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Development of a thermo-kinetic model for plutonium diffusion in the mixed oxide (U,Pu)O

Prantik Chakraborty

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Development of a thermo-kinetic model for
plutonium diffusion in the mixed
oxide (U, Pu)O₂

*Développement d'un modèle thermo-cinétique
pour la diffusion du plutonium dans l'oxyde
mixte (U, Pu)O₂*

Thèse de doctorat de l'université Paris-Saclay

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Abstract

Closing the fuel cycle in nuclear power plants has led nuclear industry to introduce the MOx fuel – uranium and plutonium mixed oxide – in actual reactors like in thermal Pressurized Water Reactor (PWR) – or to envision their use in specifically designed future reactors – like the Generation-IV Sodium-cooled Fast Reactor. The aim is to burn as efficiently as possible plutonium and minor actinides.

One of the prerequisite of using MOx in nuclear reactors is its sintering with appropriate properties: it has to show controlled plutonium composition, oxygen stoichiometry and good homogeneity. In addition, once introduced in power plants, MOx fuel experiences extreme conditions, including high thermal gradient, which drive strong redistributions of plutonium, which may have an effect on the reactor operation.

A very accurate understanding of the thermo-kinetic properties of the mixed oxide $(U, Pu)O_{2+x}$ is therefore of utmost importance for both its synthesis and in-pile behavior. Since a reliable thermodynamic model is already at hand, this thesis will focus on the development of the plutonium diffusion model in mixed oxide fuel which complement the already existing model for oxygen.

In order to approach the model development, we first have analyzed all the experimental data available in the literature for plutonium diffusion in mixed oxide fuel. We observed that the experimental data for the plutonium diffusion in mixed oxide, in spite of the stakes and interests, are rare and inconsistent. However, we selected few sets of experimental data based on their self-consistency and reliability. The lack of data is complemented using the $cB\Omega$ model. Then a full thermo-kinetic model of plutonium diffusion is further developed with DICTRA code using the selected experimental data and $cB\Omega$ results.

Using the $cB\Omega$ model, diffusion of plutonium in plutonium dioxide is extrapolated, based on the ionic radius, from the diffusion of metal ions in UO_2 and ThO_2 . The similar extrapolation scheme is also extended to apply as well on other binary oxides i.e., cerium oxide and minor actinide oxides.

Secondly, a mobility-database is constructed combining both the selected experimental data and $cB\Omega$ results of plutonium diffusion. Based on the mobility database and DICTRA code, a full and comprehensive model is finally developed for plutonium diffusion in ternary $(U, Pu)O_{2+x}$ mixed oxide fuel. The model describes the mobility of plutonium in mixed oxide fuel as a linear combination of the mobility of Pu^{3+} and Pu^{4+} ions. The mobilities of both Pu^{3+}

and Pu^{4+} are first assessed in binary plutonium dioxide and in binary uranium dioxide and in a second step in the mixed oxide. Then the mobility parameters of both Pu^{3+} and Pu^{4+} are further assessed in ternary mixed oxide fuel, i.e. $(\text{U}, \text{Pu})\text{O}_{2\pm x}$.

The typical shape of the plutonium diffusion curve against oxygen to metal ratio (which contains a plateau in the highly reduced region, a minimum near the stoichiometry 2.00 and a sharp increase in the oxidized region) is successfully reproduced with this model. In addition, the relation of each section of curve with the defects is discussed.

The model enables us to describe the plutonium self-diffusion at any temperature, plutonium content and stoichiometric ratio of the mixed oxide fuel. The model can further be used to simulate the sintering behavior, oxidation/reduction heat treatments and to improve the models in the fuel performance codes.

Synthèse en français

La fermeture du cycle du combustible a conduit l'industrie nucléaire à utiliser l'oxyde mixte d'uranium et de plutonium (le MOx) dans (i) les réacteurs nucléaires à eau pressurisée actuels (type REP : Réacteurs à Eau Pressurisée) et dans (ii) les réacteurs rapides de quatrième génération (type RNR-Na : Réacteurs à Neutrons Rapides refroidis au sodium). L'objectif est de consommer au mieux le plutonium et les actinides mineurs.

Le MOx est un oxyde mixte d'uranium et de plutonium $(U,Pu)O_{2+x}$ complexe qui doit être synthétisé avec une composition en plutonium, une stœchiométrie en oxygène maîtrisée et une répartition la plus homogène possible du plutonium. Par ailleurs, lors de son séjour en réacteur, les pastilles de MOx sont soumises à des conditions extrêmes, dont de forts gradients de température. Ces derniers produisent la redistribution radiale du plutonium qui peut avoir une influence sur les propriétés physico-chimiques du combustible et par conséquent, sur le fonctionnement du réacteur.

Il est dès lors d'une extrême importance de connaître et de modéliser avec précision le comportement thermocinétique de ce combustible pour sa synthèse et son utilisation en réacteur. La description thermodynamique de l'oxyde mixte $(U,Pu)O_{2+x}$ étant établie depuis quelques années, cette thèse se focalise sur le développement du modèle de diffusion du plutonium seulement, en complément du modèle de diffusion de l'oxygène déjà existant.

Le travail de synthèse bibliographique a montré que les données expérimentales sur la diffusion du plutonium dans le MOx sont rares et peu cohérentes entre elles. A partir de leur analyse critique, seules quelques données ont été retenues s'avérant insuffisantes pour une description complète. Pour combler ce manque de données, nous avons employé le modèle phénoménologique $cB\Omega$. Puis, nous avons établi un modèle thermocinétique complet avec le code DICTRA sur la base des données expérimentales sélectionnées et de celles générées par le modèle $cB\Omega$.

Le modèle $cB\Omega$ a permis de prédire la diffusion du plutonium dans le dioxyde de plutonium PuO_2 sur la base d'un lien entre les rayons ioniques et les données d'autodiffusion dans les dioxydes d'uranium et de thorium. Ce modèle s'est révélé pertinent pour prédire l'autodiffusion du métal dans le dioxyde de plutonium et dans d'autres oxydes (AmO_2 , BkO_2 , CeO_2 , CfO_2 , CmO_2 , NpO_2 , PaO_2).

La base de données de mobilité du plutonium dans $(U,Pu)O_{2\pm x}$ a ensuite été établie à l'aide du code DICTRA en ajustant les paramètres sur des données expérimentales sélectionnées et de celles générées par le modèle cBΩ. Le modèle décrit la mobilité du plutonium comme une combinaison linéaire des mobilités du Pu^{3+} et du Pu^{4+} . Ces mobilités sont ajustées en premier lieu sur celles des pôles purs à savoir le dioxyde d'uranium UO_2 et le dioxyde de plutonium PuO_2 . Les paramètres croisés sont ensuite affinés sur le ternaire $(U,Pu)O_{2\pm x}$ complet afin de décrire la variation en fonction de la teneur en plutonium et de la stœchiométrie en oxygène.

Un des enjeux de la description de la diffusion du plutonium dans le MOx était de reproduire la forme particulière qu'elle montre en fonction du rapport oxygène sur métal. Ainsi à une composition en plutonium donnée, la diffusion du plutonium exhibe un plateau dans le domaine sous-stœchiométrique, puis un minimum marqué proche de la stœchiométrie et enfin une augmentation rapide et importante dans le domaine sur-stœchiométrique. Cette forme est reproduite dans le modèle obtenu ici. Et mieux encore, nous avons établi un lien entre cette forme et les défauts sous-jacents qui en sont responsables.

Le modèle final donne accès à la diffusion du plutonium dans le MOx $(U,Pu)O_{2\pm x}$ en fonction de la composition, de la stœchiométrie en oxygène et de la température. Il peut être appliqué directement pour simuler des traitements thermiques d'oxydation ou de réduction à l'aide de DICTRA. Il peut également fournir des données d'entrée dans des codes multi-physiques tels que les fuel performance codes.

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CHAPTER - I

INTRODUCTION AND OBJECTIVE OF THE THESIS

This chapter aims to introduce the context, the aim and the approach adopted in the present work. After a short history on the use of MOx fuels in nuclear reactors, the motivation for the development of a plutonium mobility database for (U, Pu)O₂ fuels is presented. Then the approach used in the present work for the development of such full thermo-kinetic model is described. Finally the outline of the present manuscript is introduced.

1.1. Context:

The use of nuclear fuel is key to support the growing energy demands. The first controlled nuclear fission reaction was showcased by Enrico Fermi in 1942. Although it was a part of the Manhattan project, the interest turned to produce the energy for electricity generation after the Second World War. The primary nuclear breeder reactor was able to produce very small amount of electricity.

In 1953, President Eisenhower of USA proposed the ‘atoms for peace’ program which caused a significant effort toward generation of electricity from nuclear power commercially [1]. The USSR introduced the first reactor (Obninsk) generating 5 MWe in 1954. US implemented the PWR using the UO_2 fuel and Zr-based alloy as cladding in 1957 [2]. By 1960, the electricity generation worldwide from nuclear reactors yielded a total of 1200 MWe [3].

During 1970, many European countries began recycling the nuclear fuel elements. The reprocessing of the oxide fuel created the mixed oxide of uranium and plutonium (MOx) fuel. Initially, separated plutonium oxide was intended to use in fast breeder reactors (FBR). However, the MOx fuel was more readily used for PWRs throughout France, Belgium and Germany [2].

In the beginning of this century, an International forum was formed, known as Generation IV International Forum (GIF), to decide the future roadmap of the development of nuclear power program. The members of this forum are Argentina, Brazil, Canada, China, Euratom, France, Japan, Republic of Korea, Russia, South Africa, Switzerland, the United Kingdom and the United States of America [4]. The forum agreed on the research and development of the sodium-cooled fast reactor, with MOx as the fuel material [1].

The MOX fuel is the mixed oxide of uranium and plutonium, $(\text{U, Pu})\text{O}_{2\pm x}$, which is a continuous solid solution between $\text{UO}_{2\pm x}$ and PuO_{2-x} . The oxide exhibits a wide range of oxygen stoichiometry related to the formation of point defects that will be further described in Chapter – 2.

The plutonium content present in a typical MOx fuel for PWR is around 10%. However, the specialized fuel designed for Sodium-cooled Fast Reactor (SFR) contains more than 20% of plutonium. The study of MOx fuel with higher plutonium content could be required in future reactors.

A prerequisite to use the MOx fuel is its sintering with desired properties: controlled microstructure, desired oxygen stoichiometry and the plutonium composition of the fuel. The homogeneous distribution of elements is required in order to avoid the plutonium segregation, hence decreasing local thermal conductivity and creating non-uniform temperature distribution during reactor operation. In order to optimise the process of production, the details of the thermo-kinetic behaviour of the $\text{UO}_{2\pm x}$ – PuO_{2-x} region entirely are required.

The microstructure of MOx evolves rapidly in the initial in-pile phase in the sodium-cooled fast reactor (figure 1.1). Due to the large thermal gradient within the fuel pellet, the radial redistribution of

plutonium, uranium and oxygen occurs causing the formation of a central void in the pellet. Plutonium migrates from the central void to the cooler periphery (towards cladding) of the pellet. Both diffusion in solid state and vaporization/condensation mechanisms are majorly governing this redistribution of elements and the formation of central void in the MOx pellet due to this high temperature gradient from the centre to the periphery (cladding). But there are other minor mechanisms also at place such as, build-up of Pu agglomerates at uranium rich matrix due to neutron absorption and athermal diffusion of fuel element due to the influence of fission fragments. The coupling of the mass flux transfer and the temperature gradient is known as thermo-diffusion which calls again for the knowledge of thermo-kinetic properties in the entire $\text{UO}_{2+x}\text{-PuO}_{2-x}$ system.

There are existing plutonium diffusion models taken into account in the fuel performance codes [5, 6]. But these are macroscopic models and do not present a complete description of the plutonium diffusion in mixed oxide fuel. For example, the model used in Transuranus code does not take in to account the change of diffusion with the change of plutonium concentration in mixed oxide [6].

The existing thermodynamic model of Guéneau et al [7] using the CALPHAD method allows the description of the thermodynamic properties for the whole composition and temperature range of $(\text{U,Pu})\text{O}_2$ fuel.

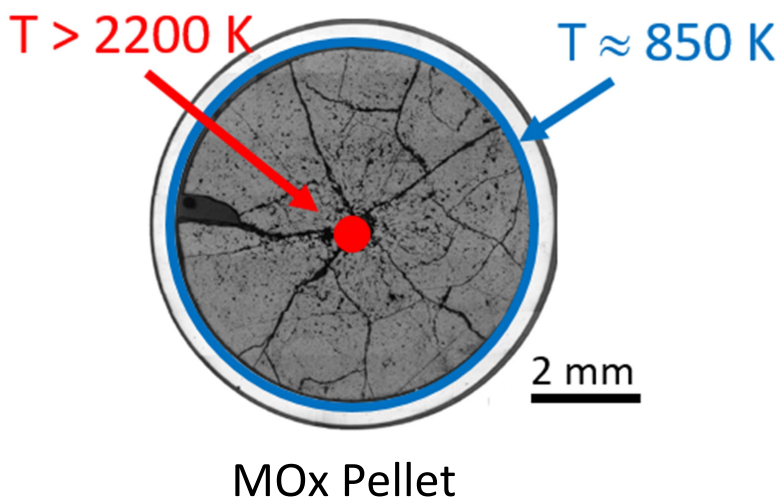


Figure 1.1: Cross section of an Irradiated MOx pellet in a Fast Breeder Reactor

In order to develop a mesoscopic model of atomic diffusion, DICTRA is a suitable code. The advantage of DICTRA is the capability to model multi-component systems and that is coupled to the CALPHAD thermodynamic model using the Thermo-Calc software as subroutine.

The mobility database is developed using diffusion coefficient data, sourced from the experimental and calculated results of other models. The mobility parameters in DICTRA framework are then

assessed by fitting the available selected data. Another advantage is that DICTRA can also be used to verify the consistency of all the data as it is a common framework for both thermodynamics and diffusion. Hence, a full thermo-kinetic model can be developed. Then the results of this model of DICTRA code developed can be used to feed the multi-physics fuel-performance code.

Two different models to describe the oxygen diffusion in MOx and uranium diffusion in UO₂ were already developed by Moore [8] using the DICTRA code. Therefore, this thesis will focus on plutonium diffusion in MOx using the DICTRA code.

1.2. Approach and Outline:

In order to approach the modelling of plutonium transport, it is of utmost need to study the thermodynamic description of $(U, Pu)O_{2\pm x}$. The available thermodynamic model describes the Gibbs energy of phase as a function of temperature, pressure, stoichiometry and plutonium content. Hence, this thesis will first discuss the thermodynamic aspects of the MOx phase in the next chapter 2. In the same chapter, the phase boundaries of UO_2 , PuO_2 and MOx are also included.

The available plutonium diffusion coefficient data in MOx are reviewed in the chapter 3. Plutonium diffusion in $(U, Pu)O_{2\pm x}$ is studied for very few plutonium contents. The results are not always consistent as well. There is no data available for plutonium diffusion coefficient in PuO_2 . However, the activation energy of plutonium diffusion was studied in PuO_2 [9, 10]. All these data and the analysis of these results (both experimental and computational) are reported in the chapter – 3. Based on the analysis, few sets of data are selected to be used in the construction of DICTRA database.

A simplistic diffusion model – ‘cBΩ’ model – is used in the chapter 4 to derive the metal diffusion coefficients in UO_2 & ThO_2 and oxygen diffusion coefficients in Li_2O . These diffusion coefficients are calculated using the fitting of a single parameter ‘c’ for each compound. Then a linear fit of ‘c’ values and ionic radii of the diffusing ions is obtained. Using this relation between c and ionic radii, the diffusion coefficient of plutonium in PuO_2 is extrapolated. The activation energy of the computed plutonium diffusion in PuO_2 is then compared with the previous results of plutonium diffusion activation energy in PuO_2 (which is presented in chapter – 3). Using the same methodology, the metal diffusion in CeO_2 , and other minor actinide oxides are also calculated.

A brief overview of the DICTRA code is presented in Chapter 5 to describe the plutonium diffusion model. In the same chapter, the principle behind the assessment of the mobility parameters using the DICTRA database (comprising of selected experimental data and cBΩ results for plutonium diffusion in PuO_2) is also described.

In chapter 6 of the thesis, the results computed using the plutonium diffusion model are presented. The results are compared with the selected experimental results of plutonium diffusion in UO_2 & $(U, Pu)O_{2\pm x}$ and cBΩ data in PuO_2 . A comparison of the calculated activation and prefactors data is performed with all available literature data. We, then, finally describe the prediction of plutonium diffusion coefficient in MOx for the variation of temperature, plutonium content and stoichiometry, using the model.

Finally, the conclusion and perspectives of the present work are presented in the Chapter 7. The model can be used to improve the fuel performance codes.

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CHAPTER - II

THERMODYNAMIC DESCRIPTION OF URANIUM & PLUTONIUM DIOXIDE PHASE

This chapter aims to introduce the thermodynamic CALPHAD method. A brief summary of the three sublattice model, in content to the U-Pu-O ternary system, is presented. Further a brief description of the existing Moore's CALPHAD model and the formulation of Gibbs energy in the model are also presented; which is followed by a detailed discussion of the concentration of species in fluorite U-Pu-O ternary system with respect to the oxygen stoichiometry and the plutonium content, based on the Moore's model. The chapter also compares the Moore's model to the other available thermodynamic models for MO_x (fluorite phase).

2.1. Introduction:

The thermodynamic calculations are very important in the perspective of our study because it determines the phase stability, phase boundary, thermodynamic data and concentrations of different components in the fluorite phase – the solid dioxide phase under investigation.

The thermodynamic model, used in this work, is based on the CALPHAD method. The CALPHAD (CALculation of PHase Diagrams) was actually developed to compute the phase equilibria. However, this method uses the mathematical model to determine the physical and chemical properties of materials at a given, temperature, pressure and composition of the model. The usage of the provisional models for assessing the phase diagram (e.g., Wagner – Schottky model or Kröger – Vink notations) are problematic in presence of several defects, which lead to a large variation of composition in material [1]. Here a compound energy formalism (CEF) framework to formulate a global expression for Gibbs energy is very often used for oxides [1, 2, 3, 4, 5]. The Gibbs energy of different phases are formulated using the compound energy formulation (CEF) and minimized and assessed to fit the phase diagram data and the thermodynamic properties (partial pressure, specific heat etc.) in this technique. This method, as claimed, is the only technique for efficient determination of physical and chemical properties of multi component and multiphase system with at par to the industrial standards [6].

In this chapter we will explain first the crystalline structure of the fluorite phase of urania, plutonia and MOx and the associated point defects in the phase. Then we will briefly explain the thermodynamic model concerning the uranium plutonium mixed oxide, used in this study. The thermodynamic model uses three sublattice model and CEF framework. Therefore, the three sublattice model is briefly explained followed by the discussion on crystallographic structure. As the CEF framework is used to formulate an expression for Gibbs energy, the compound energy formalism for the Gibbs energy of the mixed oxide of uranium and plutonium phase is also explained. After that, the phase diagram of uranium oxide, plutonium oxide and the mixed oxide of uranium & plutonium is calculated using the same thermodynamic model. Later, we will discuss the effect of the oxygen partial pressure to the concentration of cations in mixed oxide of uranium and plutonium using the Moore's model. At the end, we will compare this model to other available thermodynamic models of MOx.

2.2. Crystalline Structure and defects of (U, Pu)O_{2±x}:

The dioxides of uranium and plutonium form a solid solution above 1000 K – the mixed oxide of uranium and plutonium, i.e. (U,Pu)O₂ [7]. Both the dioxides of uranium and plutonium possess the well-known fluorite crystalline structure [8] – where eight anionic atoms arranged in a cube around cationic atom, with the cubes of anions in an edge-connected cubic array and the anionic atom is surrounded by four cationic atoms in an edge-connected face-centred cube (fcc) as well [9]). The mixed solid solution of UO₂ and PuO₂ as well forms the fluorite structure [10] (as presented in figure 2.1).

The perfect stoichiometric ratio (oxygen to total metal ratio of the system) for the mixed oxide of uranium and plutonium is O/M=2.00. Therefore, the fluorite phase of (U,Pu)O_{2±x} can be divided into hypo-stoichiometric domain (O/M<2.00) and the hyper-stoichiometric domain (O/M>2.00). The departure from the stoichiometry (=2.00) is accommodated using the defects of both oxygen and cations – either point defects or clusters [11].

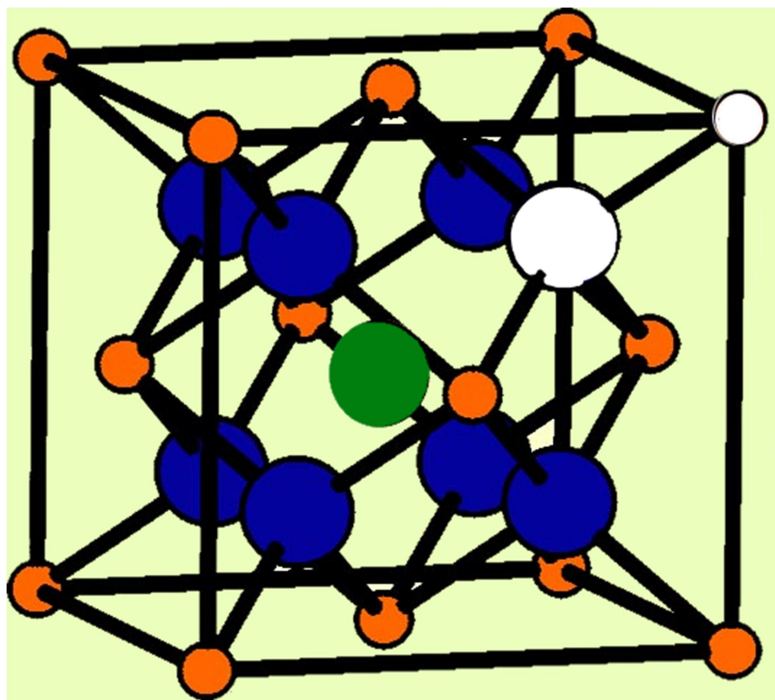


Figure 2.1: Crystal Lattice of (U,Pu)O_{2±x}. The Blue sphere represents the anions, the orange sphere represents the cations and the green sphere represents the anion at the interstitial site. The white spheres in the regular anionic/cationic site represent the vacancy at the regular site.

The defect chemistry in the actinide oxides plays major role in determining the crystal structure and composition of the solid solution. The anionic defects are of two types – the vacancy in the regular tetrahedral anionic site and the oxygen anion in the octahedral interstitial site [8]. In the hypo-stoichiometry, the oxygen vacancies are formed in due result of the low oxygen partial pressure. These

oxygen vacancies are either singly charged vacancies or doubly charged [11]. Even the hypo-stoichiometric plutonia is less complicated than the urania. In the near stoichiometry, the single doubly charged oxygen vacancy is the dominant defect. However, in the higher departure from stoichiometry, the oxygen vacancy charge is still debated (Stan et al. claims that singly charged oxygen vacancy takes over with the higher departure from stoichiometry [12]. However, Lu et al. [13] claimed that doubly charged oxygen vacancy is the only oxygen defect in hypo-stoichiometric plutonia).

In urania with stoichiometry being near 2, the major oxygen defect is usually oxygen Frenkel pair (a pair of oxygen interstitial and vacant oxygen site) [14]. Both the oxygen vacancy and oxygen interstitials are present in dioxide of plutonium [15]. Similarly, the oxygen vacancy and interstitial are also present in mixed oxide of uranium and plutonium as well [7].

On the other hand, the hyper-stoichiometric Urania is more complex than the hypo-stoichiometric domain. The departure from stoichiometry results in the formation of oxygen interstitial. However, the interstitials tend to combine and form the Willis clusters [16]. The Willis clusters (Fig 2.2) are the formation of octahedral cluster in the direction of $\langle 111 \rangle$ and comprises of two oxygen vacancy, two oxygen interstitial (displaced by holes) and two doubly charged oxygen interstitial (2:2:2) [16]. This type of clusters is dominant in higher oxygen partial pressure [17].

However, there are other octahedral clusters also formed by an oxygen vacancy and three oxygen interstitials in the direction $\langle 111 \rangle$. Two interstitials also form a di-interstitial cluster in the hyper-stoichiometric urania [18]. Although the presence of di-interstitial cluster is not experimentally proven. But theoretical calculation insisted that Willis cluster is unstable and decompose in smaller di-interstitial clusters [18].

The stability of the other oxygen clusters were studied recently [19]. Among them, two clusters are claimed to be more stable than others – I_x^4 (Figure 2.3a) and I_c^5 (Figure 2.3b), consisting of 4 and 5 oxygen interstitials respectively [20]. The stability of I_x^4 to be the most at 0 K, according to the studies of Andersson et al. [21] and Bruneval et al. [22]. However, Chen et al. [23] has calculated I_c^5 to be the most stable cluster among all at 0 K, which in accordance to the experiment as well. Soulié et al. calculated that I_x^4 is the most stable cluster at higher temperature [20].

Plutonia does not exhibit hyper-stoichiometric domain (the specification of phase boundaries of plutonia is discussed in the section 2.4). However, the cuboctahedral defect cluster of oxygen interstitials, i.e. 2:2:2 Willis cluster (as shown in figure 2.2), is also present in mixed oxides [16].

The presence of cation Frenkel defect creates cation vacancy and interstitial in the lattice crystal for UO_{2+x} [25]. In the hyper-stoichiometric urania, the uranium vacancy in the regular cationic site is resulted due to the higher oxygen partial pressure [26]. Similarly, the lower oxygen partial pressure is accommodated by the uranium interstitials, in the hypo-stoichiometry [26]. The presence of both oxygen and uranium vacancy in stoichiometric UO_2 forms the di-vacancy. The Schottky defect (which

comprises of two oxygen vacancies and one cation vacancy) is also formed in stoichiometric urania [27]. However, the ionic nature of urania requires taking the charged species into account [26]. For example, the regular state of uranium cation in UO_2 is U^{4+} . However, the hypo-stoichiometric UO_{2-x} comprises of two different uranium oxidation states, i.e. U^{3+} and U^{4+} . On the other hand, the hyper-stoichiometric UO_{2+x} comprises of U^{4+} and U^{5+} [4].

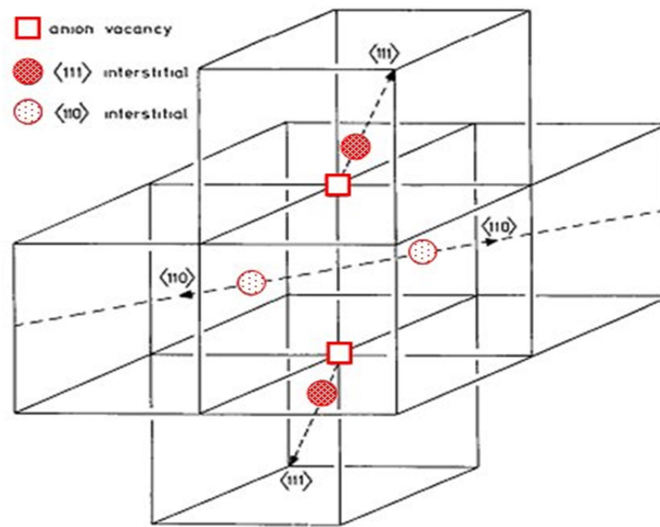


Figure 2.2: Schematic diagram of Willis Cluster (2:2:2) as presented by Welland [24]

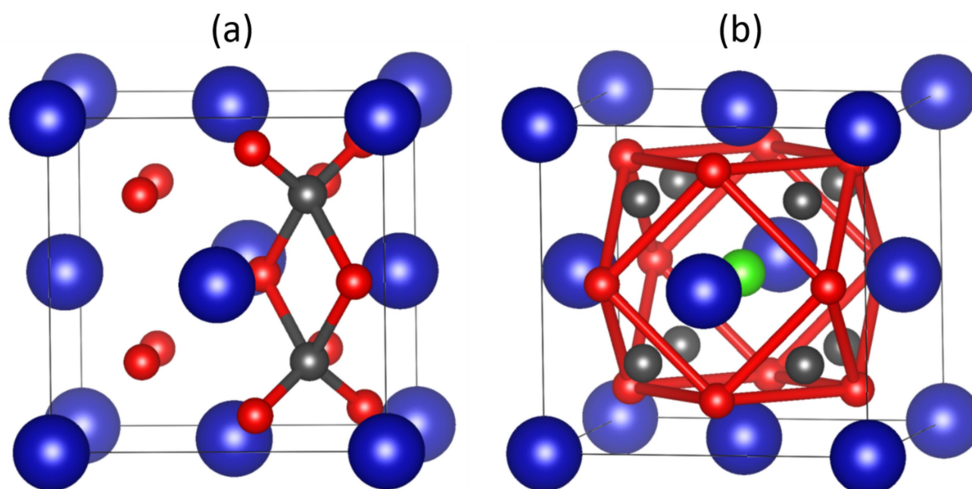


Figure 2.3: Schematic diagrams of (a) I_X^4 cluster – formed by 4 interstitial oxygens. The red spheres are oxygen ions; black sphere are the oxygen vacancy and blue spheres are the uranium ions. (b) I_C^5 cluster – formed by 5 interstitial oxygens. The red spheres are oxygen ions; black sphere are the oxygen vacancy; blue spheres are the uranium ions and green sphere is the central oxygen atom.[19].

Plutonium interstitial and plutonium vacancy are also present in stoichiometric plutonia, similar to urania [15]. However, similar to urania, the charged nature of plutonia also compels to consider the charged species in account. Hence, the stoichiometric plutonia regularly comprises of Pu^{4+} . The hypo-stoichiometric PuO_{2-x} is easily formed by reducing the Pu^{4+} cation to Pu^{3+} [28]. In the hypo-stoichiometric PuO_{2-x} ($O/M < 1.95$), the cluster formation occurs. The basic structure of this cluster consists of two Pu^{3+} ions and an oxygen vacancy. This cluster is claimed to be stable at a temperature greater than 1873 K [29]. The similar cation interstitial and vacancy, as observed in urania, are also present in $(\text{U,Pu})\text{O}_{2+x}$ [10]. However, the cation defects in both dioxides of uranium and plutonium are also represented in terms of different oxidation states of cations. The defects in mixed oxide of uranium and plutonium can also be explained as the oxidation states of uranium and plutonium. The hypo-stoichiometric MOx consists of U^{3+} , U^{4+} , Pu^{3+} and Pu^{4+} [8]. On the other hand, the hyper-stoichiometric MOx comprises of U^{4+} , U^{5+} and Pu^{4+} [8].

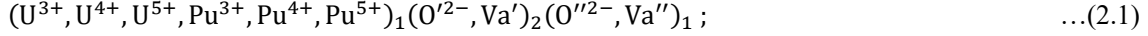
In this study, we will not consider the cationic clusters or anionic clusters. We will neither consider the variable charged anionic defects. Hence, the oxygen defects for our study, will be the doubly charged oxygen vacancy and oxygen interstitials. However, the cationic vacancies and interstitial cations are not considered in this model and the stoichiometric departure is explained in terms of the variably charged oxidation states of cations as explained previously.

2.3. Sublattice model:

Guéneau et al. formulated a CALPHAD model to calculate the phase diagram of U-Pu-O system using the three sublattice model and CEF framework [8]. Moore further modified the model of Guéneau et al. by introducing a new oxidation state of Plutonium [7]. Both models use three sublattice model to explain the crystal structure.

In sublattice model, the crystalline lattice sites are represented by different sublattices in the fluorite structure, as discussed in the previous section. The Moore's model [7], divides the lattice of uranium and plutonium mixed oxides (Figure 2.1) into three sublattices.

The first sublattice contains all the cationic species of the MOx; three uranium cations (U^{3+}, U^{4+}, U^{5+}) and three plutonium cations ($Pu^{3+}, Pu^{4+}, Pu^{5+}$). Moore modified the model of Guéneau et al. [8] by adding Pu^{5+} in the model in order to calculate the formation energy of Frenkel pair of oxygen in PuO_2 . In fact, the presence of oxygen interstitials defects required the introduction of Pu^{5+} very low, to avoid hyper-stoichiometric PuO_{2+x} to be stable [7]. The second sublattice (denoted by y') contains the anion and vacancy of regular tetrahedral anionic sites (O'^{2-}, Va'). The last sublattice (denoted by y'') contains the anion and vacancy of interstitial octahedral sites (O''^{2-}, Va''). Therefore, the full thermodynamic description of the MOx can be described using the following sublattice model [7]:



Both second and third sublattice can be filled by oxygen ions (O^{2-}) or can be vacant (Va: Vacancy). Each possible combination of above sublattices, containing a single species is called an “end-member”. Hence, end-member is a real (or, hypothetical) compound made up of one constituent from each sublattice. UO_2 is one such real end-member of Moore's model:



Similarly, the end-member can have no connection to any compound in reality and then it is utilised to describe the deviation from stoichiometry. One such key hypothetical end-member of Moore's model is $(Pu^{3+})_1 (Va')_2 (Va'')_1$ which is used to describe the boundary of hypo stoichiometric plutonia.

The end-member also is termed as the zeroth order “constituent array”, while “constituent array” is defined as the compound formed with one or more constituent from each sublattice. If two constituents are considered only from one of the sublattice and one constituent from all the other sublattices, the array is called first order array. If three constituents are considered only from one of the sublattice and two constituents from all the other sublattices, the array is called second order array and so on.

Alike, end-members, higher order constituent arrays are also used to describe key compounds with reduced and oxidised states using Moore's model [7]. For example, $(U^{3+})_1 (O'^{2-}, Va')_2 (Va'')_1$ corresponds to $UO_{1.5}$; $(Pu^{3+})_1 (O'^{2-}, Va')_2 (Va'')_1$ describes $PuO_{1.5}$; and $UO_{2.5}$ is created by

$(U^{5+})_1(O^{2-})_2(O''^{2-}, Va'')_1$. All of these constituent arrays are neutral and define the boundaries of the fluorite phase composition range in between $UO_{2\pm x}$ and PuO_{2-x} domain.

It must be noted that unlike the anions, the cation interstitial or vacancy defects are not taken into account in the Moore's model [7]. The different oxidation states for the cations are considered to describe either reduced oxide (e.g. U^{3+} or Pu^{3+} in case of $UO_{1.5}$ or $PuO_{1.5}$ respectively) or oxidized oxide (e.g. U^{5+} in case of $UO_{2.5}$). Therefore, the change in the oxidation states of uranium and plutonium allows maintaining the electro-neutrality of the MOx phase when oxygen vacancies or interstitial form.

2.4. Compound Energy Formalism and its application for MOx:

The Compound Energy Formalism (CEF) is used to describe the Gibbs energy, which can be expressed as follows [7]:

$$G_m^\theta = \sum_{I_0} P_{I_0}(Y)^\circ G_{I_0} + RT \sum_{s=1}^n \tilde{a}_s \sum_{i=1}^{n_s} y_i^{(s)} \ln(y_i^{(s)}) + G_{m,E}^\theta ; \quad \dots(2.3)$$

The first term ($P_{I_0}(Y)^\circ G_{I_0}$) describes the product of the site fraction of the constituent of the end member I_0 and the Gibbs energy of the end member. The second term of the equation ($RT \sum_{s=1}^n \tilde{a}_s \sum_{i=1}^{n_s} y_i^{(s)} \ln(y_i^{(s)})$) is the configurational entropy term. $y_i^{(s)}$ denotes the constituent site fraction, where the superscript (s) denotes the sublattice; and the number of sites in a sublattice (a_s). The constituent fraction is defined as the ratio of the number of constituent atoms to the no. of total atoms in the same sublattice [7]:

$$y_i^{(s)} = \frac{N_i^s}{N^s} ; \quad \dots(2.4)$$

The excess Gibbs energy term ($G_{m,E}^\theta$) accounts for the interaction between the higher order constituent arrays.

In accordance to the Gibbs energy of $UO_{2\pm x}$ developed by Guéneau et al. [8], the Gibbs energy of $(U, Pu)O_{2\pm x}$ is developed. Later the Gibbs energy of $(U, Pu)O_{2\pm x}$ is modified as [7]:

$$G_m^\theta = \sum_{i=U^{3+}, U^{4+}, U^{5+}, Pu^{3+}, Pu^{4+}, Pu^{5+}} y_i \sum_{j=O'^{2-}, Va'} y_j \sum_{k=O''^{2-}, Va''} y_k {}^\circ G^{(i)(j)(k)} + RT \sum_{s=1}^n \tilde{a}_s \sum_{i=1}^{n_s} y_i^{(s)} \ln(y_i^{(s)}) + G_{m,E}^{\theta, MOX} \quad \dots(2.5)$$

For pure $UO_{2\pm x}$ described by the three sublattice model, as follows,

$$(U^{3+}, U^{4+}, U^{5+})_1 (O'^{2-}, Va')_2 (O''^{2-}, Va'')_1 ; \quad \dots(2.6)$$

The Gibbs energy of pure $UO_{2\pm x}$ is expressed in accordance to the equation 2.5 as,

$$G_m^\theta = \left[y_{U^{3+}} \left(y_{O'^{2-}} y_{O''^{2-}} {}^\circ G^{(U^{3+})_1 (O'^{2-})_2 (O''^{2-})_1} + y_{O'^{2-}} y_{Va''} {}^\circ G^{(U^{3+})_1 (O'^{2-})_2 (Va'')_1} + y_{Va'} y_{O''^{2-}} {}^\circ G^{(U^{3+})_1 (Va')_2 (O''^{2-})_1} + y_{Va'} y_{Va''} {}^\circ G^{(U^{3+})_1 (Va')_2 (Va'')_1} \right) + y_{U^{4+}} \left(y_{O'^{2-}} y_{O''^{2-}} {}^\circ G^{(U^{4+})_1 (O'^{2-})_2 (O''^{2-})_1} + y_{O'^{2-}} y_{Va''} {}^\circ G^{(U^{4+})_1 (O'^{2-})_2 (Va'')_1} + y_{Va'} y_{O''^{2-}} {}^\circ G^{(U^{4+})_1 (Va')_2 (O''^{2-})_1} + y_{Va'} y_{Va''} {}^\circ G^{(U^{4+})_1 (Va')_2 (Va'')_1} \right) + y_{U^{5+}} \left(y_{O'^{2-}} y_{O''^{2-}} {}^\circ G^{(U^{5+})_1 (O'^{2-})_2 (O''^{2-})_1} + y_{O'^{2-}} y_{Va''} {}^\circ G^{(U^{5+})_1 (O'^{2-})_2 (Va'')_1} + y_{Va'} y_{O''^{2-}} {}^\circ G^{(U^{5+})_1 (Va')_2 (O''^{2-})_1} + y_{Va'} y_{Va''} {}^\circ G^{(U^{5+})_1 (Va')_2 (Va'')_1} \right) \right] + RT [y_{U^{3+}} \ln(y_{U^{3+}}) +$$

$$y_{U^{4+}} \ln(y_{U^{4+}}) + y_{U^{5+}} \ln(y_{U^{5+}}) + 2RT[y_{O'^{2-}} \ln(y_{O'^{2-}}) + y_{Va'} \ln(y_{Va'})] + RT[y_{O''^{2-}} \ln(y_{O''^{2-}}) + y_{Va''} \ln(y_{Va''})] + G_{m,E}^{\theta,UO_2} \quad \dots(2.7)$$

The excess energy term for urania is given by the following equation [8],

$$G_{m,E}^{\theta,UO_2} = y_{U^{3+}}y_{U^{4+}}y_{O'^{2-}}y_{Va''} \left[L_{(U^{3+},U^{4+})_1(O'^{2-})_2(Va'')_1}^0 + (y_{U^{3+}} - y_{U^{4+}})L_{(U^{3+},U^{4+})_1(O'^{2-})_2(Va'')_1}^1 \right] + y_{U^{4+}}y_{U^{5+}}y_{O'^{2-}}y_{O''^{2-}} \left[L_{(U^{4+},U^{5+})_1(O'^{2-})_2(O''^{2-})_1}^0 \right] \quad \dots(2.8)$$

Where L represents the interaction parameter between species in a same sublattice.

In a similar way, the three sublattice model can expand pure $PuO_{2\pm x}$ as well,

$$(Pu^{3+}, Pu^{4+}, Pu^{5+})_1(O'^{2-}, Va')_2(O''^{2-}, Va'')_1; \quad \dots(2.9)$$

Therefore, the Gibbs energy of $PuO_{2\pm x}$ is following,

$$G_m^\theta = \left[y_{Pu^{3+}} \left(y_{O'^{2-}}y_{O''^{2-}} \circ G^{(Pu^{3+})_1(O'^{2-})_2(O''^{2-})_1} + y_{O'^{2-}}y_{Va''} \circ G^{(Pu^{3+})_1(O'^{2-})_2(Va'')_1} + y_{Va'}y_{O''^{2-}} \circ G^{(Pu^{3+})_1(Va')_2(O''^{2-})_1} + y_{Va'}y_{Va''} \circ G^{(Pu^{3+})_1(Va')_2(Va'')_1} \right) + y_{Pu^{4+}} \left(y_{O'^{2-}}y_{O''^{2-}} \circ G^{(Pu^{4+})_1(O'^{2-})_2(O''^{2-})_1} + y_{O'^{2-}}y_{Va''} \circ G^{(Pu^{4+})_1(O'^{2-})_2(Va'')_1} + y_{Va'}y_{O''^{2-}} \circ G^{(Pu^{4+})_1(Va')_2(O''^{2-})_1} + y_{Va'}y_{Va''} \circ G^{(Pu^{4+})_1(Va')_2(Va'')_1} \right) + y_{Pu^{5+}} \left(y_{O'^{2-}}y_{O''^{2-}} \circ G^{(Pu^{5+})_1(O'^{2-})_2(O''^{2-})_1} + y_{O'^{2-}}y_{Va''} \circ G^{(Pu^{5+})_1(O'^{2-})_2(Va'')_1} + y_{Va'}y_{O''^{2-}} \circ G^{(Pu^{5+})_1(Va')_2(O''^{2-})_1} + y_{Va'}y_{Va''} \circ G^{(Pu^{5+})_1(Va')_2(Va'')_1} \right) \right] + RT[y_{Pu^{3+}} \ln(y_{Pu^{3+}}) + y_{Pu^{4+}} \ln(y_{Pu^{4+}}) + y_{Pu^{5+}} \ln(y_{Pu^{5+}})] + 2RT[y_{O'^{2-}} \ln(y_{O'^{2-}}) + y_{Va'} \ln(y_{Va'})] + RT[y_{O''^{2-}} \ln(y_{O''^{2-}}) + y_{Va''} \ln(y_{Va''})] + G_{m,E}^{\theta,PuO_2} \quad \dots(2.10)$$

The excess energy term for pure plutonia is as following,

$$G_{m,E}^{\theta,PuO_2} = y_{Pu^{3+}}y_{Pu^{4+}}y_*y_*' \left[L_{(Pu^{3+},Pu^{4+})_1(*)_2(*)_1}^0 + (y_{Pu^{3+}} - y_{Pu^{4+}})L_{(Pu^{3+},Pu^{4+})_1(*)_2(*)_1}^1 \right] \quad \dots(2.11)$$

Where * denotes either O^{2-} or Va in the sublattice.

The Gibbs energy of uranium and plutonium mixed oxide can then be calculated as the summation of Gibbs energy of pure $UO_{2\pm x}$ (equation 2.8), Gibbs energy of pure $PuO_{2\pm x}$ (equation 2.10) and the Gibbs energy terms for the mixed oxide phase (equation 2.11). The Gibbs energy term of the mixed oxide phase is:

$$G_m^\theta = \left[\sum_{v'=3,4,5} y_{Pu^{v'+}} \left(y_{O'^{2-}}y_{O''^{2-}} \circ G^{(Pu^{v'+})_1(O'^{2-})_2(O''^{2-})_1} + y_{O'^{2-}}y_{Va''} \circ G^{(Pu^{v'+})_1(O'^{2-})_2(Va'')_1} + y_{Va'}y_{O''^{2-}} \circ G^{(Pu^{v'+})_1(Va')_2(O''^{2-})_1} + y_{Va'}y_{Va''} \circ G^{(Pu^{v'+})_1(Va')_2(Va'')_1} \right) + \sum_{v=3,4,5} y_{U^{v+}} \left(y_{O'^{2-}}y_{O''^{2-}} \circ G^{(U^{v+})_1(O'^{2-})_2(O''^{2-})_1} + y_{O'^{2-}}y_{Va''} \circ G^{(U^{v+})_1(O'^{2-})_2(Va'')_1} + y_{Va'}y_{O''^{2-}} \circ G^{(U^{v+})_1(Va')_2(O''^{2-})_1} + y_{Va'}y_{Va''} \circ G^{(U^{v+})_1(Va')_2(Va'')_1} \right) \right]$$

$$\begin{aligned}
& y_{Va'} y_{O'^{2-}} \circ G^{(U^{V+})_1 (Va')_2 (O'^{2-})_1} + y_{Va'} y_{Va''} \circ G^{(U^{V+})_1 (Va')_2 (Va'')_1} \Big] + RT \left[\sum_{v=3,4,5} y_{U^{v+}} \ln(y_{U^{v+}}) + \right. \\
& \left. \sum_{v'=3,4,5} y_{Pu^{v'+}} \ln(y_{Pu^{v'+}}) \right] + 2RT [y_{O'^{2-}} \ln(y_{O'^{2-}}) + y_{Va'} \ln(y_{Va'})] + RT [y_{O'^{2-}} \ln(y_{O'^{2-}}) + \\
& y_{Va''} \ln(y_{Va''})] + G_{m,E}^{\theta,MOX} \quad \dots(2.12)
\end{aligned}$$

The Gibbs energy terms of the end members as well as the interaction parameters in the Excess Gibbs energy term have been adjusted to fit the available experimental data [8]. The final excess Gibbs energy term for the mixed oxide of uranium and plutonium, deduced by Guéneau et al [8], is as following,

$$\begin{aligned}
G_{m,E}^{\theta,MOX} = & y_{U^{3+}} y_{U^{4+}} y_{O'^{2-}} y_{Va''} \left[L_{(U^{3+},U^{4+})_1 (O'^{2-})_2 (Va'')_1}^0 + (y_{U^{3+}} - y_{U^{4+}}) L_{(U^{3+},U^{4+})_1 (O'^{2-})_2 (Va'')_1}^1 \right] + \\
& y_{U^{4+}} y_{U^{5+}} y_{O'^{2-}} y_{O''^{2-}} \left[L_{(U^{4+},U^{5+})_1 (O'^{2-})_2 (O''^{2-})_1}^0 \right] + y_{Pu^{3+}} y_{Pu^{4+}} y_{*'} y_{*''} \left[L_{(Pu^{3+},Pu^{4+})_1 (*')_2 (*'')_1}^0 + \right. \\
& \left. (y_{Pu^{3+}} - y_{Pu^{4+}}) L_{(Pu^{3+},Pu^{4+})_1 (*')_2 (*'')_1}^1 \right] + y_{U^{4+}} y_{Pu^{4+}} y_{O'^{2-}} y_{Va''} \left[L_{(U^{4+},Pu^{4+})_1 (O'^{2-})_2 (Va'')_1}^0 \right] + \\
& y_{U^{4+}} y_{Pu^{3+}} y_{O'^{2-}} y_{Va''} \left[L_{(U^{4+},Pu^{3+})_1 (O'^{2-})_2 (Va'')_1}^0 \right] + y_{U^{4+}} y_{Pu^{3+}} y_{Va'} y_{Va''} \left[L_{(U^{4+},Pu^{3+})_1 (Va')_2 (Va'')_1}^0 \right] + \\
& y_{Pu^{4+}} y_{U^{5+}} y_{O'^{2-}} y_{*''} \left[L_{(Pu^{4+},U^{5+})_1 (O'^{2-})_2 (*'')_1}^0 \right] \quad \dots(2.13)
\end{aligned}$$

In the previous equation * denotes either O^{2-} or Va in the sublattice. Then this model can be used to calculate the defect concentrations, oxygen stoichiometry, partial pressure of the elements and the phase diagram as well.

2.5. Calculation of Phase Diagram for U-O, Pu-O and U-Pu-O:

The phase diagram of U-O, Pu-O and U-Pu-O systems are calculated in this section, using the model of Moore [7].

2.5.1. Binary phase diagrams:

The U-O phase diagram is presented in figure 2.4. The lower boundary of the fluorite phase is found for O/U=1.67 at a temperature of 2719K. On the other hand, the upper boundary of the fluorite phase is for an O/U= 2.25 at a temperature of 1400 K. However, the melting temperature $UO_{2.00}$ is as high as 3142 K [4].

The hypo-stoichiometric UO_{2-x} is in equilibrium with the liquid enriched in uranium metal. However, the hyper-stoichiometric UO_{2+x} is in equilibrium with compounds U_3O_8 , U_4O_9 and the oxygen gas. The dioxide of uranium reduces in temperature higher than 1400 K. The uranium dioxide oxidizes from lower temperature (around 600 K). The stoichiometry of hyper-stoichiometric uranium dioxide gradually reduces for temperature higher than 1950 K [7].

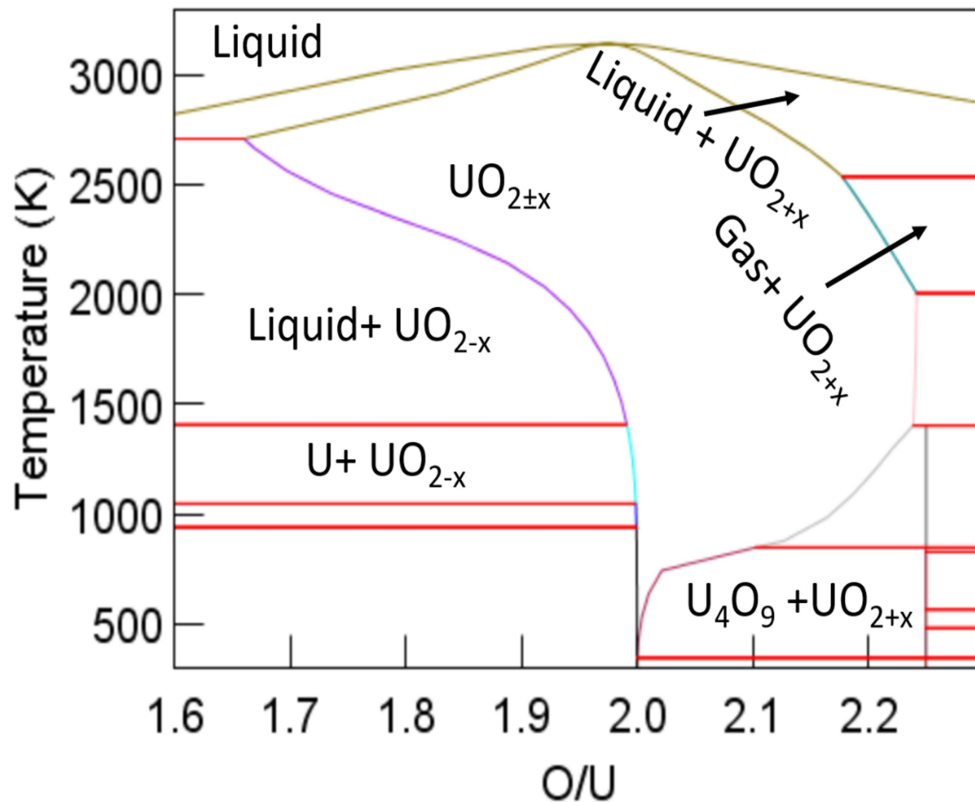


Figure 2.4: Phase diagram of U-O binary system as calculated with Moore's model [7]

The binary phase diagram of Pu-O system is represented in figure 2.5. Unlike $\text{UO}_{2\pm x}$, the dioxide of plutonium only exhibits the hypo-stoichiometry regime ranged from $\text{O}/\text{M}= 1.6$ to 2.00 . The existence of hyper-stoichiometric plutonia is still a point of debate [5].

The melting temperature of pure PuO_2 was perceived to be $2663 \text{ K} - 2700 \text{ K}$ [7]. However, the melting temperature is estimated to be 3017 K , in recent days [8]. The hypo-stoichiometric plutonia is in equilibrium with body-centred cubic structure of $\text{PuO}_{1.61}$ and with Pu_2O_3 at higher temperature. On the oxygen rich side, plutonia is in equilibrium with oxygen gas.

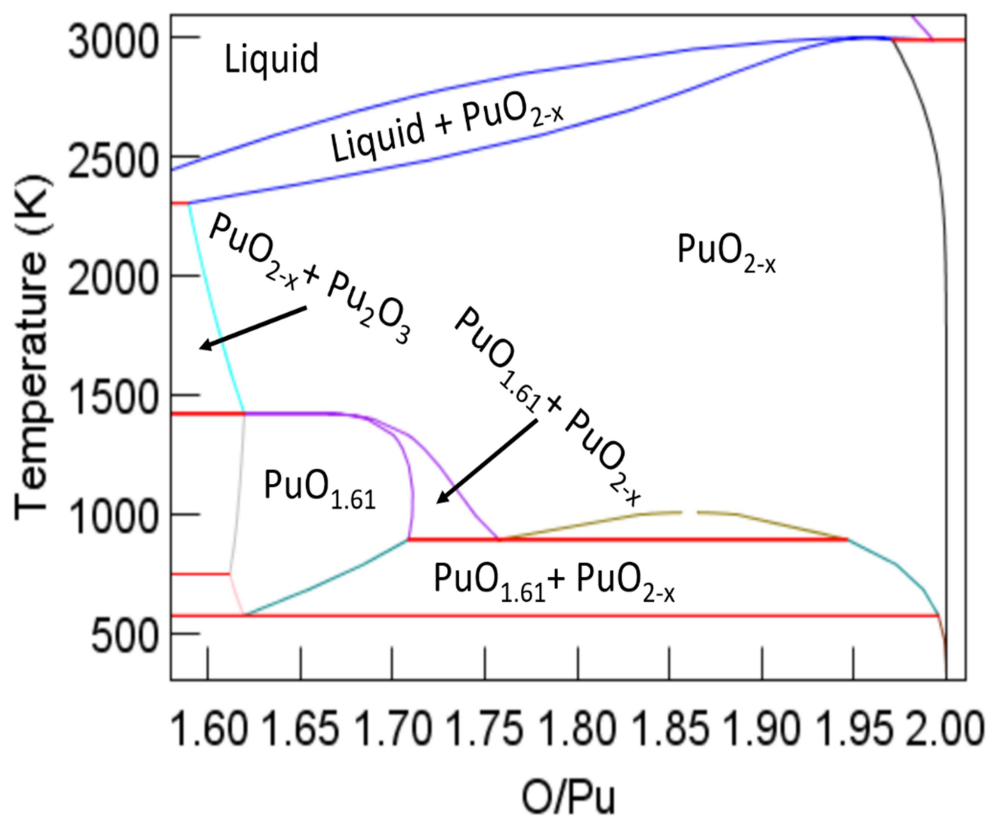


Figure 2.5: Phase diagram of Pu-O binary system as calculated with Moore's model [7]

2.5.2. U-Pu-O ternary phase diagram:

The figure 2.6 represents the isothermal section of U-Pu-O system at 1773 K . The hypo-stoichiometric MOx is mainly caused due to the reduction of Pu^{4+} to Pu^{3+} . In case of hypo-stoichiometric domain, the mixed oxide containing more than 40% Pu results two fcc phases for temperature below 900 K [30] due to the existence of a miscibility gap [31].

For the hyper-stoichiometric MOx, the uranium U^{4+} oxidizes to U^{5+} . The oxidization of Pu^{4+} to Pu^{5+} , as evident in the model of Moore, also takes place. However, the concentration of Pu^{5+} is insignificant in most cases (as discussed in the following section). The hyper-stoichiometric MOx is ranged up to

O/M= 2.2. The hyper-stoichiometric MOx is in equilibrium with oxygen and more oxidized U₃O₈ phase.

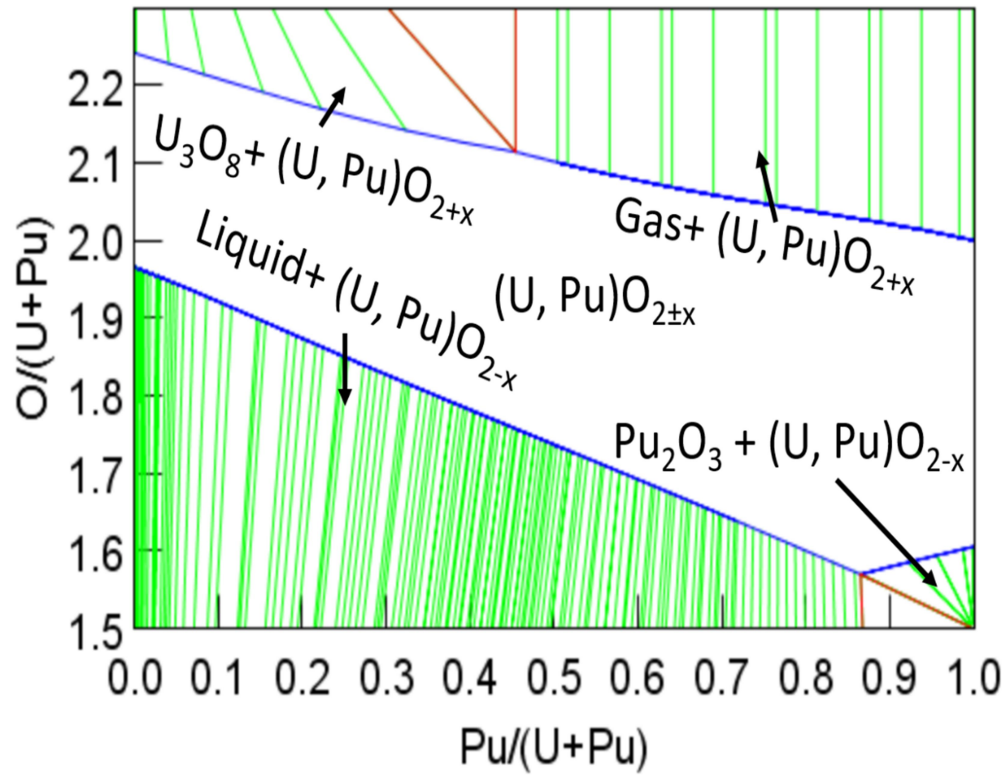


Figure 2.6: Phase diagram of U-Pu-O ternary system, calculated with Moore's model at 1773 K [7]

2.6. Cationic species distribution using CALPHAD:

As the site fraction of the different species contribute significantly in the derivation of the Gibbs energy variation with the composition, according to this model, it is also possible to calculate the population of the different constituents (or the defect fractions, in other words) from the Gibbs energy of the system using this thermodynamic model.

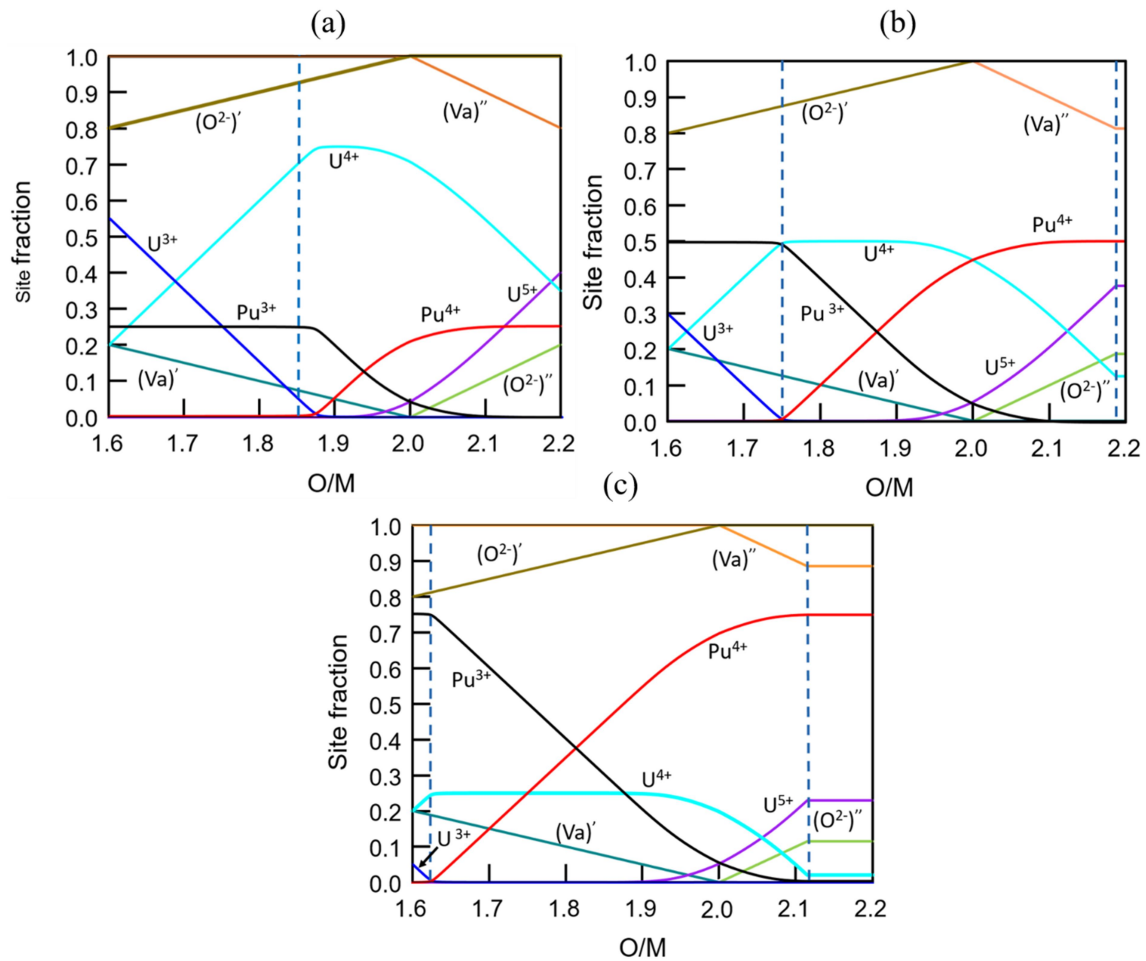


Figure 2.7: Calculated site fraction of the species at 1773 K in (a) $(U_{0.75}Pu_{0.25})O_{2\pm x}$, (b) $(U_{0.5}Pu_{0.5})O_{2\pm x}$ and (c) $(U_{0.25}Pu_{0.75})O_{2\pm x}$ as a function of O/M ratio, using the model [7]. The dashed lines indicate the phase boundaries. Calculations are performed considering only one phase (fluorite phase) in equilibrium with gaseous O_2 phase.

In the following figure 2.7, the population of the different species in $U_{0.75}Pu_{0.25}O_{2\pm x}$, $U_{0.5}Pu_{0.5}O_{2\pm x}$ and $U_{0.25}Pu_{0.75}O_{2\pm x}$ are shown. The concentration of Pu⁵⁺ is not significant and can be neglected, in both hypo and hyper-stoichiometry. However, Pu⁴⁺ is the major Pu species in the hyper-stoichiometric domain compared to Pu³⁺ species whose concentration remains very low. Therefore, the Pu⁴⁺

remains the predominant plutonium species in the hyper-stoichiometric domain for all the compositions of MO_x.

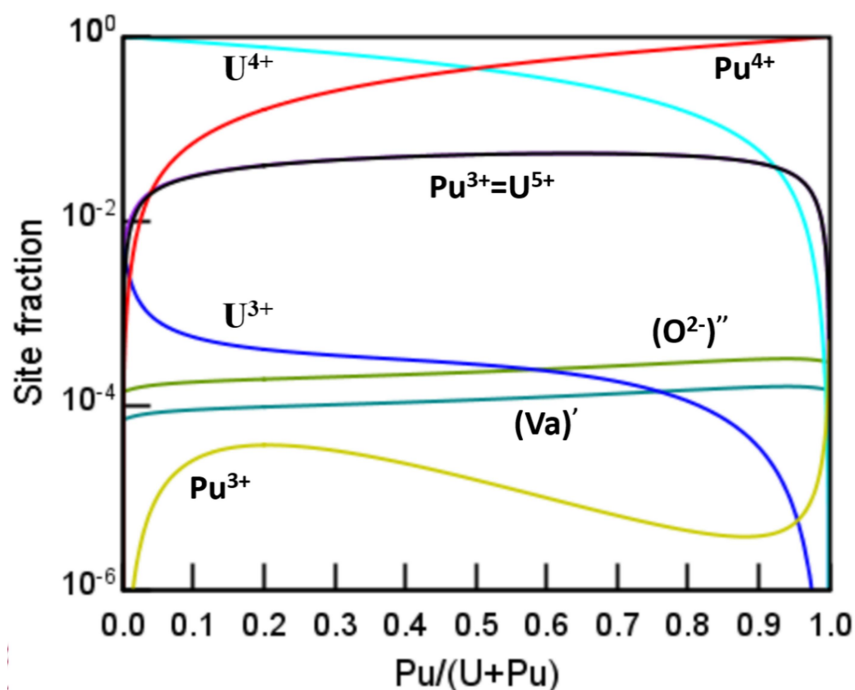


Figure 2.8: Calculated site fraction of species at 1773 K in MO_x with a fixed O/M ratio equal to 2.00 as a function of Pu/(U+Pu) ratio, using the model [7]

The population of plutonium cationic species in hypo-stoichiometry 25% MO_x can be further subdivided into two regions:

- The first region, $1.87 \leq \frac{O}{M}$, is mainly dominated by Pu³⁺ cation as a plutonium species. Whereas, the U³⁺ and U⁴⁺ are the two dominant species of uranium in this region. Therefore, Pu⁴⁺, with its lower concentration is a dormant plutonium cation in this region.
- However, in the second region, $1.87 \leq \frac{O}{M} \leq 2.0$, an equivalence between the concentration of both Pu³⁺ and Pu⁴⁺ is found for $\frac{O}{M} = 1.94$. Therefore, none of these two species can be assumed to be dormant in this region, hence cannot be neglected. Whereas, concentration of U³⁺ falls significantly in this region as well as a significant presence of U⁵⁺ can be noticed close to the stoichiometric line. Therefore, U⁴⁺ and U⁵⁺, both become the dominant uranium species but U³⁺ stays dormant in this region. However, in the initial part of this region, $1.87 \leq \frac{O}{M} \leq 1.94$, the concentration of U⁵⁺ is negligible with respect to the concentration of U⁴⁺. Therefore, in this sub-region, U⁴⁺ is the only dominant uranium species.

In the hyper-stoichiometry, the concentration of Pu^{3+} is lower than the same of Pu^{4+} . Therefore, Pu^{4+} emerges as the only dominant plutonium species in the region. However, U^{4+} and U^{5+} , both of these uranium species stay dominant in this domain.

A similar analysis can also be made for the MOx with 50% and 75% of plutonium content. The distinctive boundary of the two regions in hypo-stoichiometric domain shifts toward lower stoichiometric ratio further from the stoichiometric line. The first region emerges from $\frac{\text{O}}{\text{M}} < 1.75$, for the 50% MOx. Whereas, the second region emerges between $\frac{\text{O}}{\text{M}} = 1.75$ and $\frac{\text{O}}{\text{M}} < 2.0$. The hyper-stoichiometry domain for both the composition of MOx includes Pu^{4+} as the dominant plutonium species, whereas U^{4+} and U^{5+} , stay as the dominant uranium species in this domain. However, the concentration of U^{5+} remains significantly low till the stoichiometric value of $\frac{\text{O}}{\text{M}} = 1.95$.

On the other hand, figure 2.8 summarises the populations of the different components of the fluorite at $T = 1773 \text{ K}$, calculated as a function of plutonium concentration and at a fixed stoichiometry, $\frac{\text{O}}{\text{M}} = 2.0$. The concentration of Pu^{3+} and U^{5+} are equal and do not notably vary with the variation of plutonium concentration within the range of 5% - 95% MOx. However, the concentration of U^{3+} and U^{4+} abruptly decrease at plutonium content more than 70% plutonium MOx. Whereas, the concentration of Pu^{4+} gradually increases with the increment of plutonium content. As this calculation is made at a constant stoichiometry, the concentration of oxygen vacancy and interstitial do not show any large fluctuation. The concentration of Pu^{5+} in MOx is negligible.

Hence, we can summarize this section as,

- At the exact stoichiometry $\frac{\text{O}}{\text{M}} = 2.00$, U^{4+} and Pu^{4+} are the major species. Nevertheless, Pu^{3+} and U^{5+} have a small but significant contribution, whose concentrations are equal to maintain the electro-neutrality of the phase.
- For $\frac{\text{O}}{\text{M}} < 2$, plutonium Pu^{4+} is reduced into Pu^{3+} whose fraction increases with decreasing O/M ratio. Uranium remains U^{4+} , although a small contribution of U^{5+} exists for $\frac{\text{O}}{\text{M}} > 1.9$.
- For $\frac{\text{O}}{\text{M}} > 2$, uranium U^{4+} oxidizes into U^{5+} whose fraction increases with O/M ratio and plutonium remains as Pu^{4+} .

2.7. Comparison with Kato's model:

Moore's CALPHAD model for ternary oxide of uranium and plutonium is a useful tool to compute the concentration of the species in the system to the given atmosphere, oxygen stoichiometry as well as plutonium content in the system. In this section, we will judge the relevancy of the CALPHAD model of Moore with respect to the CALPHAD model of Guéneau et al. [8] and the other thermodynamic model of Kato et al. [32]. Figure 2.9 summarises a comparison between these three models, in terms of the resultant partial pressure of oxygen in the system as a function of oxygen stoichiometry.

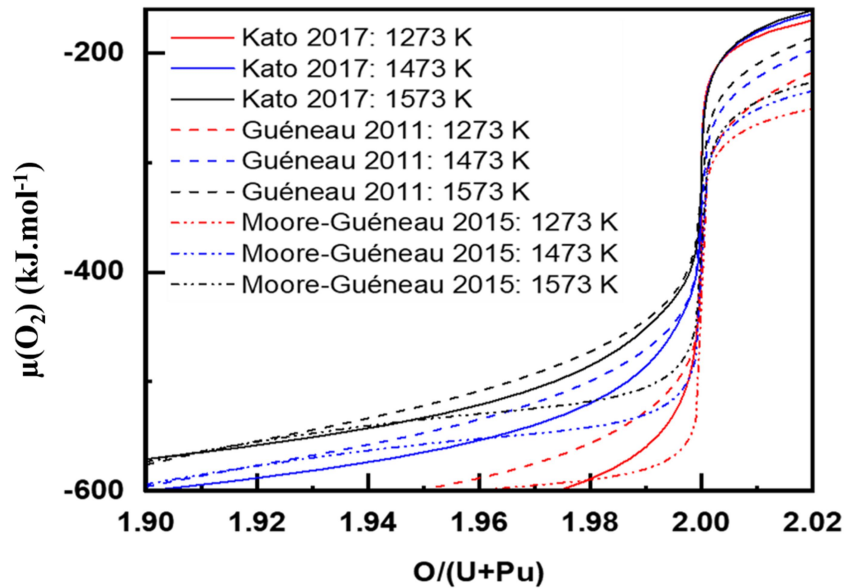


Figure 2.9: Comparison between the thermodynamic models of $(U_{0.7}Pu_{0.3})O_{2+x}$; Moore-Guéneau 2015, Guéneau 2011 and Kato 2017 represent the models corresponding to [7], [8] & [32] respectively; Dash-dot lines correspond to the Moore's model [7]; Dashed lines correspond to the Guéneau's model [8]; The solid lines correspond to the Kato's model [32].

As mentioned above, the model of Moore's CALPHAD model is a slight modification of the model of Guéneau et al. [8] – in terms of the introduction of Pu^{5+} species in the first sublattice. The introduction of a new oxidation state of plutonium induces a significant deviation between Moore's model [7] and the Guéneau's model [8]. The oxygen potential with Moore's model is around 10 – 30 kJ/mol lower in the stoichiometric range of $1.96 < \frac{O}{M} < 2.00$. In the lower oxygen stoichiometry ($\frac{O}{M} < 1.96$), the deviation is smaller. These deviation trends are universal irrespective of the temperature.

Kato et al. developed a point defect model in which the cation defects are considered as electrons and holes. Kato and co-workers already reported that their model underestimates the partial pressure of oxygen by 10-30 kJ/mol in hypo-stoichiometry than the model of Guéneau et al. [32]. In hypo-stoichiometry, the estimations of Moore's model [7] are 10 - 20 kJ/mol lesser than the estimations of Kato's model. This deviation increases with the temperature.

However, the deviation of Kato's model is large in hyper-stoichiometry to the other two models. Kato and co-worker already reported a high value of around 50 kJ/mol from their model than the model of Guéneau et al. [32]. This deviation further increases when compared the estimation of Kato's model to the estimations of Moore's model [7] (around 80 kJ/mol). The deviation between Kato's model and the two of CALPHAD models reduces with the temperature, as observed from the figure 2.9.

To conclude, the model of Moore possess some deviation to the other two models. The deviation of this model to the model of Kato et al. is very significant and needs further investigations. The model of Guéneau et al. and the Moore's model [7], in spite of having a same origin, also shows some deviation in hypo-stoichiometric regime. In this study, we will use the model of Moore in order to keep the consistency with the oxygen diffusion model on (U, Pu)O₂ developed by Moore [7].

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CHAPTER - III

PREVIOUS STUDIES ON PLUTONIUM DIFFUSION IN URANIA, PLUTONIA AND MIXED OXIDE

This chapter firstly aims to introduce the self-diffusion coefficient of an element. Then a brief summary of the previous efforts to measure the self-diffusion of plutonium in uranium dioxide, plutonium dioxide and mixed oxide of uranium and plutonium is presented. These results are reviewed with respect to the system temperature, oxygen stoichiometry and plutonium content. The analysis is further extended to compare the different data and their relevance to the actual plutonium self-diffusion. Based on this comparative analysis, a final selection of relevant data for the development of the mobility database will be presented at the end of this chapter.

3.1. Introduction:

Due to the radiotoxicity and handling problems of plutonium, there are very few experiments performed on mixed oxide of uranium and plutonium. Hence, the experimental studies of plutonium diffusion in mixed oxide of uranium and plutonium are also rare in the literature. The computational studies are also even lesser and limited to computation of the activation energy only. Therefore, in this chapter we briefly discuss each of these experiments and the computational studies performed to estimate the plutonium self-diffusion for different oxygen stoichiometric ratios and different plutonium contents (including urania and plutonia) of mixed oxides, in their chronological order. To begin with the review and analysis of the previous studies, we will introduce the Arrhenius expression for the self-diffusion coefficient very briefly.

At the end of this chapter, we obtain a series of selected experimental results to be used in our study, among the presented ones. This selection is based on the relevancy of the results to our study and global comparability of these data.

3.1.1 Arrhenius definition of Self-diffusion coefficient:

The concept of self-diffusion first introduced by Maxwell (in gases) as the diffusion process takes place even if there is only one gas molecule [1]. If the gas diffuses “into itself”, the diffusion coefficient is termed as self-diffusion. Later the introduction of diffusion of isotopic indicators, the self-diffusion coefficient was measured in solid lead using Ra indicator [2]. Therefore, the diffusion coefficient of a solid element “into itself” is the self-diffusion coefficient in solids. The self-diffusion coefficient can also be expanded in terms of Arrhenius equation as [3],

$$D_A^* = D_0 \exp\left(-\frac{Q_{act}}{k_B T}\right) \quad \dots(3.1)$$

Where, Q_{act} signifies the energy barrier of self-diffusion process and the D_0 is a prefactor term which varies with the lattice type, atomic spacing, instability of the system etc. The theoretical aspects and practical significance of Q_{act} and D_0 will be further discussed in chapter 4 and 5.

The plutonium self-diffusion in urania, plutonia and MOx was previously studied by few different experiments and very few theoretical techniques. These experiments are carried out using a tracer isotope of plutonium as ‘labelled’ atoms and the diffusion coefficient of the tracer isotope is believed to be equal to the one of normal isotope [3].

If the natural logarithm of the self-diffusion coefficient of the labelled atom is plotted against the inverse of system temperature (Arrhenius plot), then the slope of that plot signifies the activation energy of self-diffusion. In previous experimental works, different authors tried to obtain an Arrhenius plot of their data followed by an Arrhenius equation of the plutonium self-diffusion coefficient.

3.2. Pu diffusion in UO_2 and $(U, Pu)O_2$ mixed oxide:

The measurements of plutonium diffusion coefficient in UO_2 and $(U, Pu)O_2$ are reported in Table 3.1 and presented in this section. These different studies are hereafter reviewed in the chronological order. The data on plutonium diffusion in PuO_2 are reviewed in the section 3.3.

3.2.1 Lindner et al. (1967) [4]:

Lindner et al (1967) [4] measured the first set of experimental data of plutonium and uranium diffusion coefficient in stoichiometric polycrystalline $(U_{0.85}Pu_{0.15})O_2$ mixed oxide but the grain size of the material is not mentioned in the article.

The fresh oxide pellets were first annealed for several hours (the exact duration is not given in [4]) at 1773 K under a controlled atmosphere of 96% H_2 + 4% H_2O to reach the stoichiometry 2 (as per the claims of the author). Then the Pu^{238} tracer was applied by vacuum evaporation method from tantalum foil at 2773 K and 10^{-5} Torr. These tracer doped pellets were further annealed once again in the same conditions. The diffusion coefficient was determined by measuring the concentration profile of Pu^{238} tracer using α energy degradation method.

The plutonium diffusion coefficient data (as noted in Figure- 3.1) were fitted by an Arrhenius law as following:

$$D_{Pu}^* (m^2s^{-1}) = 3.45 \cdot 10^{-14} \exp \left[-\frac{138(kJ.mol^{-1})}{RT} \right] \quad \dots(3.2)$$

However, the plutonium tracer Pu^{238} is not mono-energetic (E_α : 5.49 & 5.45 MeV). Hence, the finite resolution of the alpha-spectrometer introduces an uncertainty with this technique. The limit of this uncertainty on (D.t) is reported to be $10^{-14} m^2$. Unfortunately, as the time is not given in [4], the final uncertainty on the diffusion coefficient D cannot be deduced.

The plutonium diffusion coefficient found in this experiment is significantly higher than for uranium in UO_2 . In fact the activation energy of 138 kJ/mol is much lower than for U in UO_2 (≈ 400 kJ/mol). In order to explain that, the influence of self-irradiation damage by plutonium in UO_2 has been considered. But no substantial damage was observed compared with U diffusion measurement in UO_2 . Hence, a slight increase of the oxygen to metal ratio up to ($O/M= 2.001$) was assumed. In fact, in case of a small positive deviation x , the activation energy is lowered by the free energy of formation of an anion Frenkel pair (≈ 300 kJ/mol). Therefore, the activation energy (138 kJ/mol) would only correspond to the energy for cation migration for an $O/M= 2.001$ instead of being the sum of the anion Frenkel pair formation and cation migration energies for $O/M=2$. Nevertheless it has to be mentioned that the oxygen stoichiometry has not been measured but only estimated by thermodynamic calculations.

3.2.2. Riemer & Scherff (1971) [5]:

Riemer & Scherff (1971) [5] performed an extensive experimental work to measure plutonium diffusion coefficient in hyper-stoichiometric polycrystalline $(U_{0.85}Pu_{0.15})O_{2+x}$ mixed oxide. The fresh pellets were annealed in a resistance furnace for twelve hours under a CO/CO_2 gas mixture flow in order to reach the desired oxygen stoichiometry (2.043 – 2.17).

Pu^{238} tracer was used, which was applied on the pellets by evaporation under vacuum from a tantalum foil. Then a second heat treatment in the same conditions was performed on the tracer doped samples. The α -degradation method was used to determine the tracer concentration profile after diffusion annealing.

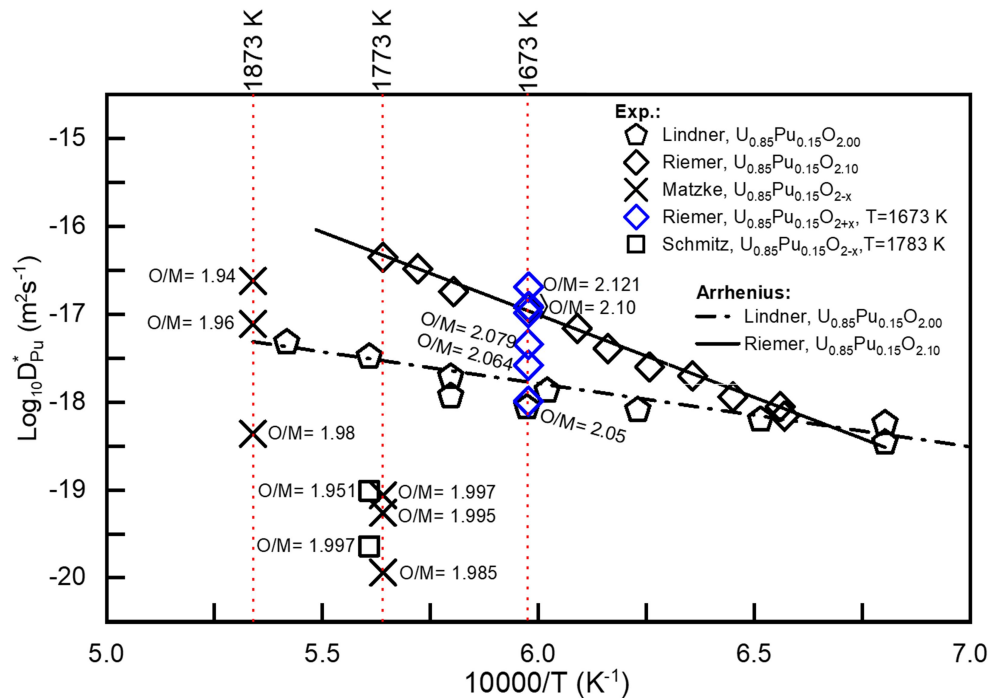


Figure 3.1: Experimental data of plutonium diffusion coefficient in $U_{0.85}Pu_{0.15}O_{2+x}$ as a function of temperature. Lindner, Riemer, Matzke and Schmitz represent the data of [4], [5], [8] & [9]. The corresponding oxygen stoichiometries are also reported. Results of the equation 3.2 and equation 3.3 are included in the graph as well.

Two different sets of measurements were performed – 1) self-diffusion coefficients in $(U_{0.85}Pu_{0.15})O_{2.10}$ as a function of temperatures (1573 K – 1773 K); 2) self-diffusion coefficients for different stoichiometric composition of hyper stoichiometric mixed oxide of $(U_{0.85}Pu_{0.15})O_{2+x}$ at a fixed temperature of 1673 K.

The measurements for plutonium self-diffusion coefficient in $(U_{0.85}Pu_{0.15})O_{2.10}$ as a function of temperature (as noted in Figure 3.1) lead to the following equation assuming an Arrhenius law:

$$D_{Pu}^* (m^2 s^{-1}) = 1.9 \cdot 10^{-6} \exp \left[-\frac{360(kJ.mol^{-1})}{RT} \right] \quad (1573 K \leq T \leq 1773 K) \quad \dots(3.3)$$

As seen in Figure- 3.1, the activation energy of 360 kJ/mol for $O/M=2.1$ is very high compared to Lindner et al. [4] (138 kJ/mol). Riemer & Scherff argued that the stoichiometry in the experiment of Lindner et al. [4] could have been wrongfully estimated and that the sample could even have been hypo-stoichiometric in oxygen (instead of hyper-stoichiometric). However, there is no conclusive evidence supporting this argument. Moreover, the prefactor for both the Arrhenius equations from Lindner et al. [4] and Riemer & Scherff [5] also exhibit a significant deviation, which can also be noticed in Figure- 3.1.

As argued by Riemer & Scherff, one would expect an activation energy of around 628 kJ/mol for the stoichiometric composition $(U_{0.85}Pu_{0.15})O_2$, in coherence to the activation energy of uranium diffusion in UO_2 . The deviation $x=0.1$ causes an expected steep decrease in the activation energy. Thus an activation energy of 360 kJ/mol at $O/M=2.10$ seems to be reasonable. Moreover this value is in agreement with the data on uranium diffusion data in hyper stoichiometric UO_{2+x} [6]. The work of Marin & Contamin [6] was performed on polycrystalline UO_{2+x} . The results were in agreement with the experiments on single-crystal urania as well. Therefore, the activation energy represents an activation energy for volume diffusion without strong grain-boundary effect. However, this agreement is not sufficient enough to conclude on the effect of grain-boundary diffusion in this experiment.

Plutonium self-diffusion coefficients were also measured by the authors as a function of the oxygen to metal ratio (2.043 – 2.17) in $(U_{0.85}Pu_{0.15})O_{2+x}$ at constant temperature, 1673 K. The plutonium diffusion coefficient is found to increase with x , the deviation from the $O/M=2$, being proportionate to $(x^{2.77})$. These results are in good agreement with the experimental data for uranium diffusion in UO_{2+x} [7].

3.2.3. Matzke (1973) [8]:

Matzke (1973) [8] investigated the plutonium self-diffusion in polycrystalline hypostoichiometric oxide $(U_{0.85}Pu_{0.15})O_{2-x}$. The fresh pellets were annealed at 1773 K and 1873 K under a commercial H_2 reducing atmosphere. Prior to the diffusion annealing, the tracer Pu^{238} was applied using an electron beam evaporation device. The α -degradation method was used to measure the tracer concentration profile. A special emphasis was given to obtain a thinner tracer layer of 10 to 20 Å. Special care was also taken to limit the surface damage and contamination in the final polishing & pre-annealing stage.

The plutonium diffusion coefficient was found to decrease from $O/M=1.94$ to 1.98 . The author compared the measured data with the uranium diffusion coefficients in urania and the plutonium diffusion coefficient measured by Riemer & Scherff [5]. The comparison between these results and the results of Lindner et al. [4], Riemer & Scherff [5] and Schmitz & Marajofsky [9] are also compared in Figure- 3.1. The results of Matzke [8] and Schmitz & Marajofsky [9] are in agreement to each other. By considering the uranium diffusion data in UO_{2+x} (proportional to $\sim x^2$) and the data of Riemer & Scherff [5] in $(U_{0.85}Pu_{0.15})O_{2+x}$, Matzke proposes the existence of a minimum at $O/M \approx 1.98$ for the cation diffusion.

3.2.4. Schmitz & Marajofsky (1975) [9]:

Measurements of plutonium diffusion coefficient in both single-crystalline UO_2 and polycrystalline $(U_{1-f_{Pu}}Pu_{f_{Pu}})O_{2-x}$ mixed oxide with $f_{Pu}=0.04, 0.1, 0.15, 0.2, 0.3$ at 1783 K were performed by Schmitz & Marajofsky [9]. During the first heat treatment, the oxygen partial pressure was fixed using mixtures of CO/CO_2 ($CO/CO_2=10^2, 10^3, 10^4$). The tracer Pu^{238} was then applied by evaporation from a Knudsen cell on the sample surface. After the second heat treatment on the doped samples, the plutonium diffusion coefficient was deduced from Pu^{238} concentration profile measured by the α -degradation method.

All the experimental data are plotted in Figure- 3.2 as a function of $(2x/f_{Pu})$. Indeed the authors considered that the oxygen potential determines the plutonium valence ($V_{Pu}=4 - 2x/f_{Pu}$) for $O/M < 2$ whereas uranium remains as U^{4+} . For a fixed oxygen partial pressure (or $2x/f_{Pu}$), the diffusion coefficient does not depend very much on the plutonium content in $(U_{1-f_{Pu}}Pu_{f_{Pu}})O_{2-x}$ for f_{Pu} ranging from 0 to 0.3. However, for a fixed plutonium content f_{Pu} , the plutonium diffusion coefficient increases with a decreasing oxygen partial pressure (or oxygen stoichiometry).

Finally, as presented in Figure- 3.2, the authors described the plutonium diffusion coefficient variation as a linear function of $(2x/f_{Pu})$ as follows:

$$\text{Log}_{10} D_{Pu}^* (m^2 s^{-1}) = \left[-(15.9 \pm 0.2) + (2.7 \pm 1) \frac{2x}{f_{Pu}} \right] \cdot 10^{-4} (\text{at } 1783 \text{ K}) \quad \dots(3.4)$$

Therefore the plutonium diffusion coefficient in $(U_{1-f_{Pu}}Pu_{f_{Pu}})O_{2-x}$ was found to increase linearly with its valence (or oxidation state). These results are interpreted by assuming the existence of a complex defect cluster constituted of two plutonium cations Pu^{3+} and Pu^{4+} associated with an oxygen vacancy V_O° .

Then the (x/f_{Pu}) ratio represents the number of clusters, thus the probability for a plutonium cation to be trapped in the cluster. The existence of the minimum for $O/M \approx 2$ is explained by the authors by a vacancy diffusing mechanism occurring for $O/M > 2$.

It has to be noted that the oxygen stoichiometry of the samples was not measured directly but deduced from a proportional relation to the partial pressure of oxygen [9].

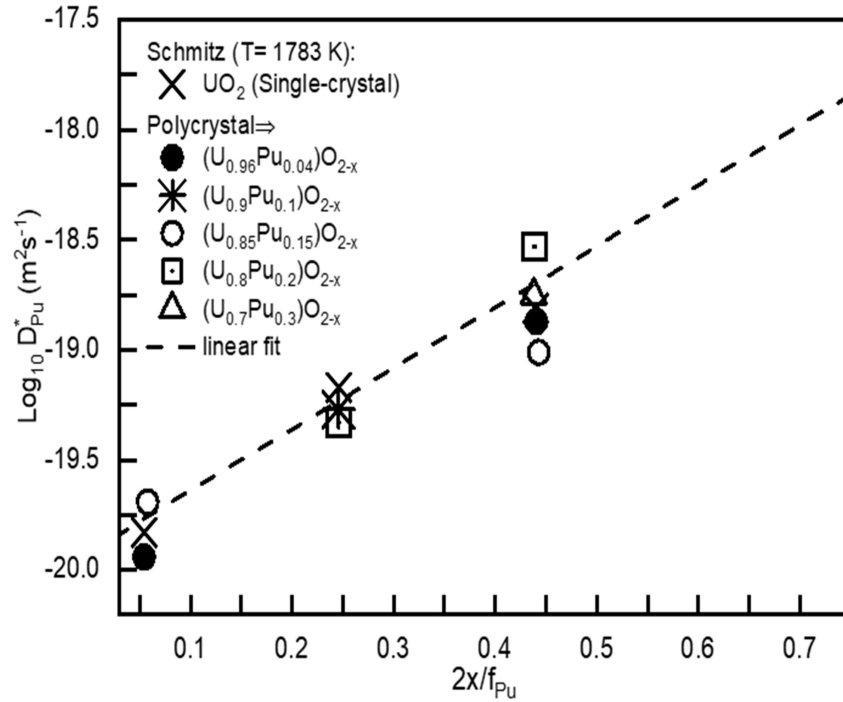


Figure 3.2: The linear relation between $2x/f_{Pu}$ and plutonium diffusion coefficient deduced by Schmitz & Marajofsky [9]; All MOx samples are polycrystalline but UO_2 sample is single-crystalline. Linear fit represents the equation 3.9.

3.2.5. Lambert (1978) [10]:

For the first time, Lambert measured the plutonium diffusion coefficient on single-crystals of both UO_2 and $(U_{0.8}Pu_{0.2})O_{2\pm x}$ mixed oxide [10]. Moreover an extensive review of the past published data was performed. Many experimental uncertainties, detailed in [10], like evaporation-condensation processes, for instance, were analysed.

The mixed oxide pellets were annealed for 18 hours in the temperature range 1873 K – 2173 K under both H_2/H_2O (for $O/M < 2$) and CO/CO_2 (for $O/M > 2$) gas mixtures to adjust the oxygen to metal ratio. The Pu^{238} tracer was applied by the evaporation method using an electron gun and the α -degradation method was used to measure the tracer concentration profile.

The following Arrhenius law was deduced for the Pu diffusion in UO_2 :

$$D_{Pu \text{ in } UO_2}^* (m^2 s^{-1}) = 0.65 \cdot 10^{-4} \exp \left[-\frac{540 \pm 55 (kJ \cdot mol^{-1})}{RT} \right] \quad \dots(3.5)$$

The activation energy is much higher than the previous literature data for uranium diffusion in UO_2 . According to Lambert, the previous diffusion coefficient data, which are quite scattered, were overestimated due to possible experimental errors and/or a slight deviation from the stoichiometry 2.

For the mixed oxide $(U,Pu)O_{2\pm x}$, the O/M ratio was deduced using thermodynamic data from Chilton and Kirkham [11] for $O/M > 2$ and from Tetenbaum [12] for $O/M < 2$. As shown in Figure- 3.3, the results at 1773 and 1873 K show the existence of a minimum of $D \sim 10^{-21} \text{ m}^2/\text{s}$ for an O/M ratio slightly below 2, as previously suggested by Matzke [8] and Schmitz and Marajofsky [9]. The position of the minimum changes with temperature, being shifted to lower O/M ratio with increasing temperature, as already found in magnetite Fe_3O_4 [13]. The existence of the minimum is interpreted by a point defect model and corresponds to a change in the cation diffusing mechanism: an interstitial one for $O/M < 1.98$ and a vacancy one for $O/M > 1.98$.

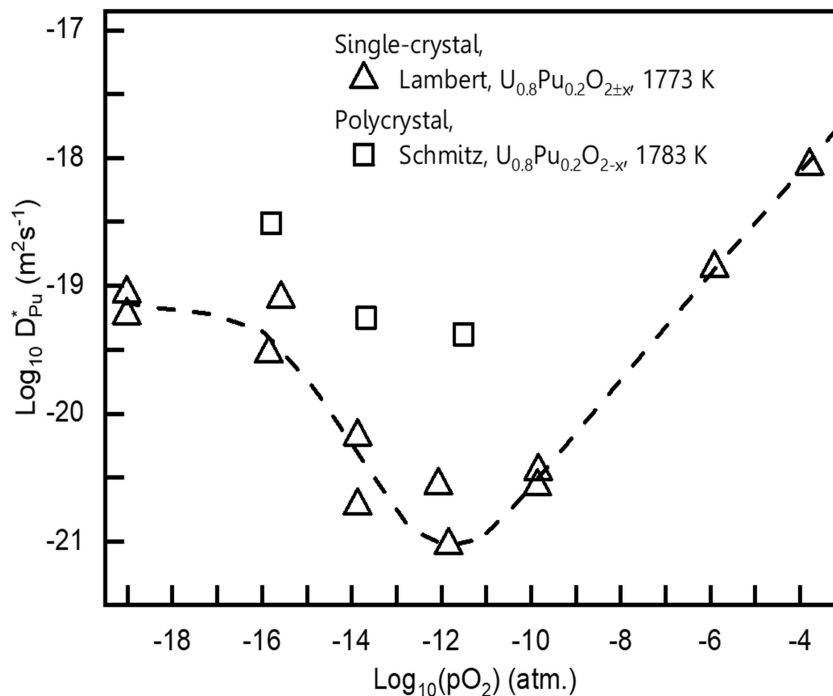


Figure 3.3: The plutonium diffusion curve of Lambert's Thesis [10] and the data of Schmitz & Marajofsky [9]. The minimum of the curves is positioned in hypo-stoichiometric regime.

Lambert also discussed the discrepancies between his data at 1773 K and the data of Schmitz & Marajofsky, at 1783 K (Figure- 3.3). Schmitz and Marajofsky obtained a higher diffusion coefficient. According to Lambert, the difference in the diffusion coefficient could be due to the use of MOx polycrystals by Schmitz & Marajofsky [9]. However, the plutonium diffusion in single crystal UO_2 , found by Schmitz & Marajofsky [9], is also higher than that of Lambert (as noted in Figure- 3.4).

A detailed analysis of the uncertainties was also performed by the author leading to the following relative error values on the penetration length δ and the diffusion coefficients D :

- For $10^{-16} < D < 10^{-17}$ (m^2/s): $\Delta\delta = 4 \%$, $\Delta D = 10 \%$
- For $10^{-20} < D < 10^{-21}$ (m^2/s): $\Delta\delta = 40 \%$, $\Delta D = 80 \%$

It can be noted that very large uncertainties are found, especially for the lowest diffusion coefficient values (found at the minimum).

3.2.6. Matzke (1983) [14]:

With the same method used by Lambert [10], Matzke studied the plutonium self-diffusion in $(U_{0.82}Pu_{0.18})O_{2\pm x}$ single crystal [14]. During the heat treatments in the temperature range 1673 K – 1973 K, the oxygen to metal ratio of the mixed oxide samples were fixed using different atmospheres: vacuum, purified argon, CO/CO_2 gas mixture, dry H_2 and H_2/H_2O mixture. An electron gun was used to evaporate Pu^{238} tracer on the samples. The tracer diffusion profile was measured using the α -degradation method. The lower limit of detection of this method was reported to be $\sim 10^{-22}$ m^2/s .

As mentioned above, oxygen potential was controlled. However, Matzke did not report the oxygen to metal ratio of the samples. Hence, in this work, the oxygen stoichiometries have been calculated using the model of Guéneau et al [15].

Like in the work of Lambert, very careful experimental conditions were used to reduce the uncertainties, as for instance, the near-surface effects. The results obtained for the plutonium diffusion in $(Pu/M)=0.18$ are in very good agreement with the results obtained by Lambert for $(Pu/M)=0.20$. The minimum in the plutonium diffusion coefficient is found at $O/M \approx 1.98$.

As in the thesis of Lambert, the plutonium diffusion coefficient variation as a function of the O/M ratio is explained using a point defect model. The cation diffusion in the mixed oxide is governed by interstitial and vacancy mechanisms. However, for very low O/M ratio (below 1.95), the diffusion process could be governed by a complex cluster of $(2Pu^{3+} - V_O)$.

3.2.7. Noyau (2012) [16]:

Noyau measured plutonium diffusion coefficient data in polycrystalline $(U_{0.55}Pu_{0.45})O_{2-x}$ samples at 1745, 1869, 1916 and 1970 K [16]. The pellets were annealed at 1753 K for 20 hours under $Ar+5\%H_2/H_2O$ atmosphere to attain oxygen to metal ratio in the range 1.95 – 1.98, corresponding to an oxygen potential $\mu(O_2)$ of -395 ± 2 kJ/mol. The O/M ratio values reported by the authors were calculated using the model of Guéneau et al [15].

It has to be mentioned that Noyau used a different tracer, Pu^{242} , as Pu^{238} was not available. Also for the first time, Noyau used another technique, Secondary Ion Mass Spectrometric (SIMS) to measure the plutonium tracer concentration profile on $(U, Pu)O_2$ samples. The benefit of this technique is that the concentration threshold is very low of the order of ppb with a resolution of the order of nanometre.

From his experimental results on polycrystalline MOx pellets, Noyau extracted two different Arrhenius laws corresponding to both the plutonium volume diffusion coefficients (D_{Pu}^*) and grain-boundary diffusion coefficients (D_{Pu}^{GB}):

$$- D_{Pu}^*(m^2s^{-1}) = (11.02_{-4.93}^{+6.41})10^{-4} \exp \left[-\frac{625_{-6.75}^{+3.86}(kJ.mol^{-1})}{k_B T} \right] \quad \dots(3.6)$$

$$- D_{Pu}^{GB} (m^2s^{-1}) = (4.51_{-2.99}^{+2.90})10^{-2} \exp \left[-\frac{507_{-11.58}^{+1.93}(kJ.mol^{-1})}{k_B T} \right] \quad \dots(3.7)$$

Noyau compared his volume diffusion coefficient results with the literature data from Lambert and Matzke. The experimental data of – Noyau for volume diffusion are lower by half order of magnitude than the plutonium diffusion data in UO_2 measured by Lambert [10] (as noted in Figure- 3.5). However, the volume diffusion coefficient in MOx is at the same order of magnitude compared to the data of Lambert on MOx with 20% Pu, as noted in Figure- 3.4 (for the mentioned temperatures), although the respective plutonium contents are different in both of these experiments. On the other hand, the grain boundary diffusion, estimated by Noyau, is significantly higher than the volume diffusion coefficients (Figure- 3.4) which is evident due to the presence of grain boundary and a high concentration of defects in the crystal. This high concentration of defects causes the decrease of migration energy of diffusion, hence, a higher diffusion coefficient is obtained [16].

3.2.8. Cheik Njifon (2019) [17]:

Recently, Cheik Njifon studied the migration barrier of both uranium and plutonium diffusion in stoichiometric $U_{0.75}Pu_{0.25}O_2$, using Nudged Elastic Band Density Function Theory (DFT). The barriers were studied for diffusion of Pu vacancy and interstitial. The author determined the activation energy of diffusion for plutonium vacancy with neutral charge and formal charge (+4). However, the activation energy of plutonium interstitial diffusion was determined only for neutral charge.

As assumed in this study, the diffusion activation energy is a summation of defect formation energy (vacancy or interstitial) and the migration energy of the defect [18]. However, for non-stoichiometric samples, the defects are already present in the sample. Hence, the formation energy of defect needs not to be considered in those samples. Even at the oxygen stoichiometry of O/M= 2.000, the mixed oxide of uranium and plutonium crystal is not free from defect (as assumed in this study) [19]. Therefore, the activation energy (as an arithmetic sum of formation energy and migration energy) of this study is not comparable with the activation energies of experimental works.

The author obtained the highest value of migration energy for the formal charged Pu vacancy, i.e. 528.74 kJ/mol. The highest experimental activation energy of Pu self-diffusion, found by Noyau [16], is 625 kJ/mol. However, these two studies are performed at two different plutonium contents (45% Pu MO_x for Noyau and 25% Pu MO_x for this study). Also, the study of Noyau [16] is performed at a different stoichiometry than this study. The different migration and activation energy values obtained in this study are tabulated in Table 3.1.

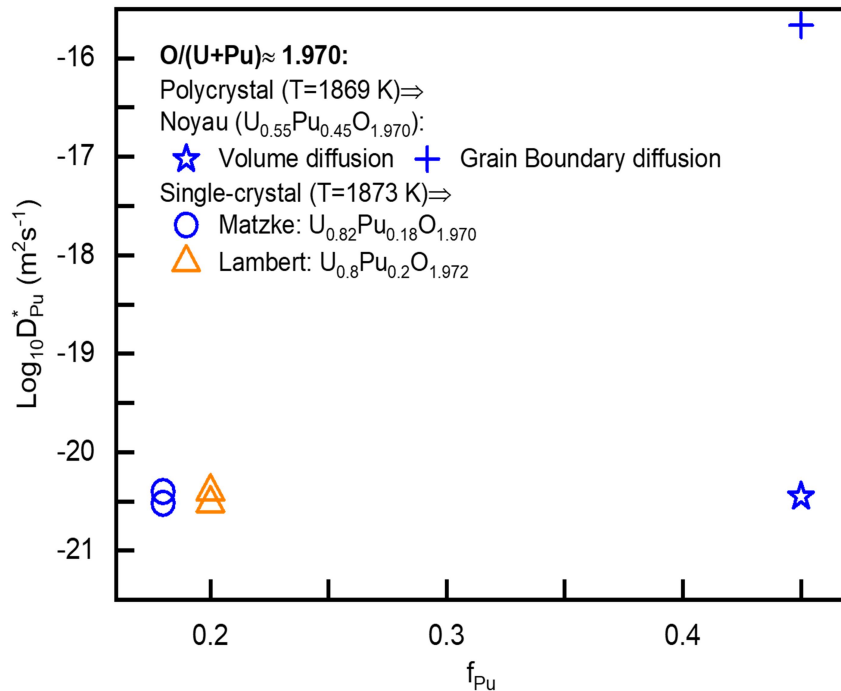


Figure 3.4: Plutonium self-diffusion coefficient as a function of plutonium content; Results are showing near stoichiometric ratio of 1.97 and plutonium content ranging from 18% to 45%. Data of Lambert [10], Matzke [14] and Noyau [16] are reported.

3.3. Pu diffusion in PuO₂:

There is no direct measurement found in literature to estimate the plutonium diffusion coefficient of plutonium dioxide. However, there are few studies performed to estimate the activation energy of self-diffusion for plutonium in plutonium dioxide.

3.3.1. Kutty *et al.* (2000) [20]:

Kutty *et al.* [19] performed an experimental work on the sintering of UO₂-PuO₂ mixtures with different fractions of PuO₂ (0%, 20%, 50%, 76% and 100%). The authors measured the shrinkage behaviour of the pellets using a dilatometer. A better sinterability was found in reducing atmosphere (Ar+8%H₂) than in oxidizing atmosphere (CO₂). The reducing atmosphere caused the formation of Pu³⁺ ion, as confirmed by XRD analysis. Hence, in reducing atmosphere, the expansion in shrinkage curve around 1173 K – 1373 K was assumed to be related to the formation of Pu³⁺ ion and the combined diffusion of both Pu³⁺ and Pu⁴⁺ ions. Based on this analysis and on point defect model [21, 22], the migration energy of Pu³⁺ and Pu⁴⁺ were estimated. The migration energies of plutonium ions (both Pu³⁺ and Pu⁴⁺) are reported in table 3.1.

3.3.2. Wang *et al.* (2020) [23]:

The migration of Pu in PuO₂ was studied by Wang *et al.* using the Nudged Elastic Band (NEB). The migration energy of Pu vacancy and interstitial were determined in this study. The migration of both the Pu defects were studied in two pathways, i.e. <100> and <110>.

The migration energy of Pu interstitial, in the direction of <100>, is the lowest one among the computed migration energies of this study, i.e. 248 kJ/mol. However, the determined migration energy of Pu vacancy in the direction of <100> is 447.69 kJ/mol and the migration energy of Pu³⁺, found by Kutty *et al.* [20], is 396.55 kJ/mol. On the other hand, the determined Pu interstitial in the direction of <110> is 592.42 kJ/mol and the migration energy of Pu⁴⁺, found by Kutty *et al.* [20], is 574 kJ/mol.

All these migration energies found in this study are tabulated in the table (Table- 3.1).

Compounds	O/M	T (K)	Atmosphere	$p(O_2)/\mu(O_2)^{\#}$	Crystal	Exp ^o	Tracer	Principle	Q_{act} (eV)	D_0	Ref
$(U_{0.85}Pu_{0.15})O_{2+x}$	~2.0	1173 – 1873	H ₂ + H ₂ O	-	PC	α	238	Arrhenius	1.4	$3.45 \cdot 10^{-14}$	Lindner (1967)
$(U_{0.85}Pu_{0.15})O_{2+x}$	2.05 – 2.10	1573 – 1773	CO/CO ₂	-	PC	α	238	Arrhenius	3.73	-	Riemer (1971)
$(U_{0.85}Pu_{0.15})O_{2-x}$	1.95 – 2.00	1773 – 1873	H ₂ reducing atmosphere	-	PC	α	238		-		Matzke (1973)
$(U_{0.96}Pu_{0.04})O_{2-x}$ $(U_{0.90}Pu_{0.10})O_{2-x}$ $(U_{0.85}Pu_{0.15})O_{2-x}$ $(U_{0.80}Pu_{0.20})O_{2-x}$ $(U_{0.70}Pu_{0.30})O_{2-x}$	1.90 – 2.00*	1783	CO/CO ₂	$p(O_2)=$ $1.6 \cdot 10^{-16}$ $2.1 \cdot 10^{-14}$ $3.1 \cdot 10^{-12}$	PC	α	238	Valence (2x/y)	-	-	Schmitz (1975)
UO ₂ $(U_{0.80}Pu_{0.20})O_{2\pm x}$	2.00 (UO ₂) 1.90 – 2.15 (MOx)	1773 – 2173	Vacuum (UO ₂) CO/CO ₂ (hyper) H ₂ /H ₂ O (hypo)	$\mu(O_2)=$ -96.65 to -642.24	SC	α	238	Arrhenius	5.6 ± 0.6 (UO ₂)	$6.5 \cdot 10^{-3}$ (UO ₂)	Lambert (1978)
$(U_{0.82}Pu_{0.18})O_{2\pm x}$	1.91 – 2.09	1673 – 1973	CO/CO ₂ H ₂ /H ₂ O Dry H ₂	$\mu(O_2)=$ -96.7 to -627.5	SC	α	238	Point-defect Model	-		Matzke (1983)
$(U_{0.55}Pu_{0.45})O_{2-x}$	1.95- 1.98*	1745 – 1970	Ar+5%H ₂ /H ₂ O	$\mu(O_2)=$ 395 \pm 2	PC	S	242	Arrhenius	$6.48^{+0.04}_{-0.07}$	$(11.02^{+6.41}_{-4.93})10^{-4}$	Noyau (2012)
PuO ₂	1.92- 2.003	-	Ar-8%H ₂ CO ₂	-	-	Sin	-	Point-defect Model	4.11(Pu ³⁺) 5.95(Pu ⁴⁺)	-	Kutty (2000)
$(U_{0.75}Pu_{0.25})O_2$	2.00	-	-	-	-	D	-	NEB	4.90(V ⁰ _{Pu}) ¹ 5.48(V ⁰ _{Pu}) ² 4.01(I ⁰ _{Pu}) ³	-	Cheik Njifon (2019)
PuO ₂	2.00	-	-	-	-	D	-	NEB	4.64(V ⁰ _{Pu}) ⁴ 3.38(V ⁰ _{Pu}) ₅ 2.57(I ⁰ _{Pu}) ⁶ 6.14(I ⁰ _{Pu}) ⁷	-	Wang (2019)

Table 3.1: Bibliography of plutonium diffusion coefficient with experimental conditions from different references;

*calculated from Taf-ID

$p(O_2)$ is in atm and $\mu(O_2)$ is in kJ/mol; whereas, $\mu(O_2)= RT\ln[p(O_2)]$;

^oExp represents the experimental techniques; α - Alpha degradation method, S- Secondary Ion Mass Spectroscopy, Sin- Sintering Experiment, D- Density Function Theory;

¹Plutonium vacancy with neutral charge; ²Plutonium vacancy with formal charge; ³Plutonium interstitial with neutral charge;

⁴Plutonium vacancy in [100] direction; ⁵Plutonium vacancy in [110] direction;

⁶Plutonium interstitial in [100] direction; ⁷Plutonium interstitial in [110] direction;

3.4. Discussion and selection of experimental data:

An overall comparison of self-diffusion coefficients in stoichiometric MOx is tabulated in Figure- 3.5, with respect to the plutonium content, starting from UO₂ (or, 0% MOx).

The plutonium diffusion coefficient value in UO₂ measured by Lambert [10] is higher than the data obtained by Schmitz [9] which is probably due to the use of polycrystal by Schmitz [9] instead of single crystals by Lambert [10]. Thus for the Pu diffusion in UO₂, the data of Lambert are selected.

For the MOx, the data of Lindner [4] and Schmitz [9] are systematically higher than the data obtained on single crystals by Lambert [10] and Matzke [14]. The results of Schmitz are higher than the results of Lambert [10] and Matzke [14] by one order of magnitude.

The diffusion coefficients of Lindner [4] is higher than the results of Schmitz [9] by two orders of magnitude. This clearly indicates that the Grain boundary effect is predominant in the case of Lindner [4]. If the diffusion coefficient in polycrystal is comparable to the self-diffusion coefficient in single-crystal then the diffusion mechanism can be assumed as volumetric diffusion [16]. However, the diffusion coefficients of Schmitz [9] can assume to be neither in agreement to the volumetric diffusion mechanism [10, 14] nor the grain boundary diffusion mechanism [4]. Therefore, the conclusion for the diffusion mechanism in the experiment of Schmitz [9] cannot be confirmed. However, this set of data is not selected but will be compared to the upcoming model under this work.

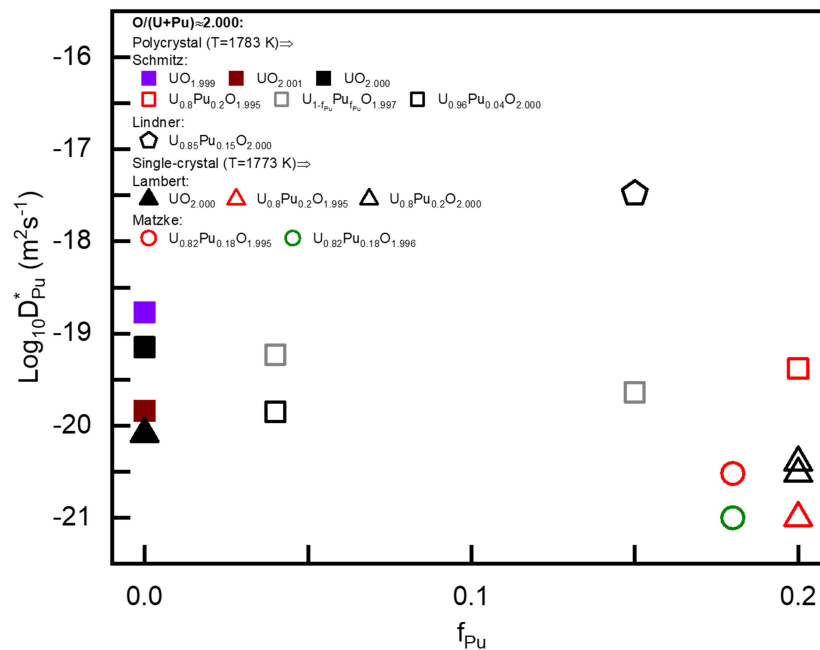


Figure 3.5: Plutonium self-diffusion coefficient as a function of plutonium content at near perfect stoichiometric ratio and the plutonium content ranging from 0% to 20%. Data of Schmitz [9], Lindner [4], Lambert [10], Matzke [14] are reported.

The only single-crystal self-diffusion coefficient data measured in MOx by Matzke [14] and Lambert [10], are reported in Figure- 3.5. Both of these results are very similar and comparable to each other (as the Pu contents are very close, 18% Pu MOx and 20% Pu MOx). As, these two experiments are performed on single-crystals, the diffusion coefficients are indicative of self-diffusion coefficients. So, these data are selected.

The plutonium diffusion coefficients value in UO_2 measured by Lambert [10] is higher than that of in $(U_{0.8}Pu_{0.2})O_{2\pm x}$ and $(U_{0.82}Pu_{0.18})O_{2\pm x}$. These data show that the plutonium diffuses faster in UO_2 than in MOx and thus that for an O/M close to 2.00, the Pu diffusion coefficient decreases with the Pu content.

An overall comparison of the plutonium diffusion data in MOx as a function of the oxygen partial pressure at comparable temperatures is represented in Figure- 3.6.

The results of Lambert [10] and Matzke [14] on single-crystal MOx with 20% and 18% Pu content clearly show that the Pu diffusion coefficient shows a minimum at about 10^{-21} m²/s for $pO_2 \sim 10^{-12}$ atm corresponding to an O/M ratio of 1.98. The diffusion coefficient data are much higher for lower and higher O/M ratio. A plateau was observed for pO_2 lower than 10^{-15} atm.

In comparison with these data, the volumetric diffusion coefficient of Noyau [16] for 45% Pu and O/M ratio of about 1.98 is about one order of magnitude lower than the diffusion coefficients of Lambert [10] and Matzke [14], which could be due to the different plutonium contents and temperature of respective experiments.

The data of Schmitz on polycrystals of MOx with 4 – 15 % Pu are higher than the data on single-crystals but the variation with oxygen partial pressure is consistent with Lambert [10] and Matzke [14] showing an increase in the Pu diffusion coefficient for pO_2 lower than 10^{-12} atm corresponding to $O/M < 1.98$.

For higher oxygen partial pressure $pO_2 > 10^{-12}$ atm corresponding to $O/M > 2$, the plutonium diffusion increases with the oxygen partial pressure. The data of Lindner [4] and Riemer [5] for 15% Pu are not consistent with the data of Lambert [10] and Matzke [14] for 20% and 18% Pu, being one and half order of magnitude higher. In the present work, the data of Lambert and Matzke are selected. A comparison of our model with the data of Riemer [5] will be performed.

To conclude, the experimental data selected for the modelling are:

- Lambert [10] data for the Pu diffusion in UO_2 ;
- Lambert [10] and Matzke [14] data for the Pu diffusion in MOx with 20% and 18% plutonium content;
- Noyau [16] data for the Pu diffusion in MOx with 45% Pu content;

The results of DFT of Cheik Njifon [17] on stoichiometric MOx will not be directly used in the modelling. However, the final results of our model will be compared with these results.

Concerning the Pu diffusion data in PuO₂, as there is no direct measurement of the Pu diffusion coefficient, a simpler model (the ‘cBΩ model’) is used to provide input data to DICTRA model (Chapter- 4). Our results will be compared with the diffusion activation energy of plutonium ions estimated by Kutty [20], and calculated by Wang [23].

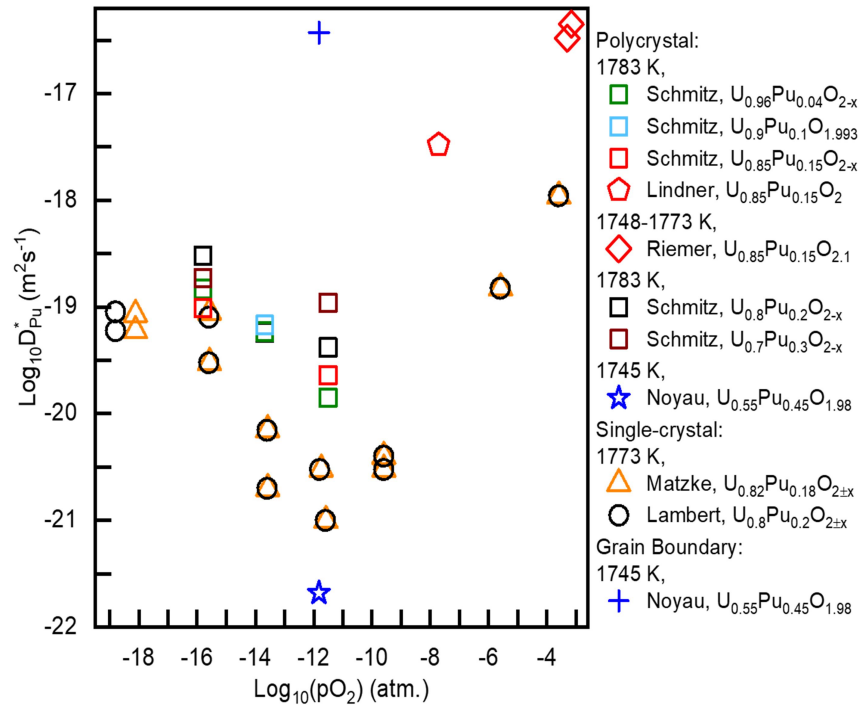


Figure 3.6: Plutonium diffusion coefficient against partial pressure of oxygen. Diffusion coefficient both through grain boundary and volumetric of [16] are included. The Lambert's results [10] and Matzke's results [14] are with single-crystal but the results of Lindner [4], Riemer [5] and Schmitz [9] are with polycrystal.

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CHAPTER - IV

SIMPLE MODELS FOR CATION DIFFUSION IN BINARY OXIDES

This chapter firstly aims to compute a substantiated diffusion coefficient for plutonium diffusion in plutonium dioxide. In due process, this will explore two simple semi-empirical models for diffusion of defects in ionic crystals. A comparative study will be performed in between these two models. One of the model will be selected and improvised further to apply for diffusion coefficient calculations of cations in few binary oxides, which were explored experimentally and respective diffusion coefficients were estimated. Then the improvisation further extended to compute the plutonium diffusion in plutonium dioxide. Further extending the scope of this chapter, we will explore cation diffusion in other dioxides of rare earth and radioactive metals, in view of the selected model.

4.1. Introduction:

In this chapter, we explore two simple empirical models, which use macro-physical parameters to quantify the self-diffusion coefficients of ions. We also discuss about those macro-physical quantities and how they are deduced to implement in these models.

The first model- Glyde's model- was derived from the relation between migration energy of a vacancy and the Debye temperature of the material [1]. A similar relation was developed by Mukherjee [2] between vacancy formation energy and Debye temperature. That was considered the point of inception of Glyde's model. We will discuss briefly the model of Mukherjee and then introduce Glyde's model theoretically in this chapter.

The second model- $cB\Omega$ model- was developed by Varotsos and co-workers. The model was first formalised a relation between Gibbs formation energy of vacancy, in relation to the volume per atom and the local bulk modulus of the deformed region (which is again assumed to be equal to the overall bulk modulus of the material), as the creation of vacancy caused a local dilation of its surroundings [3]. Based on this hypothesis, a similar relation was also formalised for the activation free energy of vacancy diffusion. This relation consists of a product of bulk modulus of material and mean volume per atom and a fitting parameter, which can be fitted over the experimental estimation of self-diffusion coefficients. However, this relation is only valid when the diffusion is assisted by single type of defect. We will also discuss the theoretical basis and the practical applicability of this model in this chapter as well. Further, we will compare both the models and will show that both the models are actuating a same (or, similar) formalism for the activation free energy of self-diffusion.

Henceforth, we will apply the experimentally deduced self-diffusion coefficient values to estimate the fitting parameter mentioned in the $cB\Omega$ model for three cases- Th^{4+} diffusion in ThO_2 , U^{4+} diffusion in UO_2 and O^{2-} diffusion in Li_2O . All these three compounds exhibit fluorite structure (Li_2O exhibits anti-fluorite structure or inverted-fluorite structure) and the corresponding cation lattices (anion lattice for Li_2O) exhibit face centred cubic (fcc) lattice structure. Then we will establish a linear fitting relation between the ionic radii of the diffusing ion and the fitting parameter. Later, using this linear fit, we will deduce the Pu^{4+} diffusion in PuO_2 (which also exhibits a fluorite structure and Pu^{4+} exhibit an fcc lattice). The linear fit relation will then again be extrapolated to deduce the cation diffusion in several other actinide and lanthanide (only Ceria) oxides.

At the end of the chapter, we will re-calculate the Arrhenius equation of each of these cation diffusion cases, which will further aid us to study the evolution of the activation energy and prefactor of the cation self-diffusion in different oxides with fluorite structure.

4.2. Glyde's Model:

The direct relation between formation energy of vacancy defect and the Debye model of solids were been theoretically explored [2, 4]. Mukherjee pointed out if the formation energy of a vacancy ($Q_f^{\text{Mukherjee}}$) surrounded by ζ nearest atoms in a closed packed metallic lattice being:

$$Q_f^{\text{Mukherjee}} = \frac{\zeta}{2} W_\infty; W_\infty = \text{work done to remove atom from site to infinity.} \quad \dots(4.1)$$

Then, the classical vibration frequency of the atom (due to the simple harmonic oscillation) can be approximated as the Debye characteristic frequency (ν_D) and can further be expressed as,

$$\nu_D = \left(\frac{1}{2\pi} \right) \left[\frac{n(n-1)Q_f^{\text{Mukherjee}}}{\zeta \mu \Omega^3} \right]^{1/2} \quad \dots(4.2)$$

Where, μ is the atomic mass; Ω is the mean atomic volume and n is the number of atoms per lattice.

However, Glyde proposed a proportional relation between Debye temperature (θ_D) (instead of Debye frequency) & vacancy migration energy (Q_m^{Glyde}) by quantifying the probability of atomic displacement to jump to the adjacent vacant site for monoatomic cubic crystals [1].

$$Q_m^{\text{Glyde}} = C_0^m \left(\frac{2\pi k_B}{h} \right)^2 \mu \theta_D^2 a_0^2 \quad \dots(4.3)$$

Where, C_0^m is the proportionality constant, h is Planck's constant, k_B is Boltzman's constant and a_0 is the lattice parameter at 0 K.

Glyde [1] further demonstrated that similar to migration energy, formation energy is also proportional to the product of $\mu \theta_D^2 a_0^2$.

$$Q_f^{\text{Glyde}} = C_0^f \left(\frac{2\pi k_B}{h} \right)^2 \mu \theta_D^2 a_0^2 \quad \dots(4.4)$$

Activation energy of self-diffusion is an arithmetic sum of formation enthalpy & migration enthalpy, a direct relation could eventually been established between Debye temperature and activation energy of self-diffusion as following:

$$Q_{\text{act}}^{\text{Glyde}} = (C_0^f + C_0^m) \left(\frac{2\pi k_B}{h} \right)^2 \mu \theta_D^2 a_0^2 = C_0^{\text{act}} \left(\frac{2\pi k_B}{h} \right)^2 \mu \theta_D^2 a_0^2 \quad \dots(4.5)$$

Hence, Siethoff re-formulated the activation energy of self-diffusion using the model of Glyde [1] for fcc lattice [5]:

$$Q_{\text{act}}^{\text{Glyde}} = C_1 \left(\frac{k_B}{h} \right)^2 n^{2/3} \mu a_0^2 (\theta_D^{0K})^2 \quad \dots(4.6)$$

Where C_1 is a proportionality constant.

Siethoff also commented that the shear modulus at 0 K (K_s^{0K}) of the material is directly related to the Debye temperature,

$$\theta_D^{0K} = C_2 \left(\frac{k_B}{h}\right)^2 n^{-1/6} \left(\frac{K_s^{0K} a_0}{\rho}\right)^{1/2} \quad \dots(4.7)$$

Where C_2 is another fitting constant. In the relation 4.6, following the work of Ledbetter [6] where it was pointed out that the use of Bulk modulus (B) instead of the Shear modulus (K_s) for cubic metals leads to a significant error. Hence, author used K_s^{0K} in equation 4.6.

Merging equations 4.6 & 4.7, author deduced an equation,

$$Q_{act}^{Glyde} = C_3 \left(\frac{a_0^3}{n}\right) K_s^{0K} \quad \dots(4.8)$$

Where $C_3 = C_1 C_2^2$; The relation was also previously derived semi-empirically [7]. On this point, the mean volume per atom at 0 K, Ω_0 , can replace $\frac{a_0^3}{n}$ of equation 4.8. Therefore, equation 4.8 develops to,

$$Q_{act}^{Glyde} = C_3 K_s^{0K} \Omega_0 \quad \dots(4.9)$$

Equation 4.9 of Glyde's model is equivalent to the following cB Ω model. However, the cB Ω model takes temperature dependence into account, which Glyde's model does not. This aspect will be discussed further in the following section.

4.3. cBΩ Model:

As explained in the chapter – 3, the self-diffusion coefficient of one species (cation in this case) in a system can be described in terms of Arrhenius expression as equation 3.1. In this relation, the activation energy (Q_{act}) does not vary with the change of temperature as it is the slope of the Arrhenius plot (plot of $\ln D^*$ vs $1/T$). However, the prefactor of the Arrhenius equation can vary with the system temperature. This variation of the prefactor with system temperature can be quantified in term of entropy as [8],

$$D_0 = D'_0 \exp\left(\frac{S_{act}}{k_B}\right); \quad \dots(4.10)$$

Where S_{act} is entropy of the system. Therefore, Arrhenius equation can be re-written as,

$$D^* = D_0 \exp\left(-\frac{Q_{act}}{k_B T}\right) = D'_0 \exp\left(-\frac{Q_{act} - TS_{act}}{k_B T}\right) \quad \dots(4.11)$$

In previous theoretical study [9], it was established that the activation energy of diffusion is the summation of defect formation enthalpy (H_F) and defect migration enthalpy (H_m) as,

$$Q_{act} = H_F + H_m = H_{act} \quad \dots(4.12)$$

Therefore, equation 4.10 can be re-written using second law of thermodynamics as,

$$D^* = D'_0 \exp\left(-\frac{G_{act}}{k_B T}\right) \quad \dots(4.13)$$

Where G_{act} is the activation free energy of self-diffusion.

D'_0 can be expanded after [8] as,

$$D'_0 = \lambda_{Geo} a_0^2 \nu \quad \dots(4.14)$$

Where λ_{Geo} is the geometric lattice correlation factor, ν is the jump frequency. It has to be noted as the D'_0 does not vary with the system temperature. Therefore, all three parameters of equation 4.14 should be evaluated at a given temperature, preferably at 0 K.

Therefore, the modified equation of self-diffusion is following,

$$D^* = \lambda_{Geo} a_0^2 \nu \exp\left(-\frac{G_{act}}{k_B T}\right) \quad \dots(4.15)$$

Our study utilizes different experimental results extensively to develop the model, within the cBΩ framework.

In the cBΩ framework, the activation free energy of self-diffusion (G_{act}) is explained as,

$$G_{act} = cB\Omega \quad \dots(4.16)$$

B is bulk modulus of the material; $\Omega = a^3/4$ for fcc lattices; c is a distinct fitting parameter fitted over the experimental results of self-diffusion coefficients [10].

4.3.1 Temperature dependence of Activation Energy:

Although Glyde's model and the $cB\Omega$ model are equivalent, they are not equal to each other. The Glyde's model define the activation energy (Q_{act}^{Glyde}) as per the following equation,

$$Q_{act}^{Glyde} = H_F + H_m \quad \dots(4.17)$$

Where, H_F and H_m are the enthalpy of formation and enthalpy of migration respectively. Therefore, Q_{act}^{Glyde} is basically the activation enthalpy of self-diffusion (H_{act}).

However, the activation free energy (G_{act}) of $cB\Omega$ model can be represented by both activation enthalpy (H_{act}) & activation entropy (S_{act}) as,

$$G_{act} = H_{act} - TS_{act} \quad \dots(4.18)$$

Hence, the activation energy given by the Glyde's model (Q_{act}^{Glyde}) is not temperature dependent but the activation free energy of $cB\Omega$ model (G_{act}) is dependent on temperature. Therefore, the equation 4.15 can be rewritten as,

$$D^* = \lambda_{Geo} a_0^2 v \exp\left(\frac{cB_0\Omega_0}{k_B T}\right) \exp\left(\frac{cf_T(B\Omega)}{k_B T}\right) \quad \dots(4.19)$$

Where, B_0 and Ω_0 are the bulk modulus and mean volume per atom at 0 K; $f_T(B\Omega)$ is the temperature dependence function of the product $B\Omega$. Therefore, $f_T(B\Omega)$ can be defined as,

$$B \times \Omega = (B_0 + b_1 T + b_2 T^2 + \dots)(\Omega_0 + \omega_1 T + \omega_2 T^2 + \dots) = B_0 \Omega_0 + f_T(B\Omega) \quad \dots(4.20)$$

Hence, the temperature dependence of B and Ω also needs to be studied for $cB\Omega$ model.

Now, we will discuss each parameter of equation 4.19 in the following subsections.

4.3.2 Geometric correlation factor (λ_{Geo}):

Bardeen and Herring noted that the diffusion of particles in solids follow a correlation factor [11]. The principle of Bardeen & Herring was applied by Compaan & Haven to calculate the correlation factor (λ_{Geo}). However, the results of Compaan & Haven achieved a better convergence in due process. The geometric correlation factor reported in [12], i.e. 0.78149 for fcc lattice, is utilized in this section of our study.

4.3.3 Jump frequency:

The jump frequency can further be approximated to the Debye frequency (ν_D) as reported in literature [13, 14]. The Debye frequency is related to the Debye Temperature (θ_D^{0K}) with the following equation [15],

$$\theta_D^{0K} = \frac{h\nu_D}{2\pi k_B} \quad \dots(4.21)$$

In the study of Actinide Oxides by Willis, it was found that Debye frequency is approximately constant against the temperature variation of the system [16].

However, the variation of Debye temperature with the change of system temperature was studied further for different fluorite compounds [17, 18]. The Debye temperature is quantified as a fourth-order polynomial of system temperature by Huffman & Norwood as [18]:

$$\theta_D = \theta_1 + \theta_2 T^2 + \theta_3 T^4 \quad \dots(4.22)$$

Where θ_1 , θ_2 & θ_3 are fitted constants.

As explained in the previous section, the Debye frequency needs to be considered at 0 K in our study. The Debye temperature is assumed to be approximately constant against the temperature variation of the system and the Debye temperature at 0 K is assumed to be the same at room temperature, in our study.

4.3.4 Lattice Parameter & Mean volume per atom:

As mentioned above, mean volume per atom and lattice parameter of fcc lattice share a direct relation. We calculate Ω from the value of lattice parameter directly in our study. Hence, mean volume per atom, Ω varies with the variation of system temperature as the lattice parameter varies.

The anharmonicity in the vibration of the atoms brings an expansion of the lattice due to heating of the system [19]. Lattice expansion coefficient (α) is directly related to the rate of change of lattice parameter as follows,

$$\alpha = \frac{1}{a_0} \left(\frac{da}{dT} \right) \quad \dots(4.23)$$

Where, a_0 is the lattice parameter at 0 K. The relation is implying that the thermal expansion coefficient can be utilized to deduce a temperature dependent function for lattice parameter [20].

A formulation of lattice parameter was previously deduced as a third-order function of system temperature [21] as:

$$a = a_0 + A_1 T + A_2 T^2 + A_3 T^3 \quad \dots(4.24)$$

Where A_1 , A_2 & A_3 are fitting constants exclusive for different compounds. In our study, we utilize different variations of equation 4.24 for different compounds, recommended by different authors [22, 23, 24]. These variations of lattice parameter are further discussed for different compounds, later of this chapter.

4.3.5 Bulk Modulus:

In literature, Elastic constants of fluorites were previously expressed as a second-order polynomial of temperature based on the empirical data [25]. Hence, the Bulk modulus (B_T) also can be deduced using a second order polynomial as,

$$B_T = B_0 + b_1T + b_2T^2 \quad \dots(4.25)$$

where, the B_0 , b_1 , b_2 are constants and their values are exclusive for different fluorite compounds. This equation, similar to lattice parameter, consists of two parts, i.e. temperature independent B_0 (or, bulk modulus at 0 K) & the temperature dependent part.

4.3.6 Determination of fitting parameter c :

The estimation of fitting parameter is done using a database of experimental estimation of self-diffusion coefficients (D-1 of figure 4.1). This database is further discussed in the next section. The fitting process calls for some re-writing of the governing equations of the $cB\Omega$ using equation 4.19.

$$\ln(D^*) - \ln(\lambda_{\text{Geo}}v_D a_0^2) = -\frac{c}{k_B T} [B_0\Omega_0 + f_T(B\Omega)] \quad \dots(4.26)$$

From equation 4.11 & equation 4.26, it is straightforward that

$$TS_{\text{act}} = f_T(B\Omega); \quad \dots(4.27)$$

In our fit, for the simplicity of calculations, we consider $f_T(B\Omega) = 0$; which implies that the bulk modulus and mean volume per atom does not vary as well with the temperature for our calculation. However, the self-diffusion coefficient still varies with the system temperature.

Further for the fit, a database (D-2 of figure 4.1) containing B_0 , Ω_0 , a_0 , v_D and λ_{Geo} for each compound is prepared in the following section. Then using these two databases, the value of c is calculated in the first phase of the calculation, as shown in the first bloc (B-1) of figure 4.1. Therefore, all of these parameters (as described in the following section) are extrapolated to 0 K to be used as input in the fitting scheme.

The Levenberg-Marquardt algorithm is used in the fitting of first bloc in our study because of its simple implementation and prompt convergence even from a far-off initial guess [26]. We implement Levenberg-Marquardt Algorithm using *curve fit* function of *optimize* module from *scipy* library to estimate c . The python code to determine the c value and the diffusion coefficient, as per the scheme of figure 4.1, is included in the appendix A.1.

In the second stage of our study, we then calculate the self-diffusion coefficient at different system temperature, using the fitted c value and the second database (D-2) as shown in the second bloc (B-2) of figure 4.1.

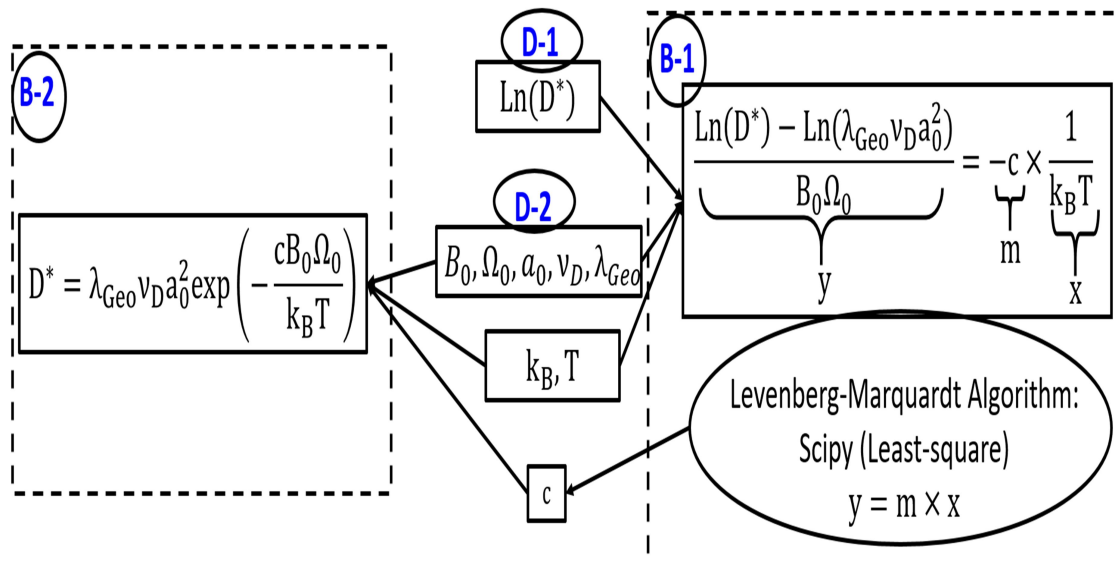


Figure 4.1: Flow diagram of the least-square minimization process of fitting constant, c and the self-diffusion coefficient calculated from $cB\Omega$ formalism implemented in our study;

4.4. Application of cBΩ model:

In this section we will first discuss the input databases (D-1 & D-2), as mentioned in the previous section, for each compound then present the results of the fit for c, followed by the estimated results of diffusion coefficients.

4.4.1 UO_2 :

The diffusion of Uranium in UO_2 was most extensively explored experimentally among all actinide oxides. In 1961, Auskern & Belle measured the self-diffusion of uranium in UO_2 using the surface-activity decrease method and U_{92}^{235} tracer element [27]. The experiment was performed for the temperature range of 1723 K – 2058 K. Lindner & Schmitz were the second to measure the self-diffusion of uranium in UO_2 [28]. They used α -absorption method to measure the self-diffusion coefficient for the temperature range of 1573 K – 1873 K. However, unlike Auskern & Belle, they used the U_{92}^{233} as the tracer element due to its higher activity with respect to the other isotope (U_{92}^{238}) of uranium. In 1965, Lindner & Schmitz performed the same experiment once again with U_{92}^{235} tracer [29]. Alcock et al. used α -ray Spectrometry technique and U_{92}^{233} tracer element for their experiment. However, they quantified the final diffusion profile in two methods – surface activity decrement method and concentration profile analysis method [30].

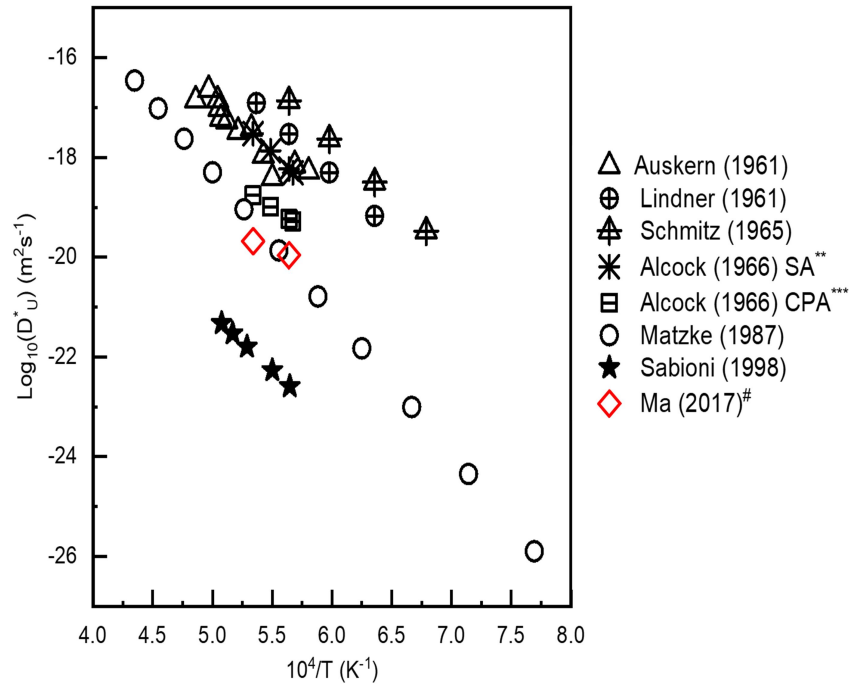


Figure 4.2: Experiments of U self-diffusion in single-crystal $UO_{2,00}$;

**SA - Surface Activity method;

***CPA - Concentration Profile Analysis;

#This experiment is performed for $UO_{2,001}$ composition;

Matzke recommended an Arrhenius equation for a temperature range of 1300 K- 2300 K for cation self-diffusion in UO_2 [31]. This recommendation was based on the previous researches done by the same author [32], which was a U_{92}^{233} α -ray Spectrometry experiment on single crystals. The recommendations were corrected for the surface effect and fast-tracer penetration effect.

Sabioni et al. measured the uranium self-diffusion in UO_2 for the temperature range of 1771 K – 1970 K using Secondary Ion Mass Spectrometry (SIMS). This is the first SIMS measurement for U self-diffusion in UO_2 [33]. In 2017, Ma experimentally measured uranium self-diffusion in $\text{UO}_{2.001}$ using SIMS [34]. Despite its deviation in stoichiometry, the measurement of Ma is consistent with the recommendation of Matzke (Figure- 4.2). Therefore, we computationally utilize the recommendation of Matzke in our work.

The Debye temperature of UO_2 was found to be 385 K at 0 K by Fritz [35]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $5.039 \cdot 10^{13} \text{ s}^{-1}$.

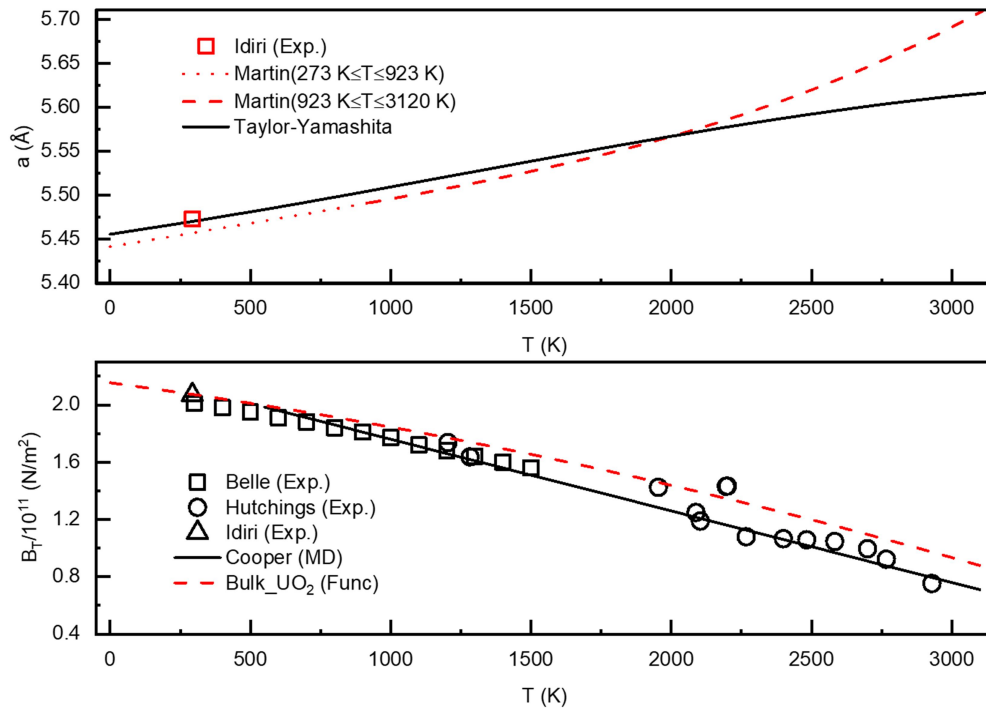


Figure 4.3: Temperature dependent evolution of Bulk modulus and Lattice parameter for UO_2 . The data of Hutchings (Exp.) and Belle (Exp.) represent the experimental estimations of [40] and [41] respectively. The data of Cooper (MD) represent the linear relation suggested by [39]. The Functions of Bulk_UO₂ (Func) refers to the Bulk modulus function of equation 5.2. Two sets of data from Martin represent the recommended equation of [23] for lattice parameter, distributed in two distinct temperature range; The data of Taylor-Yamashita represents the recommendation of [21] using the a_0 recommended by Yamashita et al. [22]. Idiri (Exp.) represents data estimated by Idiri et al. [37].

Martin proposed a polynomial fit for the temperature dependence of lattice parameter in UO_2 [23]. In order to obtain a better fit, he divided the model into two regions of temperature, e.g. 273 K – 923 K &

923 K – 3120 K. Later, Fink re-examined the consistency of this model along with some new data and found it to be consistent [36]. The model is analogous to the equation 4.24. The constants of the equation 4.24 for lattice parameter of UO₂, as per Martin [23], are following,

$$a(\text{\AA}) = (9.9734 \cdot 10^{-1} + 9.082 \cdot 10^{-6} T - 2.705 \cdot 10^{-10} T^2 + 4.391 \cdot 10^{-1} T^3) a_{273} \quad (273 \text{ K} \leq T \leq 923 \text{ K}) \quad \dots(4.28)$$

$$a(\text{\AA}) = (9.9672 \cdot 10^{-1} + 1.179 \cdot 10^{-5} T - 2.429 \cdot 10^{-9} T^2 + 1.219 \cdot 10^{-12} T^3) a_{273} \quad (923 \text{ K} \leq T \leq 3120 \text{ K}) \quad \dots(4.29)$$

Furthermore, Guthrie et al. recently checked the consistency of the Martin's model along with their newly measured results [38]. The deviation of the newly measured results (for relative linear expansion) is still less than 1% from the results of Martin's model.

As per Taylor's recommendation, Yamashita et al. [22] also calculated a polynomial for the lattice parameter of UO₂ as,

$$a(\text{\AA}) = 5.456 + 4.581 \cdot 10^{-5} T + 10.355 \cdot 10^{-9} T^2 - 2.736 \cdot 10^{-12} T^3 \quad \dots(4.30)$$

Idiri et al. calculated the lattice parameter of UO₂ at room temperature [37]. All these different relations are compared with the deduction of Idiri et al., in the figure- 4.3. We considered Martin's model to compute the lattice parameter of UO₂ down to 0 K.

Cooper et al. described a model for the evolution of Bulk modulus with temperature for several Actinide Oxides, using the newly developed many-body empirical potential [39]. The model is analogous to the equation 4.25 (where b₂= 0),

$$B_T \left(\frac{\text{N}}{\text{m}^2} \right) = 226.01 \cdot 10^9 - 5 \cdot 10^7 T \quad \dots(4.31)$$

Hutchings et al. experimentally estimated the bulk modulus of UO₂ [40]. The bulk modulus of UO₂ at room temperature (2.07.10¹¹ N/m²) was also estimated by Idiri et al [37]. Hence, we calculate a second order polynomial (as per equation 4.25), using the slope of the results of Hutchings and considering the value of Idiri to calculate B₀,

$$B_T \left(\frac{\text{N}}{\text{m}^2} \right) = 2.154 \cdot 10^{11} - 2.599 \cdot 10^7 T - 4.8848 \cdot 10^3 T^2 \quad \dots(4.32)$$

The experimental results of Belle and Berman [41] are also in accordance with this relation as well. All these results are compared in Figure-4.3. Therefore, this above mentioned relation is used to compute the bulk modulus in UO₂ at 0 K.

4.4.2. ThO_2 :

Thorium self-diffusion in single crystal ThO_2 was less studied than U self-diffusion in UO_2 . Few experiments were performed to determine the diffusion coefficient in single crystal ThO_2 . All the experiments were carried out using the α -spectrometry techniques with different tracers (Th_{90}^{228} , Th_{90}^{230}). King and Matzke performed their respective experiments with arc-fused single crystals of ThO_2 and Th_{90}^{228} tracer [42, 43].

The results of King and Matzke are in agreement to each other. Whereas, the results of Hawkins & Alcock are not in agreement with the same of King. Hence, it was argued before that the results of Hawkins & Alcock [44] are not representative of the volume diffusion [43]. Hence, those results are not been computationally utilized for our study. Matzke, in his detailed study, argued that the volume diffusion could not be correctly measured without the correction of fast surface relaxation effect. The results obtained by Matzke, without the correction of fast surface relaxation effect, shows an agreement with the results of Poteat and Morgan [45].

Hence, the results of Poteat & Morgan also cannot be acknowledged as the representative of the volume diffusion [43]. Therefore, the results of King and Matzke can only be considered as the correct results of the volume diffusion and are used in this work. The results of these two experiments are tabulated in Table-4.1.

The Debye temperature of ThO_2 was found to be 393 K at 0 K in literature [46]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $5.147 \cdot 10^{13} \text{ s}^{-1}$.

Yamashita and Mathews measured experimentally the evolution of lattice parameter with temperature less than 1500 K [22, 47]. Both the results are consistent to each other. These results show an excellent agreement (Figure-4.4) with the regression model recommended by Taylor [22] as well (equation 4.33).

$$a(\text{\AA}) = 5.583 + 4.628 \cdot 10^{-5} T + 0.471 \cdot 10^{-9} T^2 + 2.512 \cdot 10^{-12} T^3 \quad \dots(4.33)$$

T (K)	D_{Th}^* (m^2/s)	Reference
2326	$4.37 \cdot 10^{-19}$	[42]
2262	$2.0 \cdot 10^{-19}$	[42]
2208	$5.01 \cdot 10^{-20}$	[42]
2208	$4.07 \cdot 10^{-20}$	[42]
2137	$2.95 \cdot 10^{-20}$	[42]
2114	$3.09 \cdot 10^{-20}$	[42]
2439	$4.68 \cdot 10^{-18}$	[43]
2273	$1.0 \cdot 10^{-18}$	[43]

Table 4.1 : Experimental estimations of Th self-diffusion in single-crystal $ThO_{2,00}$:

Recently, Szpunar & Szpunar also developed a model for the temperature dependant evolution of lattice parameter up to 3300 K, based on first-principle molecular dynamics [48]. All of these experimental results and models are presented in the Figure- 4.4.

In higher temperature (more than 1000 K), Taylor’s model and Szpunar’s model are in agreement. Whereas, the deviation is significant in the lower temperature. However, the result of Idiri at room temperature is in accordance to the Taylor’s model. Therefore, we consider the Taylor’s regression model to extrapolate lattice parameter at 0 K in this study.

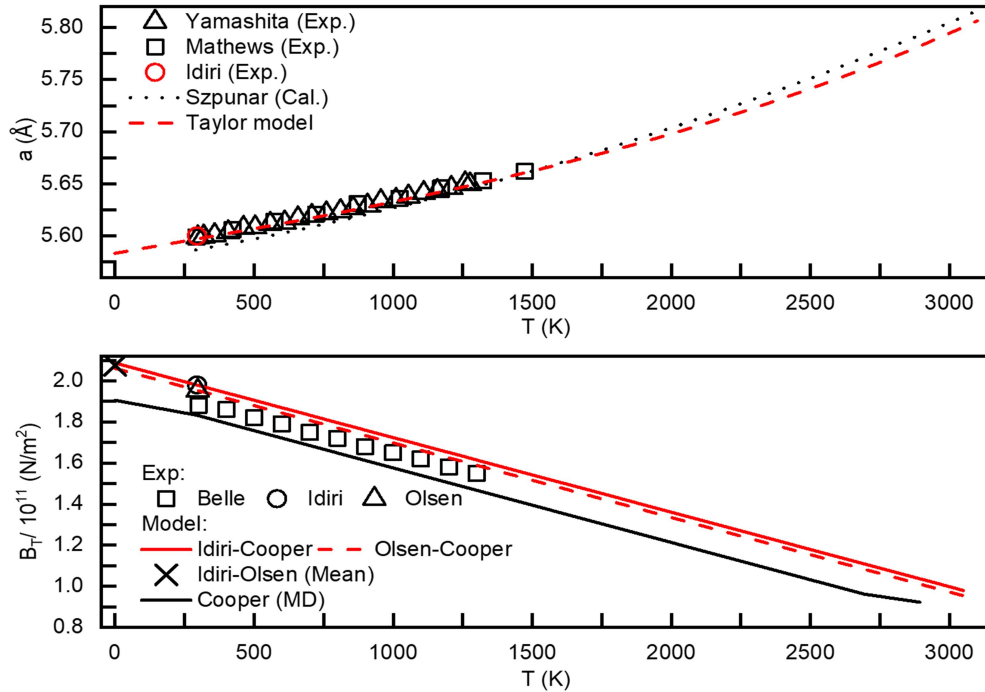


Figure 4.4: Temperature dependent evolution of Bulk modulus and Lattice parameter for ThO_2 . The data of Belle (Exp.) represents the experimental estimations of [41]. The data of Cooper (MD) represent the linear relation suggested by [39]. Idiri (Exp.) represents the experimental results of [37]. Olsen represents the experimental results of [49]. Yamashita (Exp.) and Mathews (Exp.) represent the lattice parameter experimental results of [22] & [47] respectively. Szpunar (Cal.) represents the data of lattice parameter estimated by Szpunar & Szpunar [48]. The data of Taylor model represents the recommendation of [21] using the a_0 recommended by [22];

Similar to UO_2 , Cooper et al. also derived a linear relation for the Bulk modulus of ThO_2 .

$$B_T \text{ (N/m}^2\text{)} = 201.19 \cdot 10^9 - 3.63 \cdot 10^7 T \quad \dots(4.34)$$

The experimental results of Belle and Berman are in agreement with the Cooper's linear relation as presented in Figure-4.4. However, the recent experimental results of Idiri et al [37] and Olsen et al [49] are not in agreement with the Cooper’s model. Therefore, by taking into account of Cooper’s rate of change of temperature ($b_1 = -3.63 \cdot 10^7$ N/m², in equation 4.25) and having fitted to the experimental

data of Idiri et al and Olsen et al respectively, we obtain two new linear relations (Idiri-Cooper & Olsen-Cooper). Using the relations of Idiri-Cooper & Olsen-Cooper the bulk modulus up to 0 K is extrapolated. The average bulk moduli (at 0 K) obtained from these two linear relations are considered in this study. The accepted values are reported in table- 4.2.

4.4.3. Li_2O :

On contrary to the Actinide oxides, there are abundance of data for the cation diffusion (Li^+) in Li_2O . However, because of its anti-fluorite structure, the O^{2-} ion forms the fcc lattice for Li_2O . The diffusion of oxygen in Li_2O was investigated by Ando et al. using gas-solid isotope exchange technique with ^{18}O tracer. The Li_2O samples were annealed in an ^{18}O enriched oxygen gas atmosphere. Diffusion coefficient was determined by determining the $^{18}\text{O}/^{16}\text{O}$ ratio in the atmosphere after diffusion anneal [50]. This experiment was conducted for polycrystalline Li_2O . However, the author pointed out that the oxygen self-diffusion coefficient in polycrystalline Li_2O & single-crystalline Li_2O exhibit an agreement, at $T= 1233$ K. Although, in higher temperature, D^*_o of Li_2O for poly-crystal is greater than that for single-crystal. However, we decide to use the value of D^*_o of poly-crystalline Li_2O for our study because of the rarity of the D^*_o of single-crystalline Li_2O .

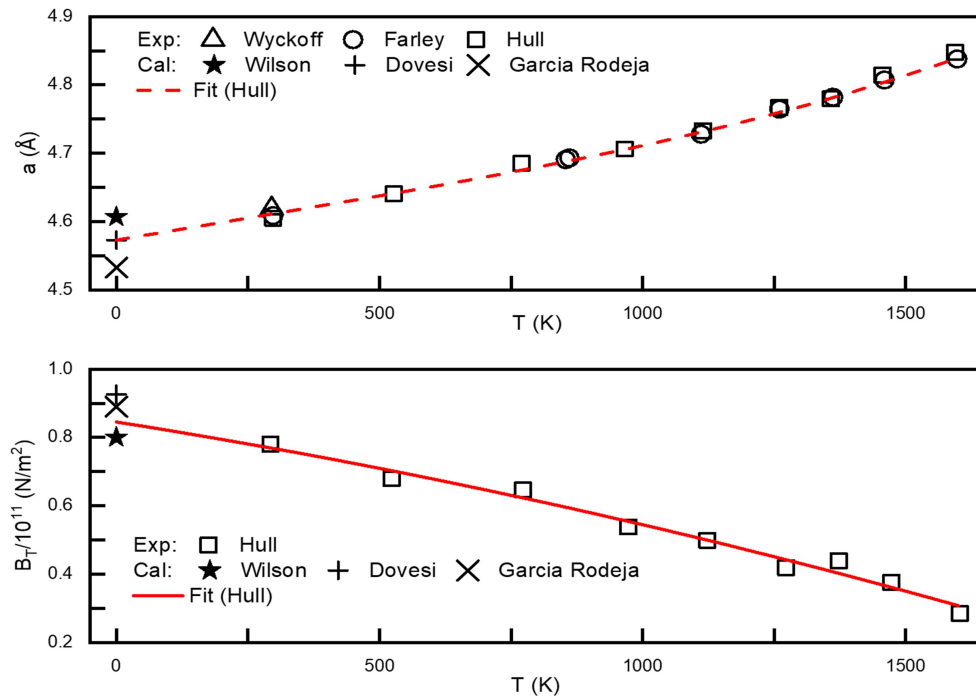


Figure 4.5: Temperature dependent evolution of Bulk modulus and Lattice parameter for Li_2O . The data of Wyckoff (Exp.), Hull (Exp.), Farley (Exp.), Wilson, Dovesi and Garcia Rodeja represent the estimations of [52], [24], [51], [54], [53] and [55] respectively. The function of [24] for lattice parameter of Li_2O is noted by Hull (Poly). The fitted function of B_T over the estimated data of Hull et al. [24], under the framework of equation 4.36, is referred by coin 'Fit'.

The Debye temperature of Li₂O was found to be 1080 K at 0 K by Hull et al. [24]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $1.415 \cdot 10^{14} \text{ s}^{-1}$.

Hull et al. formulated a third degree polynomial between lattice parameter and temperature for Li₂O [24]. The relation was deduced from two sets experiments- a neutron scattering experiment [24] and a neutron diffraction experiment [51]. This reported polynomial is utilized to determine the variation of lattice parameter of Li₂O against temperature.

$$a (\text{\AA}) = 4.611 + 1.283 \cdot 10^{-4} (T - 293) + 2.729 \cdot 10^{-11} (T - 293)^3 \quad \dots(4.35)$$

This relation is also in accordance to the lattice parameter calculated by Wyckoff [52], at room temperature as noted in the figure- 4.5. However, at 0 K, the relation of Hull is in accordance to the calculation of [53]. Therefore, this relation is implemented to extrapolate the lattice parameter at 0 K.

Hull et al. have reported the temperature variation of the stiffness constants for Li₂O [24]. Hence, they computed the Bulk modulus of Li₂O at various temperature. We fitted a second-order polynomial relation between the bulk modulus and the temperature reported by the author. The results are noted in Fig- 4.5. The fitted relation is following,

$$B_T (\text{GPa}) = 84.51 - 0.0242 T - 5.878 \cdot 10^{-6} T^2 \quad \dots(4.36)$$

Although, the relation is not in accordance to the calculated results of [53], [54] & [55], the fit is in accordance to the experimental results. Therefore, this relation is applied to extrapolate the bulk modulus of Li₂O at 0 K.

4.4.4. PuO₂:

Pu self-diffusion coefficient in PuO₂ was not experimentally measured in literature. However, the activation energy of Pu self-diffusion was estimated by two different methods that have been discussed in Chapter-3. Hence, we subsequently extrapolate the cBΩ model for PuO₂ by applying a linear law to the parameter c with respect to the ionic radii of cations, using the values of c of previous compounds. This process is further discussed in the next sub-section.

The Debye temperature of PuO₂ was found to be 415 K at 0 K in literature [46]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $5.435 \cdot 10^{13} \text{ s}^{-1}$.

For PuO₂, The experimental data of lattice parameter, calculated by Yamashita et al., are at the temperature less than 1300 K [22]. A set of data was also calculated recently for an elevated temperature (300 K – 2000 K) using molecular dynamics and empirical potential of Arima [56]. The regression model of Taylor for lattice parameter (using the recommended constants of [22]) of PuO₂ fits well with both the experimental results of Yamashita and the results of molecular dynamics. These results are as well presented in the Figure-4.6. Hence, the model of Taylor for PuO₂ is adapted as well, in this study, to extrapolate the lattice parameter at 0 K.

There is no experimental data found, in the literature, for the evolution of B_T in PuO_2 . Though, Rahman et al. and Cooper et al. both presented respective sets of results calculated from the molecular dynamics using the same many-body empirical potential [57, 39]. As both the molecular dynamics calculations were performed using the same empirical potential, the results are in accordance to each other. Cooper et al. also deduced a linear relation for Bulk modulus of PuO_2 as per equation 4.25.

$$B_T = 220.8 \cdot 10^9 - 4.63 \cdot 10^7 T; \quad \dots(4.37)$$

By taking into account of Cooper's rate of change of temperature ($b_1 = -4.63 \cdot 10^7 \text{ N/m}^2$, in equation 4.25) and fitting to the experimental data of Idiri et al, we obtain a new linear relation (Cooper-Idiri).

Minamoto et al. reported another set of results for the temperature evolution of B_T in PuO_2 , using a combination of first-principles and lattice dynamics [58].

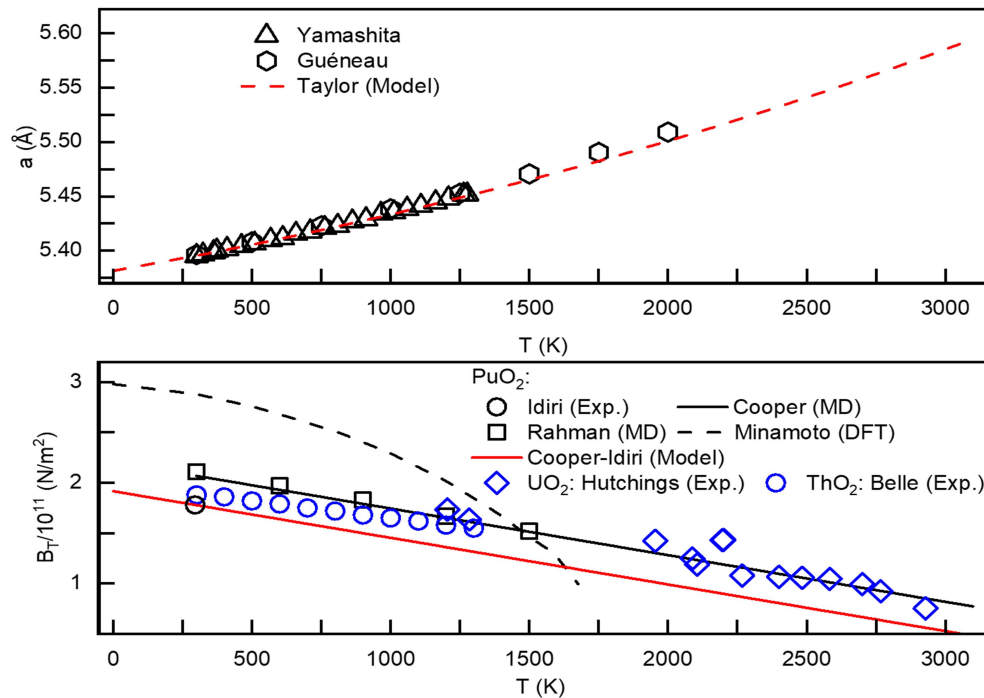


Figure 4.6: Temperature dependent evolution of Bulk modulus and Lattice parameter for PuO_2 . The data of Rahman (MD) represents the calculated estimations of [57]. Idiri (exp.) represents the experimental results of [37]. The data of Cooper (MD) represents the linear relation suggested by [39]. Minamoto (DFT) represents the results of [58]. Yamashita represents the lattice parameter experimental results of [22]. Guéneau represents the data of lattice parameter estimated using potential of Arima [56]. The data of Taylor (Model) represents the recommendation of [21] using the a_0 recommended by Yamashita et al. [22]. Hutchings (Exp.) and Belle (Exp.) represent the results for UO_2 [40] & ThO_2 [41] respectively.

Minamoto's results are completely in contrast to the results calculated by both Cooper-Idiri model, Cooper et al. and Rahman et al. In fact, the results of Minamoto et al. contradicts the trend of the

experimental results of B_T for UO_2 and ThO_2 as well. Therefore, Cooper-Idiri model is used to extrapolate the bulk modulus at 0 K.

All the exclusive parameters and constants used in this work are tabulated in the table-4.2 aligned with their respective compounds. The melting temperature in the table is mentioned to point out the phase boundary of fluorite phase. It is also worth to be noted that the mean volume per atom (Ω), which is added in the table, is directly calculated from the $\Omega_0 = a_0^3/4$ relation, in our study.

Parameter	UO_2	ThO_2	Li_2O	PuO_2
v_D (THz)	50.4	51.4	141.5	54.4
a_0^2 (\AA^2)	28.96	29.74	31.18	20.91
B_0 (GPa)	215.4	207.5	84.5	191
Ω_0 (\AA^3)	40.52	43.52	23.90	38.96
c (#)	0.0982	0.1094	0.2131	0.0859
r_i (\AA) [59]	1.00	1.05	1.42	0.96
T_m (K)	3120 [56]	3651 [56]	1603 [24]	2674 [56]

Table 4.2: Input data for $cB\Omega$ model of UO_2 , ThO_2 , Li_2O & PuO_2 . v_D – Debye temperature (at 0 K); a_0 – lattice parameter (at 0 K); B_0 – bulk modulus (at 0 K); Ω_0 – mean volume per atom ($a_0^3/4$); c – fitting parameter; r_i – ionic radii of cations; T_m – melting temperature;

4.4.5. Results:

The values of c , estimated for UO_2 , ThO_2 & Li_2O , are calculated using the method explained in section 4.2.6. Though the anti-fluorite of Li_2O perceive a substantially higher value for parameter c than that of the fluorite structured oxides, the values of c for all these three compounds exhibit a linear relation with respect to the respective ionic radii of the diffusing ions, i.e. ionic radius of U^{4+} for UO_2 , ionic radius of Th^{4+} for ThO_2 and ionic radius of O^{2-} for Li_2O . This linear relation is presented in figure- 4.7.

The self-diffusion coefficient of U in UO_2 , Th in ThO_2 and O in Li_2O are then estimated using the respective c values, the $cB\Omega$ equation described in the bloc-2 of sub-section 4.3.6 and inputs of Table-4.2. The results for these three compounds are presented in Figure- 4.8. The experimental data (used to estimate the fitting parameter, c) for all three compounds are also included in the figure. The results of the $cB\Omega$ calculation is in agreement with the respective experimental data.

Using the linear fitting equation between fitting parameter c and the ionic radii of the diffusing species, the fitting parameter (c) for Pu diffusion in PuO_2 is also estimated (noted in Table- 4.2). Hence, the Pu diffusion coefficients in PuO_2 are also calculated using the $cB\Omega$ model and the inputs of table- 4.2. The diffusion coefficient results of Pu in PuO_2 are also presented in figure- 4.8.

Based on the calculated results of diffusion coefficients for all the four compounds (UO_2 , ThO_2 , PuO_2 & Li_2O), the activation energy of self-diffusion (Q_{act}) and self-diffusion prefactor (D_0) were calculated (as Q is the slope and $\ln D_0$ is the intercept of the diagram 4.8).

For UO_2 , the activation energy & prefactor estimated by Matzke [31] are in agreement with the one estimated in this work. For ThO_2 , Matzke estimated the activation energy of Th diffusion [43] & the estimation of prefactor were based on the work of King [42]. Both these two values are in agreement with the results calculated by our model. As discussed before, there is no experimental self-diffusion coefficient data available for Pu in PuO_2 . However, the activation energy calculated by this work is compared with the migration energy of Pu^{4+} in PuO_2 , found by Kutty et al [60], which is an estimation made by the sintering experiment (as discussed in chapter- 2). Both the values are in agreement.

Compounds	UO_2	ThO_2	Li_2O	PuO_2
D_0 (m^2/s)	$7.53956 \cdot 10^{-5}$	$2.74208 \cdot 10^{-5}$	$3.43471 \cdot 10^{-5}$	$1.51644 \cdot 10^{-5}$
Exp.	$6.5 \cdot 10^{-5}$ [34]	$3.5 \cdot 10^{-5}$ [45]	$1.5 \cdot 10^{-1}$ [50]	-
Q_{act} (eV)	5.71	6.25	2.74	4.00
Exp.	5.6 [34]	6.5 [43]	3.6 [50]	4.1 – 6.0 [60]

Table 4.3: Activation energy and self-diffusion pre-factor calculated by $cB\Omega$ model for UO_2 , ThO_2 , Li_2O & PuO_2 ;

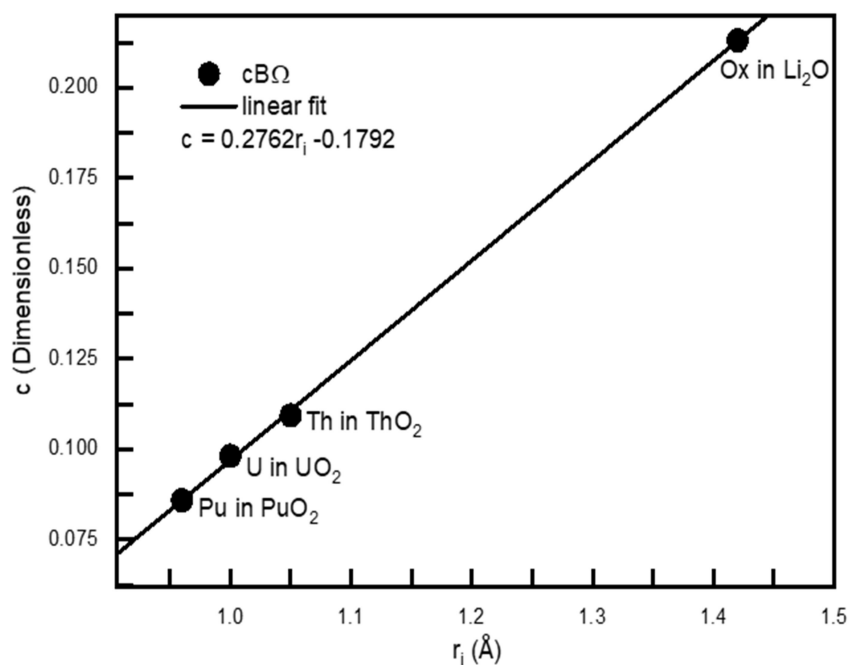


Figure 4.7: The linear fit between c (fitting parameter of $cB\Omega$) and ionic radii (r_i) of diffusing species [59] in UO_2 , ThO_2 , Li_2O ; Relational equation is also indicated (solid line); Extrapolated value of c , in case of Pu^{4+} self-diffusion in PuO_2 , is also included in the diagram;

The activation energy & prefactor for the O diffusion in Li_2O are based on the results of Ando et al [50]. It can be observed that both prefactor & activation energy for this case are under estimated with

our method. However, it has to be noted that the experimental results of O diffusion in Li_2O is based on the diffusion results in polycrystal sample.

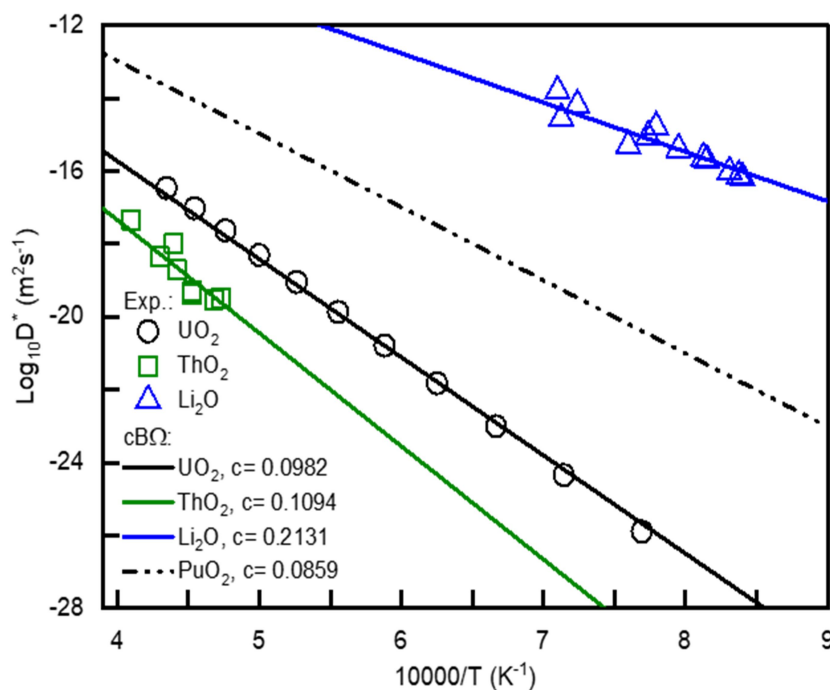


Figure 4.8: The $cB\Omega$ results of self-diffusion coefficients of U in UO_2 , Th in ThO_2 and O in Li_2O . Experimental results used in the estimation of c using equation 4.25 are also included. The calculated value of c are indicated in the legends. The extrapolated results of Pu self-diffusion in PuO_2 (dashed) are included as well and the extrapolated value of c is also indicated in the legend;

Using the activation energy & prefactor of the literature (as noted in table- 4.3), D^*_O in Li_2O valued as $8.77 \cdot 10^{-12} \text{ m}^2/\text{s}$ at $T=1773 \text{ K}$. whereas, the D^*_O in Li_2O valued as $5.59 \cdot 10^{-13} \text{ m}^2/\text{s}$ at $T=1773 \text{ K}$, using the activation energy & prefactor found in this work. However, at a lower temperature (at 1173 K), D^*_O calculated using the diffusion parameter of the literature & the parameter of our study, value $5.11 \cdot 10^{-17} \text{ m}^2/\text{s}$ and $5.80 \cdot 10^{-17} \text{ m}^2/\text{s}$ respectively.

As noted by Ando et al, the D^*_O , in higher temperature, values are higher for polycrystal Li_2O than the single-crystal Li_2O . On contrary, in both poly-crystal & single-crystal Li_2O shows a similar value of D^*_O , at a lower temperature [50]. Hence, the grain boundary effect could lead to this discrepancy found in our study and the estimated D^*_O of our study can be more relevant for single-crystal Li_2O . Although no conclusion can be drawn due to the vacuum of experimental data of D^*_O in single-crystal Li_2O .

4.5. Extrapolation of $cB\Omega$ in other binary oxides:

In this section, we extend the scope of $cB\Omega$ model and its relation to the ionic radii of the diffusing species. Using the extrapolation framework, applied for PuO_2 in the previous section, we also compute the values of c for different cation diffusions in other oxides with fluorite structures. However, the wider application of $cB\Omega$ -ionic radii framework was deemed to be further explored.

The c value is essentially computed using the following linear fit as deduced in the previous section for the following oxides.

$$c \text{ (dimensionless)} = 0.2762r_i - 0.1792 \quad \dots(4.38)$$

The calculated values of c for the following oxides with fluorite structures are also presented in the figure 4.9. The results that are pertinent to this section are presented in the figure. All the cations, which are the mobile species for our study, are ideally in +IV ionic state at exact stoichiometry.

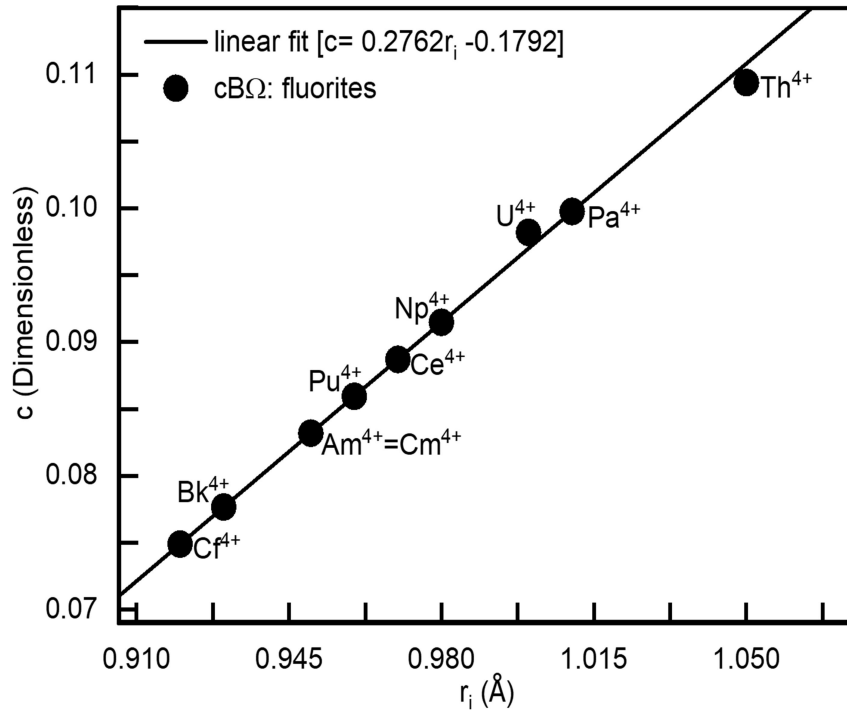


Figure 4.9: Calculation of c using the linear relation with ionic radius of mobile cation (equation 4.38) for different binary oxides with fluorite structure.

Hereon, we will discuss about the choice of inputs for Debye frequencies, lattice parameters and bulk moduli for each compound, one by one.

4.5.1 CeO₂:

The cation diffusion of CeO₂ was also not experimentally estimated previously. However, the activation energy cation diffusion was calculated using DFT method [61]. The value of c is calculated using the equation 4.38 and the ionic radius of Ce⁴⁺ [59]. The respective value of c and the ionic radius are also presented in the Table- 4.4.

The Debye temperature of CeO₂ was found to be 480 K at 0 K in literature [62]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $6.291 \cdot 10^{13} \text{ s}^{-1}$.

For CeO₂, the change of lattice parameter (Δa), normalised to its reference (lattice parameter at 293 K), is linear to the system temperature [62]. The lattice parameter at any temperature, therefore, can be calculated using the slope of ($\Delta a/a_{293}$) vs T. We have used this relation in our study to estimate the lattice parameter at 0 K. This value of lattice parameter at 0 K is adapted in our study. The used value of lattice parameter is given in Table- 4.4.

Similar to actinide oxides, Cooper et al [39], using the many body potential, computed the bulk modulus variation of CeO₂ with respect to the system temperature using linear descending relation.

$$B_T(\text{N/m}^2) = 203.86 \cdot 10^9 - 3.94 \cdot 10^7 T \quad \dots(4.39)$$

However, in experiment, the bulk modulus at room temperature found to be $2.36 \cdot 10^{11} \text{ N/m}^2$ [63]. Therefore, using the rate of change of bulk modulus, suggested by [39] and the experimental value of bulk modulus at room temperature, the bulk modulus of CeO₂ at 0 K is deduced in this work. The used value of bulk modulus is given in Table- 4.4.

4.5.2 NpO₂:

Similar to PuO₂, Np self-diffusion in NpO₂ was not measured experimentally in literature. Hence, we subsequently extrapolated the $cB\Omega$ model for NpO₂ by computing the parameter c with respect to the ionic radii of Np⁴⁺ [59]. The respective value of c and the ionic radius are also presented in the Table- 4.4.

The Debye temperature of NpO₂ was found to be 435 K at 0 K in literature [64]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $5.699 \cdot 10^{13} \text{ s}^{-1}$.

For NpO₂, the lattice parameters calculated against temperature by Yamashita et al [22] using Taylor's regression model [21] were found to be in agreement with other experimental results, as shown by Yamashita et al.

$$a(\text{\AA}) = 5.4203 + 4.276 \cdot 10^{-5} T + 9.075 \cdot 10^{-9} T^2 - 1.362 \cdot 10^{-12} T^3 \quad \dots(4.40)$$

Therefore, the model of Taylor is as well adapted in this study to calculate the lattice parameter at 0 K. The used value of lattice parameter is given in Table- 4.4.

Cooper et al [39], using the many body potential, computed the bulk modulus variation of NpO₂ with respect to the system temperature using linear descending relation.

$$B_T \text{ (N/m}^2\text{)} = 210.59 \cdot 10^9 - 3.89 \cdot 10^7 T \quad \dots(4.41)$$

In experimental study, the bulk modulus of NpO₂ was already calculated for room temperature as 2.10¹¹ N/m² [37, 65]. Using the rate of change of bulk modulus, suggested by [39] and the experimental value of bulk modulus at room temperature, the bulk modulus of NpO₂ at 0 K is deduced in this work. The used value of bulk modulus is given in Table- 4.4.

4.5.3 AmO₂:

Alike NpO₂ & PuO₂, Am self-diffusion in AmO₂ was not measured experimentally in literature. However, a set of diffusion coefficient data was computed using molecular dynamics and parameters suggested by Arima et al. [66]. The calculation was performed considering different numbers of Schottky defect pairs (0, 1, 3, and 5). Evidently, the calculations are performed at so high temperature that the system temperature for computation is higher than the melting temperature of AmO₂ (fluorite phase), noted in table- 4.4. Hence, the calculated results cannot be considered for the fitting of c. Therefore, similar to NpO₂, the value of c is calculated using equation 4.38 and the ionic radius of Am⁴⁺[59]. The respective value of c and the ionic radius are presented in the Table- 4.4.

The Debye temperature of AmO₂ was found to be 336 K at 0 K in literature [67]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as 4.398.10¹³ s⁻¹.

The temperature dependence of lattice parameter of AmO₂ was represented by a second order polynomial previously [56]:

$$a \text{ (\AA)} = 5.3733 + 4.34 \cdot 10^{-5} T + 1.43 \cdot 10^{-10} T^2 \quad \dots(4.42)$$

Therefore, we adapt equation 4.40 to compute the lattice parameter of AmO₂ at 0 K. The used value of lattice parameter is given in Table- 4.4.

Similar to NpO₂, Cooper et al [39], using the many body potential, computed the bulk modulus variation of AmO₂ with respect to the system temperature using linear descending relation.

$$B_T \text{ (N/m}^2\text{)} = 217.96 \cdot 10^9 - 4.39 \cdot 10^7 T \quad \dots(4.43)$$

In experimental study, the bulk modulus of AmO₂ was already calculated for room temperature as 2.05.10¹¹ N/m² [37]. Using the rate of change of bulk modulus, suggested by [39] and the experimental value of bulk modulus at room temperature, the bulk modulus of AmO₂ at 0 K is deduced in this work. The used value of bulk modulus is given in Table- 4.4.

4.5.4 CmO₂:

Similar to NpO₂, Cm self-diffusion in CmO₂ was not measured experimentally in literature. Hence, we subsequently extrapolated the cBQ model for CmO₂ by computing the parameter c with respect to the

ionic radius of Cm^{4+} [59]. As the ionic radii of AmO_2 and CmO_2 are same, the values of c are also found to be same. The respective values of c and the ionic radii are also presented in the Table- 4.4.

The Debye temperature of CmO_2 was found to be 337 K at 0 K in literature [68]. This value is being used in equation 4.21 of our study, which indicates the value of Debye frequency as $4.4149 \cdot 10^{13} \text{ s}^{-1}$.

A linear descending relation previously represented the temperature dependence of lattice parameter of CmO_2 [56]:

$$a (\text{\AA}) = 5.37873 + 1.016 \cdot 10^{-5} T \quad \dots(4.44)$$

Therefore, we adapt equation 4.44 to compute the lattice parameter of AmO_2 at 0 K. The used value of lattice parameter is given in Table- 4.4.

Cooper et al [39], using the many body potential, computed the bulk modulus variation of CmO_2 with respect to the system temperature using linear descending relation.

$$B_T (\text{N/m}^2) = 241.03 \cdot 10^9 - 5.09 \cdot 10^7 T \quad \dots(4.45)$$

In experimental study, the bulk modulus of CmO_2 was already calculated for room temperature as $2.18 \cdot 10^{11} \text{ N/m}^2$ [37]. Using the rate of change of bulk modulus, suggested by [39] and the experimental value of bulk modulus at room temperature, the bulk modulus of CmO_2 at 0 K has been deduced in this work. The used value of bulk modulus is given in Table- 4.4.

4.5.5: BkO_2 , CfO_2 & PaO_2 :

Due to the experimental complexity, the trans-curium dioxides are mostly computationally studied. Even the experimental studies are not often performed on PaO_2 as well. Hence, the cation self-diffusion coefficient of none of these three compounds are estimated previously. Therefore, the values of c are calculated using equation 4.38 and the ionic radius of Bk^{4+} , Cf^{4+} and Pa^{4+} [59]. The respective values of c and the ionic radii are presented in the Table- 4.4.

The Debye temperature of BkO_2 , CfO_2 and PaO_2 were found to be 325 K, 305 K and 388 K respectively, at 0 K in literature [68]. These values are used in equation 4.21 of our study, which indicate the values of respective Debye frequencies. The values of the Debye frequencies are also included in the Table- 4.4.

The temperature dependence of lattice parameter was studied only for BkO_2 among these three actinide oxides. The dependence was represented by the following second order polynomial [56]:

$$a (\text{\AA}) = 5.3304 + 4.32 \cdot 10^{-5} T + 1.6 \cdot 10^{-10} T^2 \quad \dots(4.46)$$

Therefore, we adapt equation 4.46 to compute the lattice parameter of BkO_2 at 0 K. The used value of lattice parameter is given in Table- 4.4.

Though, the temperature dependence of lattice parameter for CfO_2 and PaO_2 were not calculated before, the room temperature lattice parameter of all the actinide oxides are found to be linearly related to the ionic radii [56].

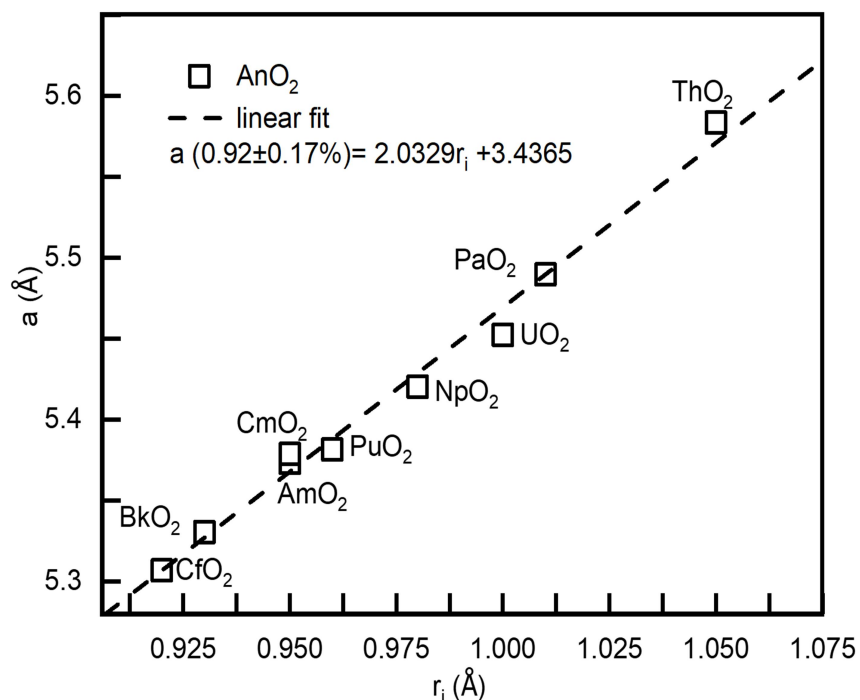


Figure 4.10: Evolution of lattice parameters of actinide oxides at 0 K as a function of the cationic radii plotted with the linear fit of equation 4.47;

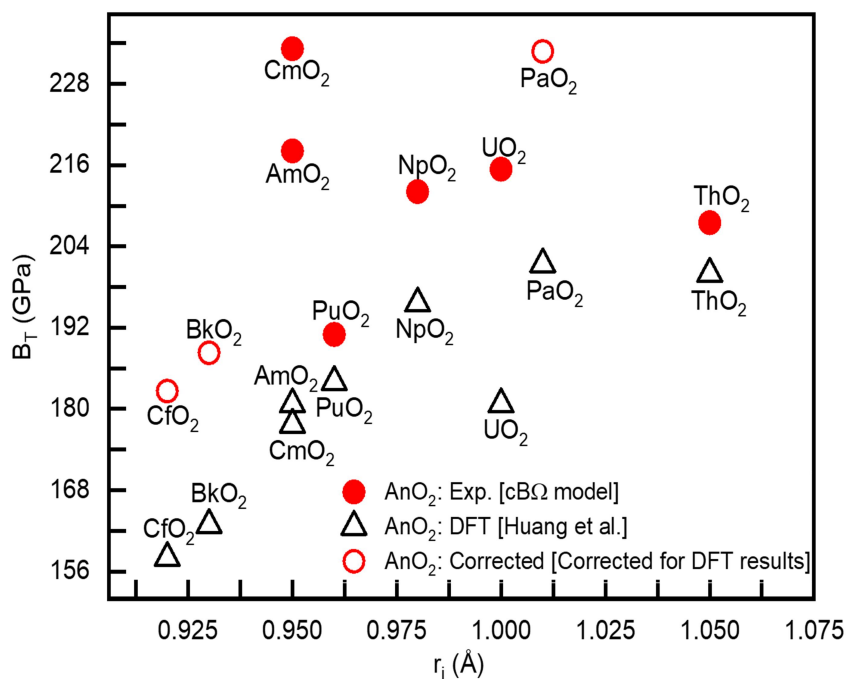


Figure 4.11: Estimation of bulk modulus for actinide oxides at 0 K – calculated by [68]; and the corrected values of bulk modulus used in this study;

Assuming the similar linear relation between the lattice parameter at 0 K and the cationic radii of the actinide oxides, the lattice parameter of CfO₂ and PaO₂ are extrapolated. The linear fit between the lattice parameter at 0 K and the cationic radius [59] is presented by the following equation:

$$a_0 (\pm 0.92 \pm 0.17\%) = 2.0329 r_i (\text{\AA}) + 3.4365 (\text{\AA}); \quad \dots(4.47)$$

The extrapolated values along with the other values of lattice parameter (used in this study) of other actinide oxides and this linear fit are presented in figure- 4.10. The deviation of less than 1% from the fit validates our hypothesis (the linearity between lattice parameter at 0 K and the cationic radius). The used values of lattice parameter for CfO₂ and PaO₂ are also given in Table- 4.4.

Unlike previous actinide oxides, bulk modulus of trans-curium oxides are not studied by Cooper et al. However, Huang et al. studied the stiffness coefficients of all the actinide oxides (AnO₂; An= Ac – No) using first-principle density functional theory (DFT) and generalized gradient approximation (GGA) [68].

Instead of using the results of Huang et al directly, we have calculated the mean deviation of the bulk modulus calculated by Huang et al (results calculated by DFT) from the bulk modulus used in this work for actinide oxides up to Curium (AnO₂ = ThO₂, UO₂, NpO₂, PuO₂, AmO₂, CmO₂). The mean deviation found to be -12.02 % ±3.07 %. Hence, the bulk modulus of these three oxides found by [68] is corrected for the calculated deviation. Therefore, these corrected bulk modulus at 0 K are adapted for our study. The deviation in the values of bulk modulus and their corrected values for three AnO₂ oxides (BkO₂, PaO₂ & CfO₂) are presented in figure- 4.11. The used corrected values of bulk modulus for BkO₂, PaO₂ & CfO₂ are also given in Table- 4.4.

4.5.6. Results:

The estimation of self-diffusion coefficients for the aforementioned fluorite oxides are performed using the input data reported in Table- 4.4.

The calculated results are presented in figure- 4.12. The results are also compared with the same calculated in the previous section (for UO₂, ThO₂, Li₂O & PuO₂) as well. The available experimental values are also included in the figure. The results which are extrapolated using the linear relation between ionic radius and c parameter, are indicated by dashed lines. The results which are calculated directly by fitting the c parameter over experimental data, are indicated by solid lines. Different compounds are indicated with different colours which are mentioned in the legends.

In spite of different values of input parameters, the self-diffusion coefficient of UO₂ (black solid line) and CeO₂ (red dashed line) are equal in values. Whereas, the equal ionic radius of Am⁴⁺ and Cm⁴⁺, led to equal value of c, does not produce equal self-diffusion coefficient and a significant difference is observed. The Cf⁴⁺ diffusion in California is the fastest among all the fluorites, we are studying. On the other hand, Th⁴⁺ diffusion in Thoria is the slowest among all the fluorites of this work. It does not

imply that the self-diffusion coefficient of cation in actinide oxides increases with the increment of atomic number of the cation. Because the pattern we can observe from the figure- 4.12 for the magnitude of D^* for actinide oxides is following:

$$D_{\text{Th}^{4+}}^* < D_{\text{Pa}^{4+}}^* < D_{\text{U}^{4+}}^* < D_{\text{Np}^{4+}}^* < D_{\text{Cm}^{4+}}^* < D_{\text{Am}^{4+}}^* < D_{\text{Pu}^{4+}}^* < D_{\text{Bk}^{4+}}^* < D_{\text{Cf}^{4+}}^*$$

When, the D^* signifies the self-diffusion coefficient of the specified cation in its stoichiometric dioxide phase.

Parameters	CeO ₂	PaO ₂	NpO ₂	AmO ₂	CmO ₂	BkO ₂	CfO ₂
ν_D (THz)	62.9	50.8	56.9	43.9	44.2	42.6	40.0
a_0^2 (Å ²)	29.1	30.1	29.4	28.8	28.9	28.4	28.2
B_0 (GPa)	247.5	231.9	212.1	218.1	233.2	187.5	181.9
Ω_0 (Å ³)	39.15	41.35	39.80	38.73	38.90	37.88	37.35
c (#)	0.0887	0.0998	0.0915	0.0832	0.0832	0.0777	0.0749
r_i (Å)	0.97	1.01	0.98	0.95	0.95	0.93	0.92
T_m (K)	2873	2784	2820	2655	2602	2407	2253

Table 4.4: Input data for $cB\Omega$ model for dioxides of cerium and minor actinides; ν_D – Debye temperature (at 0 K); a_0 – lattice parameter (at 0 K); B_0 – bulk modulus (at 0 K); Ω_0 – mean volume per atom ($a_0^3/4$); c – fitting parameter; r_i – ionic radii of cations; T_m – melting temperature;

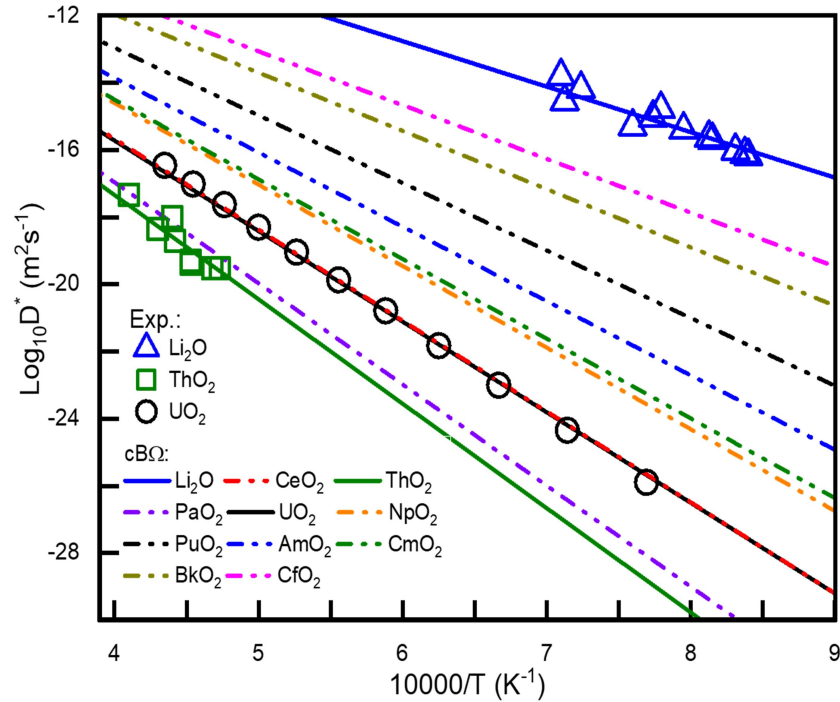


Figure 4.12: The $cB\Omega$ results of self-diffusion coefficients of cation diffusion in oxides with fluorite structure (anion diffusion for Li_2O due to its anti-fluorite structure); available experimental results are also included; the calculated values of D^* , directly fitted over experimental results, are indicated by solid lines. The extrapolated results D^* are indicated by the dashed lines;

The activation energy (Q) and the self-diffusion prefactor (D_0) of cation diffusion are also calculated for the respective fluorite structured oxides, from figure- 4.12. These results are reported in the Table-4.5. The results are compared with the available activation energies, sourced from DFT (for CeO_2) and MD (for AmO_2) calculations. The previously calculated activation energy and the activation energy calculated in this work are in agreement to each other. However, the available data are extremely rare and for other compounds, the data is not available at all. Therefore, this study factually has calculated the Arrhenius equations of self-diffusion of cation in several actinide oxides, for the first time.

	CeO_2	PaO_2	NpO_2	AmO_2	CmO_2	BkO_2	CfO_2
D_0 (m^2/s)	$1.43 \cdot 10^{-5}$	$1.20 \cdot 10^{-5}$	$1.31 \cdot 10^{-5}$	$9.92 \cdot 10^{-6}$	$9.98 \cdot 10^{-6}$	$9.45 \cdot 10^{-6}$	$8.79 \cdot 10^{-6}$
Exp.	-	-	-	-	-	-	-
Q (eV)	5.37	5.99 (5.19)	4.82	4.39	4.71	3.47 (2.99)	3.19 (2.76)
Previous Calculations	4.35- 7.3 (vacancy <110>) (DFT) [61]	-	-	4.74 (5 pair) 4.80 (1 pair) (MD) [66]	-	-	-

Table 4.5: Activation energy and prefactor calculated using the extrapolation of equation 4.38 for dioxides of cerium and minor actinides. The ‘Previous calculations’ represents the results of computational works for activation energy of cation diffusion in fluorite crystals. The activation energy calculated using the uncorrected values of bulk modulus (from [68]) are mentioned in the brackets.

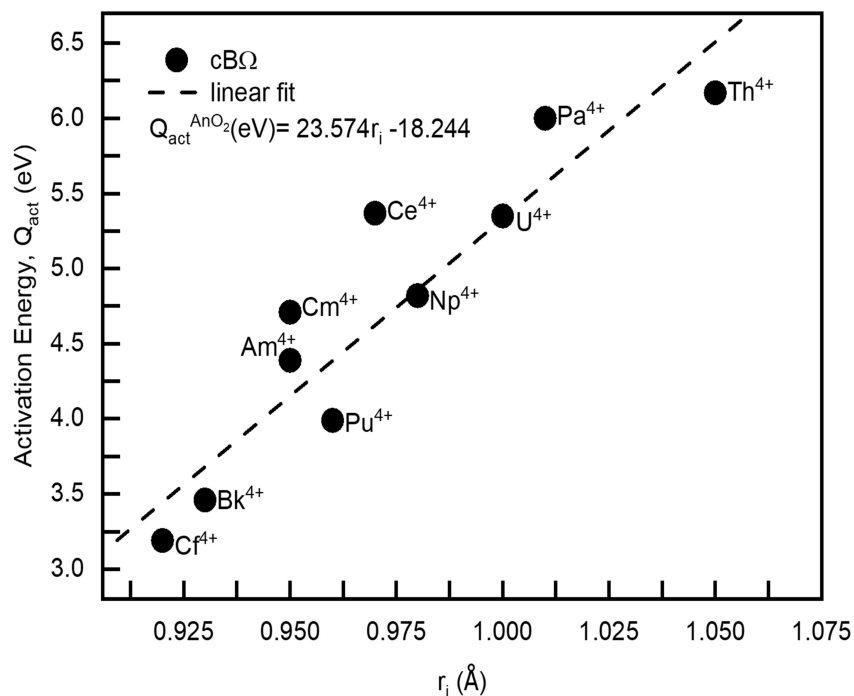


Figure 4.13: Comparison of cationic radii and activation energy of self-diffusion of cation in their respective stoichiometric dioxides. Activation energy of Ce^{4+} in CeO_2 is not considered for the linear fit.

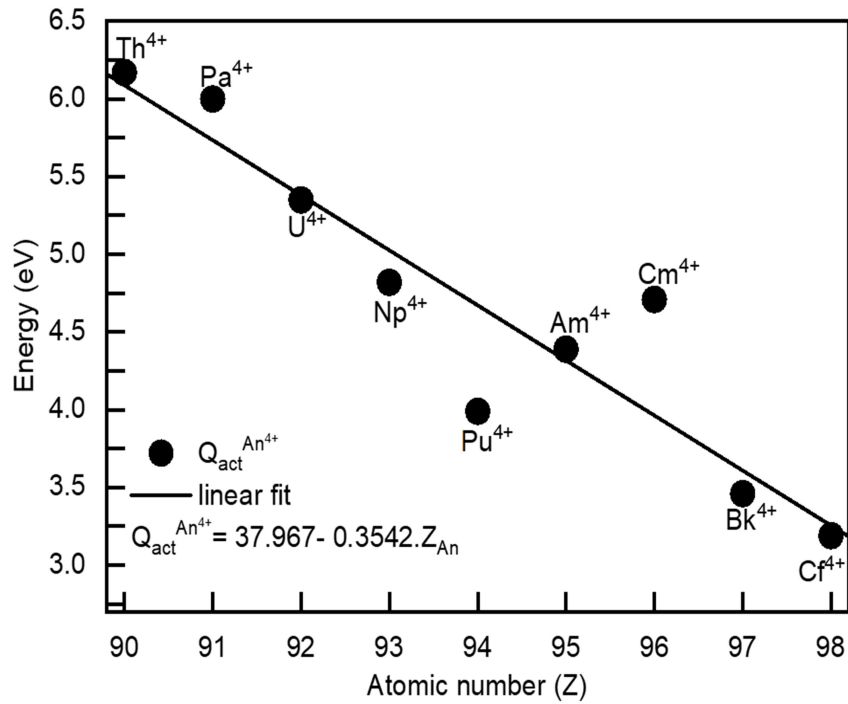


Figure 4.14: Comparison of activation energy and cationic atomic number of AnO_2 . The linear relation between atomic number of An and activation energy of self-diffusion of cation in AnO_2 is also fitted; the solid line indicates the fit.

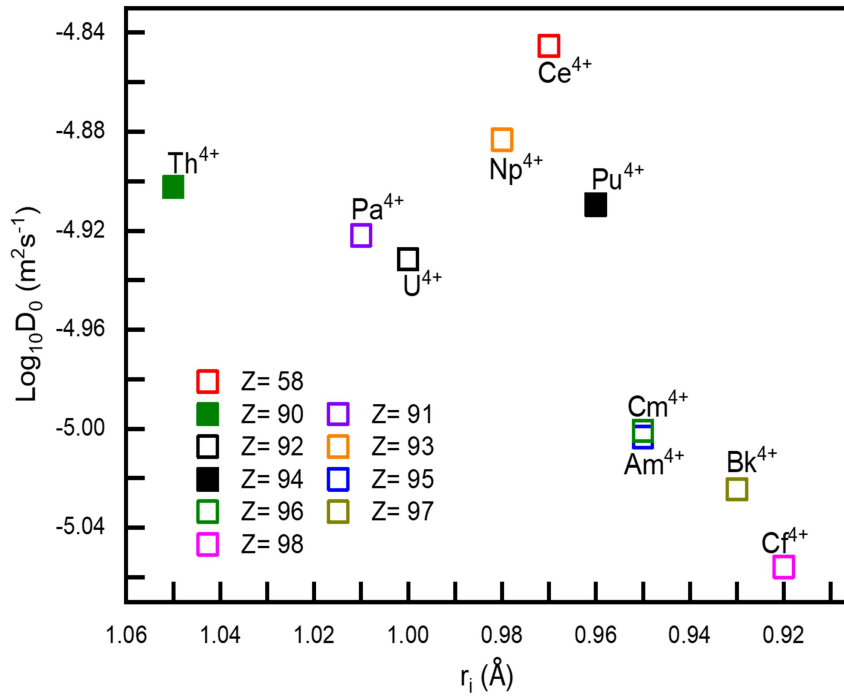


Figure 4.15: Prefactor of cation self-diffusion (D_0) for dioxides of cerium & other minor actinides and its relation to the cationic radii (r_i) and atomic number of cation (Z).

The correction of the bulk modulus applied in the section 4.5.5, for PaO₂, BkO₂ & CfO₂, does not have any effect on the prefactor of the Arrhenius equation. However, a substantial effect can be traced in the value of activation energy. The activation energy calculated using the uncorrected value of bulk modulus, sourced from [68], are mentioned in bracket in the table- 4.5

The activation energy and prefactor calculated for the actinide oxides are clearly related with the ionic radii of the cations. A linear relation is fitted for the activation energy of the cation as following,

$$Q_{\text{act}}^{\text{AnO}_2} \text{ (eV)} = 23.574 r_i - 18.244 \quad \dots(4.48)$$

The linear relation is presented in figure 4.13 along with the fitting equation. However, the error for the Cm⁴⁺ diffusion in CmO₂ is maximum (-11.9%). The average error for the fit is ±6.2%. The activation energy of self-diffusion of Ce⁴⁺ in CeO₂ shows a significant deviation from the linear fit (equation 4.48).

The activation energy variation with the variation of the atomic number of cationic atoms in actinide oxides are also reported in the figure 4.14. The activation energy with the increase of atomic number (for actinides only) gradually decreases. A linear quantification of decrement of activation energy is reported using a linear fit against the atomic number of actinides. The linearly fitted relation is as following,

$$Q_{\text{act}}^{\text{An}^{4+}} \text{ (eV)} = 37.967 - 0.3542 Z_{\text{An}}; Z_{\text{An}} \text{ is the atomic number of An in AnO}_2; \quad \dots(4.49)$$

The averaged error in the linear fit of equation 5.12 is ±5.7%.

Similar to activation energy, the prefactor also studied as a function of the ionic radii of cations and the atomic numbers of cations (figure- 4.15). The increase in ionic radius causes a decrease in the value of cation self-diffusion prefactor. However, the descending pattern is not universal as D₀^{Np⁴⁺} and D₀^{Pu⁴⁺} does not follow the pattern among the actinide dioxides. On the other hand, the prefactor of self-diffusion is studied as a function of atomic number of the actinide for actinide dioxides (figure- 4.15). A descending pattern can also be noticed with the increment of atomic number but the pattern again is not universal. D₀^{Ce⁴⁺} values significantly higher than the prefactors of actinide dioxides.

4.6. Summary & Conclusion:

The chapter briefly summarises the theoretical basis of both the empirical models. The inherent difference of $cB\Omega$ model and Glyde's model is in the consideration of system entropy. In our study, we have ignored the effect of entropy over self-diffusion for the simplicity of our estimations. However, the diffusion entropy was not largely explored for metal diffusion in the oxides either (especially for fluorite structures).

Zener pointed out that the entropy is proportional to the product of activation enthalpy and inverse of melting temperature ($\Delta S \propto H_{act}/T_m$) [69]. Later, the relation of Zener was further explored in metal for self & impurity diffusion [70].

For fluorite structure, King and Moerman tried to quantify the entropy of diffusion in CaF_2 . They recommended a value of 15 to 20 k_B [71]. Lambert tried to implement Zener's relation for UO_2 and found an entropy value of 10.7 k_B [72]. However, this value of entropy is not in accordance to other experiments on UO_2 [72]. The cavity in entropy estimation demands further study.

Mullen established a relation between the activation energy of self-diffusion and ionic radius of diffusing species in several halide crystals [73]. That was later successfully applied for cation diffusion in MgO [74]. This model considers ions as a hard sphere and assumes that the hopping of atom is governed by elastic strain. Hence, the model is also developed with similar hypothesis to $cB\Omega$ model. Therefore, the linear fit of ionic radius and c (also, activation energy) can be argued as a simplified assertion based on Mullen's model. This linearity can further be used to study other compounds as well.

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CHAPTER - V

THE PRINCIPLE OF MOBILITY DATABASE DEVELOPMENT USING DICTRA CODE

This chapter aims to introduce the newly developed plutonium mobility database using DICTRA code. A brief discussion of the basic principle of DICTRA code is presented. Further the model along with the database of mobility parameters for plutonium diffusion, subjected to assessment, are also presented for the mixed oxide of uranium and plutonium. At the end, the scheme applied to assess the mobility terms are briefly discussed.

5.1. Introduction:

DICTRA (Diffusion Controlled TRAnsformation) is a software package to simulate phase transformation controlled by diffusion in multi-component systems. It is based on the one-dimensional numerical solution of the multi-component diffusion equation. DICTRA is directly linked to the Thermocalc software that supply all the required thermodynamic calculations [1].

As mentioned in the chapter – 2, CALPHAD method uses the assessed thermodynamic parameters for model of Gibbs energy. These parameters are assessed by minimization process. This assessment is mostly done using the PARROT program [2] in the Thermocalc software.

In the same spirit of CALPHAD, Andersson and Ågren modelled the atomic mobility of each component, in a multicomponent system. The frequency and activation energy of atomic mobility was described using the Redlich-Kister expansion [3]. Similar to Thermocalc, the mobility parameters of the DICTRA code are also assessed in the PARROT program under the DICTRA code.

In the model of plutonium diffusion, the same principles are applied and the mobility parameters are assessed using the experimental data mentioned in the chapter – 3 and the results of $cB\Omega$ calculations, (as described in the chapter – 4)

In this chapter, we will first briefly explain this general equations of diffusion and report the established relation between the Gibbs energy of the system and the diffusion coefficients of the elements of the system. We will also report the simple relation between diffusion coefficient and the atomic mobility. Then we will discuss the set of principles and equations used in DICTRA code to model the mobility parameters for the plutonium diffusion in MOx.

A database containing the mobility parameters for the diffusion of plutonium in mixed oxide of uranium & plutonium is discussed in the following section. The discussion of this section will also include the relevant approximation and assumptions and reductions taken for the development of the model. At the end of this chapter, we will finally explain the scheme applied for the assessment of the mobility parameter.

5.2. Model development:

5.2.1. Equation of diffusion:

Flux of diffusion of an element k is proportional to the concentration gradient of that element ($\frac{\partial c_k}{\partial x}$) which acts as a driving force of diffusion and this flux of diffusion (J_k) was quantified by Fick's law as [3],

$$J_k = -D_k \frac{\partial c_k}{\partial x} \quad \dots(5.1)$$

Where, D_k is the diffusion coefficient of element k.

In definition, the self-diffusion coefficient (D^*) is the diffusion coefficient of an element without any chemical gradient [4]. It is related to the diffusion coefficient as follows:

$$D_k = D_k^* \left(\frac{n_k}{RT} \right) \frac{\partial \mu_k}{\partial n_k} \quad \dots(5.2)$$

However, we have witnessed in Chapter-3 that the tracer diffusion coefficient of isotopically labelled species is considered to be the self-diffusion coefficient, in practice.

Fick's first law of diffusion defines, for a definite element (Pu) the diffusion coefficient (D_{Pu}) in terms of net diffusion flux (J_{Pu}) and concentration gradient ($\frac{\partial c_k}{\partial x}$) of a monophasic binary system as per equation 5.1.

Whereas, the diffusion coefficient of this equation is termed as practical diffusion coefficient which can be synonymous to both chemical or inter-diffusion coefficient, depends on the system and type of diffusion. The diffusion flux, hence the diffusion coefficient as well, are measured in respect to the reference frame as well as the driving force (F) [5]. The diffusion velocity of the species $V_{F,Pu}$ (which arises from the driving force) is directly proportional to the Flux as,

$$J_{Pu} = C_{Pu} V_{F,Pu} \quad \dots(5.3)$$

In linear theory of irreversible process, this velocity is also defined in terms of the Gibbs energy gradient [5] (or, an appropriate potential gradient, which can be chemical potential as well [3]) as,

$$V_{F,Pu} = -M_{Pu} \frac{\partial G_{Pu}}{\partial x} \quad \dots(5.4)$$

Where, the parameter M_{Pu} is the mobility of the diffusing species. The mobility of the species is directly related to the self-diffusion coefficient by Nernst-Einstein equation as,

$$D_{Pu}^* = M_{Pu} RT \quad \dots(5.5)$$

Now, by combining all these equations, we can define the flux of diffusion as,

$$J_{Pu} = -C_{Pu}M_{Pu} \frac{\partial G_{Pu}}{\partial x} \quad \dots(5.6)$$

Hence, the self-diffusion coefficient of a species is directly related to the diffusion flux of that species. The product $C_{Pu}M_{Pu}$ is known as the Phenomenological coefficient (L_{Pu}) of the species. Hence, the linear expression of flux comprising phenomenological coefficient is,

$$J_{Pu} = -L_{Pu} \frac{\partial G_{Pu}}{\partial x} \quad \dots(5.7)$$

It is evident that the practical diffusion coefficient of equation 5.1 is again directly related to the phenomenological coefficient with and hence the self-diffusion coefficient is also related to the practical diffusion coefficient in following relation.

$$D_{Pu} = L_{Pu} \left(\frac{\partial G_{Pu}}{\partial C_{Pu}} \right) = D_{Pu}^* \left(\frac{C_{Pu}}{RT} \right) \left(\frac{\partial G_{Pu}}{\partial C_{Pu}} \right) \quad \dots(5.8)$$

5.2.2 Application in DICTRA:

According to Andersson & Ågren [3], when there is a vacancy (V_a) associated to the diffusing species atom under lattice fixed frame of reference then the mobility of the species in thermal equilibrium can be defined as:

$$M_{Pu} = y_{Va} \Phi_{Pu} \quad \dots(5.9)$$

y_{Va} is the fraction of vacancy and Φ_{Pu} is a kinetic parameter that gives the rate of exchange between the atom and the vacant site adjacent to the atom. However, for the diffusion carried out by the interstitial mechanism, the mobility parameter, M_{Pu} , is defined as:

$$M_{Pu} = \Phi_{Pu} \quad \dots(5.10)$$

However, the thermodynamic description of MOx suggested by Guéneau et al., which is utilized in this work, does not identify any vacancy or interstitial defect for Pu in MOx [6]. Rather different oxidation states of Pu (+III, +IV, +V) act as the Pu defects in MOx. Hence, the kinetic parameter is irrelevant and the mobility parameter directly is modelled in this work. This has already been discussed in details in Chapter-2. However, several parameters increase the complexity of the model.

We present an example of pure plutonia only and reduces the sublattices as required here for the sake of simplicity and suitability of understanding. The example is presented in figure – 5.1. The example contains 12 end-members including both real and hypothetical compounds. A similar chart can be developed for the pure urania (without any plutonium ion in the first sublattice). In this study, we will assess the plutonium diffusion in each of these end-members, which is explained in the following sections.

As we have presented that self-diffusion coefficient and mobility parameters are strongly interrelated (phenomenological coefficient as well), we have modelled the mobility of the species Pu in MOx. Using the Arrhenius definition, the mobility parameter can be modelled as:

$$M_{Pu} = M^0 \exp\left(-\frac{Q_{act}^m}{RT}\right) \Gamma_{mg} \quad \dots(5.11)$$

Q_{act}^m represents the activation energy of mobility of the species which is equal to the activation energy of self-diffusion (Q_{act}). M^0 represents the prefactor of the mobility parameter and Γ_{mg} represents the effect of ferromagnetic transition. However, the ferromagnetic effect in diffusion is negligible for the fcc crystals [7]. Hence we considered $\Gamma_{mg} = 1$.

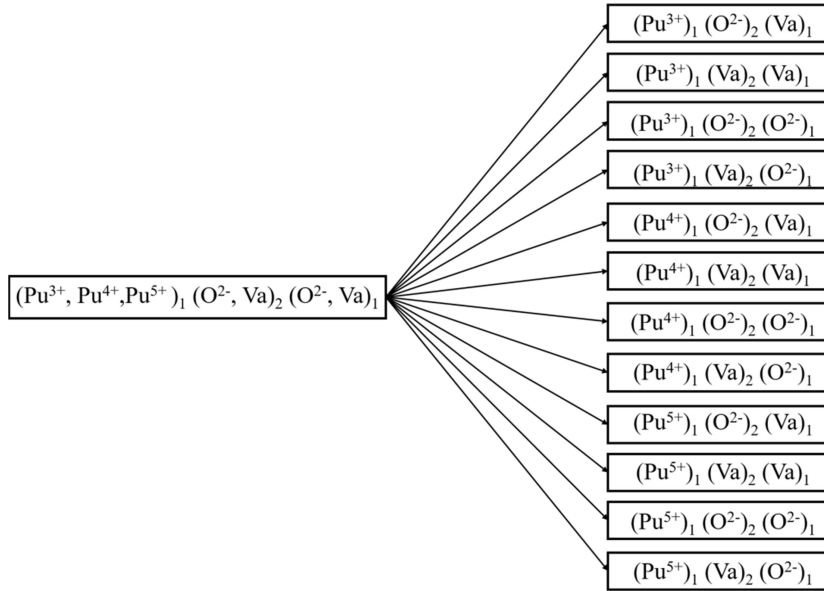


Figure 5.1: All endmembers of pure plutonia which are considered for cationic diffusion in this work;

The mobility of Pu in MOx is an aggregate of the mobility of different cations of Pu, similar to the case of mobility of U in Urania [8]. As described in Chapter-2, the concentration of Pu⁵⁺ is very low irrespective of the composition of MOx. Therefore, the mobility of Pu is further expressed in terms of the mobility of Pu³⁺ and Pu⁴⁺ cations under the scope of this work. The mobility of Pu⁵⁺ is neglected due to its low concentration in the following expression of mobility of Pu.

$$L_{Pu} = C_{Pu} M_{Pu} = \frac{1}{V_m} [y_{Pu^{3+}} M_{Pu^{3+}} + y_{Pu^{4+}} M_{Pu^{4+}}] \quad \dots(5.12)$$

In the equation, V_m is the molar volume of Pu. The mobility of each cation of Pu is computed using the equation 5.11. Activation energy of the mobility (or self-diffusion, Q_{act}) and the mobility prefactor (M^0) of each Pu cation can again be decomposed as a function of all possible endmembers under the

CEF framework, described in chapter- 2. Although Pu^{5+} is ignored as a diffusing species, the end-members with +V charge state of plutonium is considered in the following equations.

$$\text{Ln}(M_{\text{Pu}^{v+}}^0) = \sum_{(i=\text{Pu}^{3+}, \text{Pu}^{4+}, \text{Pu}^{5+}, \text{U}^{3+}, \text{U}^{4+}, \text{U}^{5+})} Y_i \sum_{(j=\text{O}^{2-}, \text{Va}')} Y_j \sum_{(k=\text{O}^{2-}, \text{Va}'')} Y_k \text{Ln}(M_{\text{Pu}^{v+}}^0)^{(i)(j)(k)} \dots(5.13)$$

$$Q_{\text{act}}^{\text{Pu}^{v+}} = \sum_{(i=\text{Pu}^{3+}, \text{Pu}^{4+}, \text{Pu}^{5+}, \text{U}^{3+}, \text{U}^{4+}, \text{U}^{5+})} Y_i \sum_{(j=\text{O}^{2-}, \text{Va}')} Y_j \sum_{(k=\text{O}^{2-}, \text{Va}'')} Y_k \times (Q_{\text{act}}^{\text{Pu}^{v+}})^{(i)(j)(k)} \dots(5.14)$$

5.3. DICTRA database:

The mobility of Pu^{4+} in pure plutonia depends upon $(M_{\text{Pu}^{4+}})^{(i)(j)(k)}$ associated to all endmembers, and their site fractions y_i, y_j & y_k with $i \in (\text{Pu}^{3+}, \text{Pu}^{4+})$ and $j, k \in (\text{O}^{2-}, \text{Va})$. Here after, we will going to use the symbol * to signify either O^{2-} or Va in both 2nd and 3rd sublattices, i.e. $(\text{Pu}^{3+}, \text{Pu}^{4+}, \text{Pu}^{5+})_1 (*)_2 (*)_1$.

For the assessment of the diffusion of Pu^{3+} and Pu^{4+} in MOx, both the mobilities in $\text{PuO}_{2\pm x}$ and $\text{UO}_{2\pm x}$ need to be assessed. In order to assess diffusion in both Plutonia & Urania endmembers, 96 parameters needs to be assessed (48 activation energies & 48 mobility prefactors, see Table – 5.1).

Diffusion Cation Cationic end-member	Pu^{3+}		Pu^{4+}	
Pu^{3+}	$M_{\text{Pu}^{3+}}^0 (\text{Pu}^{3+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{Pu}^{3+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{Pu}^{3+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{Pu}^{3+})(*)(*)}$
Pu^{4+}	$M_{\text{Pu}^{3+}}^0 (\text{Pu}^{4+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{Pu}^{4+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{Pu}^{4+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{Pu}^{4+})(*)(*)}$
Pu^{5+}	$M_{\text{Pu}^{3+}}^0 (\text{Pu}^{5+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{Pu}^{5+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{Pu}^{5+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{Pu}^{5+})(*)(*)}$
U^{3+}	$M_{\text{Pu}^{3+}}^0 (\text{U}^{3+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{U}^{3+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{U}^{3+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{U}^{3+})(*)(*)}$
U^{4+}	$M_{\text{Pu}^{3+}}^0 (\text{U}^{4+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{U}^{4+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{U}^{4+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{U}^{4+})(*)(*)}$
U^{5+}	$M_{\text{Pu}^{3+}}^0 (\text{U}^{5+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{3+}(\text{U}^{5+})(*)(*)}$	$M_{\text{Pu}^{4+}}^0 (\text{U}^{5+})(*)(*)$	$Q_{\text{act}}^{\text{Pu}^{4+}(\text{U}^{5+})(*)(*)}$

Table 5.1: The list of Mobility Parameter for Pu in MOx.

We assume that the activation energy and the mobility prefactor of Pu cations depend on the cationic species of the endmembers, i.e. $\text{U}^{3+,4+,5+}$ & $\text{Pu}^{3+,4+,5+}$, rather than the oxygen sublattices. Hence, the role of oxygen in the plutonium diffusion is negligible. However, it has to be noted that the negligible role of oxygen does not imply negligible role of stoichiometric ratio. The mole fractions of different cationic stages are determined the stoichiometric ratio of the compound which is discussed in detail in Chapter- 2. A list of mobility parameters, which are assessed in our study, are given in table- 5.1.

In order to further simplify the model development, we have set up few additional relations within the assessing parameters of table-5.1.

- The lack of the Pu diffusion data in $\text{PuO}_{2\pm x}$ has been repeatedly mentioned before. Hence, to minimize the complexity of assessing the different mobility parameters for that case, we have

set the mobility of Pu³⁺ equals in all the endmembers of pure plutonia; mobility of Pu⁴⁺ equals in all the endmembers of pure plutonia;

$$M_{\text{Pu}^{3+}}^0 (\text{Pu}^{3+})(*)(*) = M_{\text{Pu}^{3+}}^0 (\text{Pu}^{4+})(*)(*) = M_{\text{Pu}^{3+}}^0 (\text{Pu}^{5+})(*)(*) \quad \dots(5.15)$$

$$Q_{\text{act}}^{\text{Pu}^{3+}} (\text{Pu}^{3+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{3+}} (\text{Pu}^{4+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{3+}} (\text{Pu}^{5+})(*)(*) \quad \dots(5.16)$$

$$M_{\text{Pu}^{4+}}^0 (\text{Pu}^{3+})(*)(*) = M_{\text{Pu}^{4+}}^0 (\text{Pu}^{4+})(*)(*) = M_{\text{Pu}^{4+}}^0 (\text{Pu}^{5+})(*)(*) \quad \dots(5.17)$$

$$Q_{\text{act}}^{\text{Pu}^{4+}} (\text{Pu}^{3+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{4+}} (\text{Pu}^{4+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{4+}} (\text{Pu}^{5+})(*)(*) \quad \dots(5.18)$$

➤ As mentioned in details in the chapter-2, Pu³⁺ are the predominant Pu cation species in low O/M ratio. Whereas, in O/M ≥ 2, Pu⁴⁺ is the major Pu cation species. Hence, the Pu³⁺ mobility against all endmembers containing U³⁺ & U⁴⁺ are taken into equal. On the other hand, the mobility of Pu⁴⁺ against all endmembers containing U³⁺ & U⁴⁺ are also taken into account. This presumption is necessary to reproduce the plateau observed for low O/M value (O/M < 1.9). We will discuss further about this phenomenon in the following chapter.

$$M_{\text{Pu}^{3+}}^0 (\text{U}^{3+})(*)(*) = M_{\text{Pu}^{3+}}^0 (\text{U}^{4+})(*)(*); Q_{\text{act}}^{\text{Pu}^{3+}} (\text{U}^{3+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{3+}} (\text{U}^{4+})(*)(*) \quad \dots(5.19)$$

$$M_{\text{Pu}^{4+}}^0 (\text{U}^{3+})(*)(*) = M_{\text{Pu}^{4+}}^0 (\text{U}^{4+})(*)(*); Q_{\text{act}}^{\text{Pu}^{4+}} (\text{U}^{3+})(*)(*) = Q_{\text{act}}^{\text{Pu}^{4+}} (\text{U}^{4+})(*)(*) \quad \dots(5.20)$$

On the other hand, to get an agreement with the experimental results of Pu diffusion in MOx with O/M = 2.0, we have introduced a necessary interaction parameter between Pu⁴⁺ and U⁴⁺, i.e. Ψ_{Pu⁴⁺,U⁴⁺}. Introduction of this interaction parameter hence modifies the estimating equation of M_{Pu⁴⁺}^{(U⁴⁺)(*)(*)} as following:

$$M_{\text{Pu}^{4+}}^{(\text{U}^{4+})(*)(*)} = y_{\text{U}^{4+}} M_{\text{Pu}^{4+}}^0 (\text{U}^{4+})(*)(*) \exp \left[\frac{Q_{\text{act}}^{\text{Pu}^{4+}} (\text{U}^{4+})(*)(*) + y_{\text{Pu}^{4+}} y_{\text{U}^{4+}} \Psi_{\text{Pu}^{4+}, \text{U}^{4+}}}{RT} \right] \quad \dots(5.21)$$

Using these relations, the mobility of Plutonium cations in MOx is assessed using the DICTRA add-on module of Thermo-Calc software [7]. Further, the Self-diffusion coefficient (D_{Pu}^{*}) is also calculated using the Nernst-Einstein relation (equation 5.5).

5.4. Assessment technique for the mobility parameters:

The assessment of the mobility parameters were performed using the PARROT module of the DICTRA code. Even after the reduction of the substantial numbers of parameters, as discussed in the preceding section, a total of 12 mobility parameters (6 for Pu³⁺ mobility and 6 for Pu⁴⁺ mobility) needs to be assessed.

The assessment is done in two fold (as shown in figure – 5.2) – first, for the plutonium diffusion (both Pu³⁺ and Pu⁴⁺) in binary UO₂ and PuO₂; which means the mobility parameters under consideration are those which play a role for the plutonium diffusion in perfectly stoichiometric urania and plutonia. In the second step, the mobility parameters of plutonium diffusion in mixed oxide of uranium and plutonium, (U, Pu)O_{2±x} (including the deviation of stoichiometry) are assessed.

In the initial step, we assessed the mobility of the plutonium diffusion in UO₂ and PuO₂, independently. The assessment of the plutonium diffusion in UO₂ was performed using the assessment of $M_{Pu^{4+}}^{(U^{4+})(*)}$, as described in the previous section. The assesment were performed in order to fit the diffusion data of Pu in UO₂, measured by Lambert [9]. An interaction parameter, introduced in the equation 5.11, is also used to fit the Pu diffusion data in UO₂.

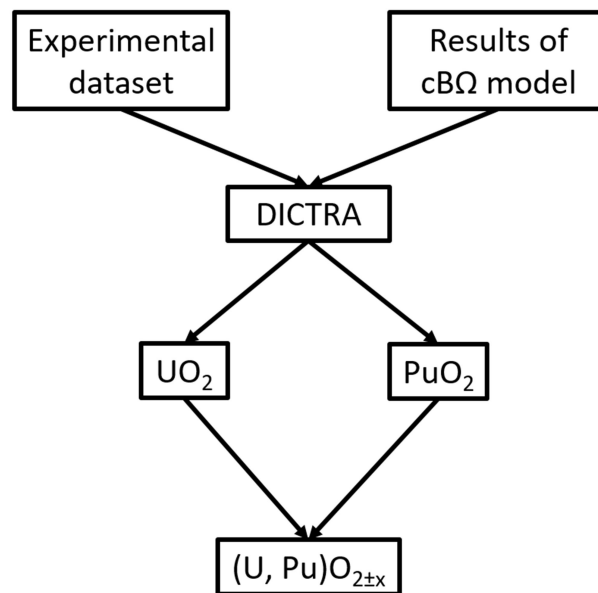


Figure 5.2: Assessment Scheme for mobility parameters using DICTRA

In parallel, the Pu diffusion in PuO₂ calculated using cBΩ model (Chapter – 4) is used to assess the $M_{Pu^{4+}}^{(Pu^{4+})(*)}$. Chapter – 4 of this study extensively discussed about the correlation of ionic radius and the diffusion coefficient of the ion. Hence, the ionic radius ratio Pu³⁺/Pu⁴⁺ has been taken into

account in order to model the diffusion coefficient and the activation energy of diffusion for Pu^{3+} in PuO_2 is considered to be 1.04 times higher than that of the Pu^{4+} ($r_{\text{Pu}^{3+}} = 1.00 \text{ \AA}$, $r_{\text{Pu}^{4+}} = 0.96 \text{ \AA}$).

The diffusion coefficient varies not only with the variation of temperature but also with the variation of oxygen stoichiometry of the system. After fixing the Pu diffusion coefficient in the stoichiometric urania and plutonia, the deviation from stoichiometry is accommodated by assessing the plutonium (both Pu^{3+} and Pu^{4+}) mobility parameter for U^{3+} , U^{5+} , Pu^{3+} and Pu^{5+} ions in the cation sublattice.

The variation of oxygen stoichiometry produces a diffusion curve which is similar to the figure – 3.3. The curve consists of a lower leg (in the hypo-stoichiometric regime), a minima (near the $\text{O}/\text{M} = 2.00$) and an upper leg (in the hyper-stoichiometric regime). Using this characteristic shape of the curve and the diffusion coefficient data already discussed in the chapter – 3, the mobility parameter of plutonium diffusion in non-stoichiometric mixed oxide is assessed.

In the cation sublattice, the main contribution of Pu^{3+} diffusion against U^{3+} is significant in the stoichiometry $\text{O}/\text{M} < 1.9$. So, the mobility parameter $M_{\text{Pu}^{3+}}^0 (\text{U}^{3+})(*)(*)$ is optimized in low stoichiometric ratio.

On the other hand, the contribution of Pu^{3+} against U^{5+} in the cation sublattice, is significant in the stoichiometry near 2.00. Hence, the mobility parameter $M_{\text{Pu}^{3+}}^0 (\text{U}^{5+})(*)(*)$ is optimized accordingly. The mobility of Pu^{4+} diffusion against U^{5+} in the cation sublattice, i.e. $M_{\text{Pu}^{3+}}^0 (\text{U}^{5+})(*)(*)$, is assessed as such this mobility parameter can capture the faster diffusion process observed in the experiments (upper leg of the curve), for stoichiometric ratio $\text{O}/\text{M} > 2.00$ [9, 10]. The results of these assessments are shown in the next chapter.

5.5 Conclusion:

This chapter serves as a brief introduction to the newly developed DICTRA framework. The plutonium model which is developed under the scope of this thesis is described in this chapter as well. The details of all the required mobility parameters are then discussed as well. It has been pointed out that there are a total of 97 mobility parameters, associated to the 24 end-members, involved in the model of Pu diffusion (48 prefactors, 48 activation energies and 1 interaction term). The overwhelming number of parameters increases the degree of freedom of the model. Hence, a set of assumptions was postulated to reduce the mobility parameters. Finally, 12 parameters have been selected for further optimization. At the end, the assessment scheme of these 12 parameters is also detailed in this chapter.

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CHAPTER - VI

THE RESULTS OF THE MODEL OF PLUTONIUM DIFFUSION IN MIXED OXIDE

This chapter aims to present the results of the plutonium diffusion in binary urania & plutonia and in ternary MO_x, computed from the newly developed model using DICTRA code. The assessed mobility parameter values are firstly presented in this chapter. Then the computed results of diffusion coefficients are compared with the experimental data of both binary and ternary oxides, when available. The final activation energy and prefactor of plutonium diffusion in MO_x are calculated and compared with literature data. Finally, the effect of plutonium content, stoichiometric ratio and temperature on the plutonium diffusion coefficient in MO_x is predicted using the model.

6.1. Introduction:

The results of our model are presented in this chapter. The calculated data are compared with the selected experimental data and cBΩ results which are already discussed in detail in the chapter – 3 and 4. The model is used to predict the variation of the plutonium diffusion coefficient with the variation of oxygen stoichiometry, plutonium content and temperature. Hence, it will be qualified as the first full thermo-kinetic model for plutonium diffusion in MOx.

The chapter will first report the assessed mobility parameters for plutonium diffusion. The assessment technique has already been discussed in the previous chapter. So, this chapter will only present the values of the optimized parameters and then analyze the parameter values.

In the following section, we will present the assessment results, calculated from our model in binary oxide UO₂ & PuO₂ and compare them with the selected experimental data and the results of cBΩ model. In this section we will also report the predicted variation of plutonium diffusion coefficient with oxygen stoichiometry, calculated from our model.

In the next section, we will calculate the plutonium diffusion coefficient in mixed oxide of uranium and plutonium and compare the results with the selected experimental data at different plutonium content, stoichiometry and temperature. This section will also analyze the variation of plutonium diffusion against the oxygen stoichiometry and Pu content from the concentration of different species in the mixed oxide.

We will then discuss the diffusion activation energy and prefactor, calculated from our model and compare them with the available data found in the literature (both via experiment and computation). At the last section, we will finally discuss the effect of the plutonium content, stoichiometric ratio and the system temperature on the plutonium diffusion coefficient in the system.

6.2. Assessed Mobility Parameters:

The previous chapter discussed the assessment scheme of the mobility parameter. In this section, the assessed results are presented. The mobility parameters are reduced to 12. A detailed discussion of the reduction of parameters is carried out in the previous chapter. An additional interaction parameter between Pu^{4+} and U^{4+} (in the first sublattice) is also introduced and assessed. These results are reported in table- 6.1.

Diffusing Cation Cationic end-member		Pu ³⁺		Pu ⁴⁺	
		Mobility prefactor (M^0), m ² /s	Activation energy (Q_{act}), kJ/mol (eV)	Mobility prefactor (M^0), m ² /s	Activation energy (Q_{act}), kJ/mol (eV)
PuO ₂	(Pu ³⁺) ₁ (*) ₂ (*) ₁	1.10 ⁻¹⁰	393.6 (4.1)	3.10 ⁻¹⁰	370 (3.85)
	(Pu ⁴⁺) ₁ (*) ₂ (*) ₁	1.10 ⁻¹⁰	393.6 (4.1)	3.10 ⁻¹⁰	370 (3.85)
	(Pu ⁵⁺) ₁ (*) ₂ (*) ₁	1.10 ⁻¹⁰	393.6 (4.1)	3.10 ⁻¹⁰	370 (3.85)
(U, Pu)O ₂	(U ³⁺) ₁ (*) ₂ (*) ₁	2.10 ⁻⁸	560 (5.8)	4.10 ⁻⁹	540 (5.6)
	(U ⁴⁺) ₁ (*) ₂ (*) ₁	2.10 ⁻⁸	560 (5.8)	4.10 ⁻⁹	540 (5.6)
	(U ⁵⁺) ₁ (*) ₂ (*) ₁	1.10 ⁻²⁰	1000 (10.4)	1.10 ⁻³	350 (3.65)
	(Pu ⁴⁺ ,U ⁴⁺) ₁ (O ²⁻) ₂ (Va) ₁				-450 (4.66)

Table 6.1: The assessed values of mobility parameters for Pu diffusion in plutonia and mixed oxide of uranium and plutonium;

In this section, it also has to be explained that the mobility of plutonium in any of these endmembers (as mentioned in table 6.1) has no practical significance in isolation. Even many of these end-members are not real compounds (as also explained in chapter – 2). The plutonium mobility, as whole, in the mixed oxide of uranium and plutonium, is an aggregation of these end-member mobility parameters all together. This will be further discussed in the next section. So, we will now focus on the analysis of the values of the parameters in this section.

The mobility of Pu³⁺ in plutonia is set to a higher activation energy than the mobility of Pu⁴⁺ in plutonia. This is because the ionic radius of Pu³⁺ is larger than that of Pu⁴⁺ (as per the discussion of the chapter – 5). However, the mobility prefactor (M^0) of both Pu⁴⁺ and Pu³⁺ are assessed and exhibit the same magnitude of values. It means the Pu⁴⁺ diffuses faster in plutonia than Pu³⁺. The Pu³⁺ mobility prefactor and the activation energy are assumed to be same in the presence of all three plutonium cations in first sublattice, i.e. Pu³⁺, Pu⁴⁺ and Pu⁵⁺. Similarly, the Pu⁴⁺ mobility prefactor and the activation energy are assumed to be same in the presence of all three plutonium cations in first

sublattice, i.e. Pu^{3+} , Pu^{4+} and Pu^{5+} . This assumption is postulated due to the lack of experimental results of plutonium diffusion in plutonia (especially in non-stoichiometric PuO_{2-x}).

The hypo stoichiometric mixed oxide of uranium and plutonium has majorly of two uranium cations in the first sublattice (as per the discussion in chapter – 2), i.e. U^{3+} and U^{4+} . The mobility parameters of Pu^{3+} in the presence of both U^{3+} and U^{4+} are assumed to be the same (as discussed in Chapter – 5). Similarly, the mobility parameters of Pu^{4+} in the presence of both U^{3+} and U^{4+} are also assumed to be the same (as discussed in Chapter – 5). The values of these activation energies and mobility prefactors are assessed using the PARROT module of DICTRA.

The activation energy of Pu^{3+} mobility in the presence of U^{3+} reports a higher activation energy of 0.2 eV than that of the Pu^{4+} mobility activation energy. The mobility prefactor of Pu^{3+} in the presence of U^{3+} is one order higher than the mobility prefactor of Pu^{4+} in the presence of U^{3+} .

Similarly, the deviation between the mobility activation energy of Pu^{4+} and Pu^{3+} in the presence of the U^{4+} (similar to the case of U^{3+}) in the first sublattice is less than 4%. The prefactor of mobility shows an increase of one order of magnitude for Pu^{3+} than that of Pu^{4+} with U^{4+} in the first sublattice. The presence of both Pu^{4+} and U^{4+} in the first sublattice exhibit a negative interaction term (as shown in the table 6.1). This negative interaction term reduces the activation energy of mobility of Pu^{4+} (as per the equation 5.21) and increases the mobility rate of Pu^{4+} . The mobility of Pu^{3+} in perfectly stoichiometric charged compound (a constituent array) $(\text{U}^{4+})_{0.8}(\text{Pu}^{3+}, \text{Pu}^{4+})_{0.2}\text{O}_2$ at 1773 K is 1.06 times higher than the mobility of Pu^{4+} in the same compound. Therefore, the Pu^{3+} is a bit more mobile than Pu^{4+} in presence of U^{4+} as a first sublattice cation in the mixed oxide of uranium and plutonium.

In the hyper stoichiometry mixed oxide of uranium and plutonium has a total of four cations in the first sublattice (as per the discussion in chapter – 2), i.e. U^{4+} , U^{5+} , Pu^{4+} , and a minute concentration of Pu^{5+} . Among these four cations, the Pu^{3+} is less mobile than Pu^{4+} in presence of two plutonium cations in the first sublattice (Pu^{4+} and Pu^{5+}).

The Pu^{3+} concentration reduces with the increase of stoichiometry as a detailed discussion has been carried out in the chapter – 2. On the contrary, the concentration of U^{5+} increases with the increase of stoichiometry. The change of concentration of Pu^{3+} and U^{5+} with respect to both stoichiometric ratio and plutonium content is laid down in figure 6.1, at a fixed temperature of 1773 K. The concentrations of other cations and anions are intentionally suppressed in the figure 6.1 to reduce the complexity of the figure.

The presence of both Pu^{3+} and U^{5+} are noted in the hypo-stoichiometric regime ($\text{O}/\text{M} > 1.9$) for low plutonium MOx (30% or less of plutonium content). With increase of plutonium content, the presence of both Pu^{3+} and U^{5+} are noted in the hyper-stoichiometric regime as well.

The concentration of U^{4+} in $U_{0.75}Pu_{0.25}O_{1.95}$ is 100 times higher than the concentration of U^{5+} , at a temperature of 1773 K (figure 2.7 of chapter – 2). Thus, the contribution of the mobility of Pu^{3+} in the presence of U^{4+} in the first sublattice is higher than the contribution of the mobility of Pu^{3+} in the presence of U^{5+} in the first sublattice, for computing the overall Pu^{3+} mobility in stoichiometry higher than $O/M= 1.9$.

Although Pu^{3+} is present in the hyper-stoichiometric MO_x with a higher plutonium content, the concentration of Pu^{4+} is always higher than that of Pu^{3+} (44 times higher in $U_{0.25}Pu_{0.75}O_{2.05}$ at 1773 K). However, the significance of Pu^{3+} mobility parameters in the presence of U^{5+} as a first sublattice cation cannot be ignored. Therefore, the very high activation energy and mobility prefactor (as shown in table 6.1) abnormally reduces the mobility of Pu^{3+} in the presence of U^{5+} in the first sublattice. In order to obtain a good agreement with the previously measured experimental results of plutonium diffusion (the selected data from chapter – 3) and to retain the prescribed shape of the diffusion curve with the minimum around 1.98 (as discussed in the Chapter – 5), very high value of activation energy (10.4 eV) and very low value of mobility prefactor ($1.10 \cdot 10^{-20} \text{ m}^2 \cdot \text{s}^{-1}$) for Pu^{3+} mobility in the presence of U^{5+} as first sublattice cation, is accepted in this model.

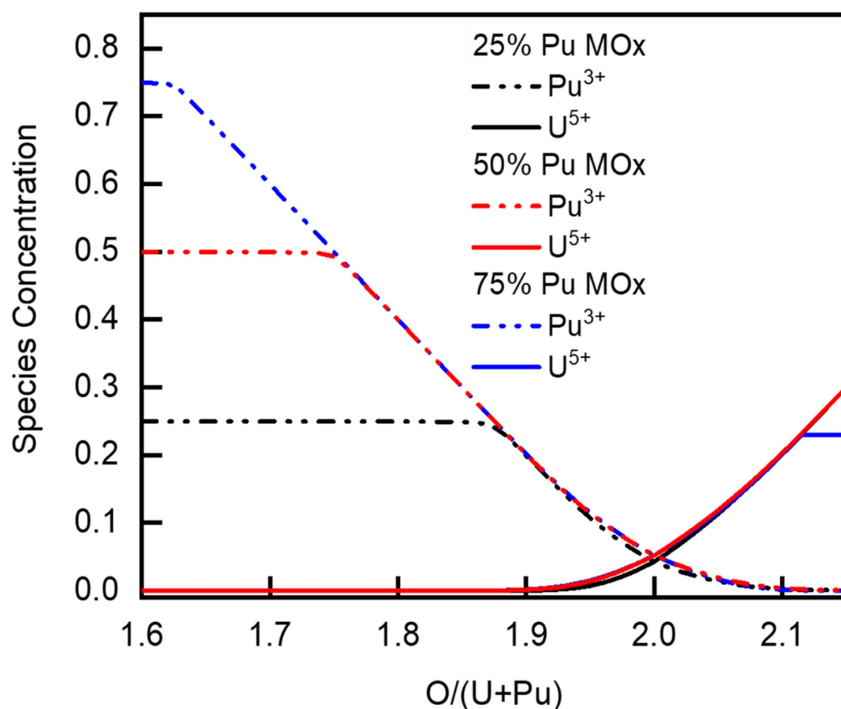


Figure 6.1: Comparison of concentration of Pu^{3+} and U^{5+} with respect to the stoichiometric ratio at 1773 K.

On the other hand, the assessed mobility prefactor of Pu^{4+} in the presence of U^{5+} is higher than the Pu^{4+} mobility prefactor in U^{4+} . The activation energy of Pu^{4+} in the presence of U^{5+} is lower than the

Pu^{4+} activation energy in U^{4+} . This value of mobility parameters of Pu^{4+} in the U^{5+} present in the first sublattice can be reasoned by the lower ionic radius of U^{5+} (0.84 Å) than that of U^{4+} (1 Å).

From the values of activation energy in table 6.1, it is evident that the mobility of Pu^{3+} is higher in the presence of any of the Pu ions in the first sublattice than the presence of any of the uranium cations as the activation energy. The Pu^{4+} mobility is also higher in the presence of any of the three plutonium ions in first sublattice than the presence of either U^{3+} or U^{4+} in the first sublattice because of the values of activation energy. However, the Pu^{4+} mobility is highest in the presence of U^{5+} in the first sublattice as the activation energy is highest. From this observation one can conclude that the Pu^{3+} mobility in PuO_2 is higher than in UO_2 . Even the Pu^{4+} mobility is also expected to be higher in highly reduced plutonia than the highly reduced urania. But it can never be concluded that the mobility of Pu^{3+} varies linearly with respect to plutonium content from UO_2 to PuO_2 as the mobility heavily depends on the concentration of each ion (both cation and anion) in the system.

6.3. Pu diffusion in binary UO₂ and PuO₂ :

The mobility parameters of Pu diffusion are first assessed in the binary PuO₂ and UO₂. In this section we are reporting the results calculated from the assessment in both binary oxides UO₂ and PuO₂ (figure 6.2). The results are also compared with the experimental data of Lambert [1] for Pu diffusion in UO₂ and the calculated cBΩ data (chapter – 4) for the Pu⁴⁺ diffusion in PuO₂.

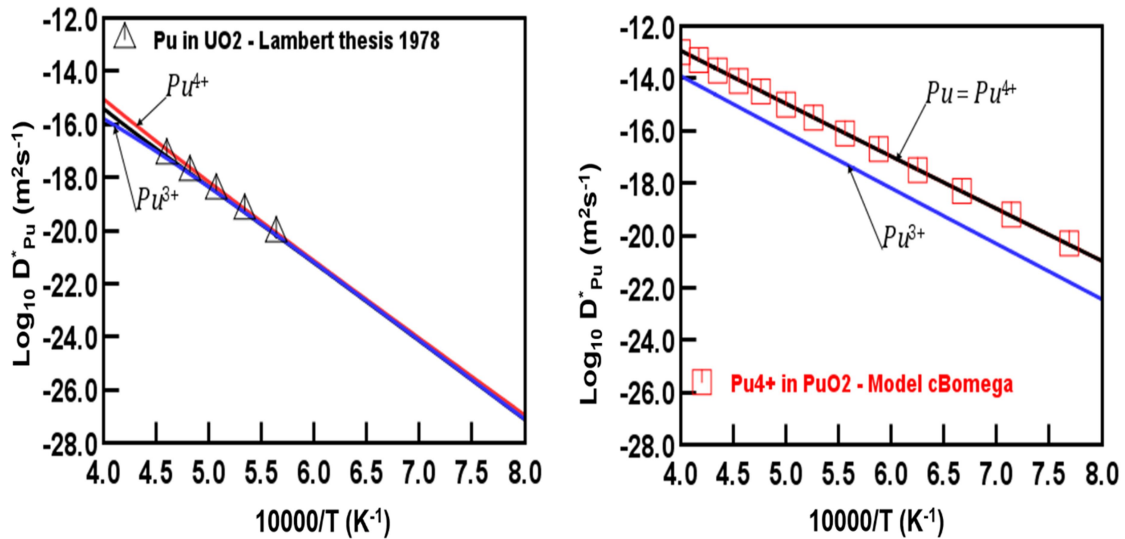


Figure 6.2: Pu, Pu³⁺ and Pu⁴⁺ diffusion coefficient in UO₂ (Left) and in PuO₂ (right).

The figure represents the diffusion coefficient of Pu (or each cation of Pu) as a function of the inverse of temperature. Therefore, the slope of the figure represents the activation energy of the Pu diffusion. In case of the Pu diffusion in UO₂, the diffusion coefficient of Pu calculated by this model is in agreement with the experimental data of Lambert [1]. The diffusion coefficient of Pu is an aggregation of the diffusion coefficient of Pu³⁺ and the diffusion coefficient of Pu⁴⁺ (as per the equation 5.12). In case of lower temperature, both the value of Pu³⁺ and Pu⁴⁺ diffusion coefficients are the same. In the higher temperature a minute deviation in the value of Pu³⁺ and Pu⁴⁺ diffusion coefficient can be observed.

On the other hand, the Pu⁴⁺ diffusion in PuO₂ (calculated by our model) is in agreement with the results of cBΩ model (also calculated under the scope of this work). As mentioned in the chapter – 5, the activation energy of diffusion of Pu³⁺ in PuO₂ is analytically calculated by considering the ratio of the ionic radius of Pu³⁺ and Pu⁴⁺. However, the diffusion coefficient results obtained using this activation energy (for Pu³⁺) reports a significant deviation from that of Pu⁴⁺.

At a fixed temperature, the diffusion rate of Pu in UO₂ is always less than the diffusion rate of Pu in PuO₂. It can be explained by the higher equilibrium oxygen partial pressure of the PuO₂ than the one

of UO_2 . It is known that the partial pressure of oxygen in PuO_2 is higher than that of the UO_2 at a fixed temperature [2].

It is evident that the partial pressure of oxygen influences the oxygen and vacancy concentrations of second and third sublattice [3] which finally effects in influencing both the mobility prefactor and activation energy of Pu (as per the equations 5.13 and 5.14). Hence, it can be concluded that the higher partial pressure of oxygen is the reason for higher diffusion coefficient of Pu in plutonia than that of urania.

In the figure 6.3 the plutonium diffusion in both urania and plutonia are reported with respect to the deviation of stoichiometric ratio in the system. The figure reports not only the Pu diffusion but also the diffusion of Pu^{3+} and Pu^{4+} . As mentioned before, the Pu diffusion is an aggregation of the Pu^{3+} diffusion and Pu^{4+} diffusion. It can be observed in figure 6.3 as well.

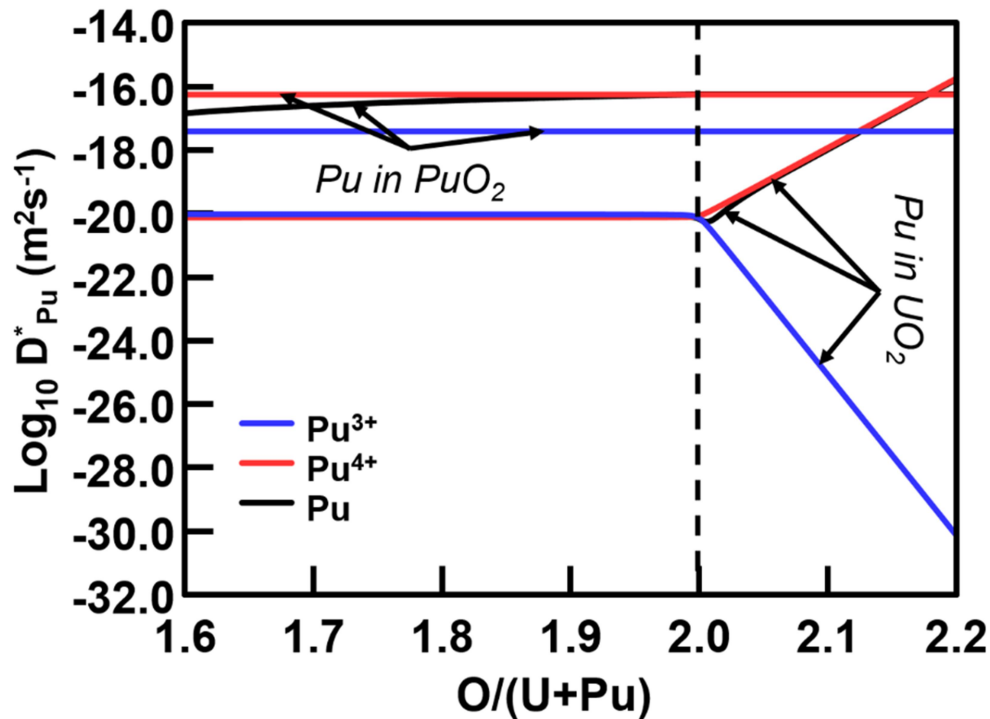


Figure 6.3: Pu, Pu^{3+} and Pu^{4+} diffusion in urania and plutonia with respect to the stoichiometric ratio, at 1773 K.

The Pu diffusion in UO_{2-x} has no variation with the change of the stoichiometry because the mobility parameters of either Pu^{3+} or Pu^{4+} do not vary with the change of uranium cations (either U^{3+} or U^{4+}). The Pu^{4+} diffusion coefficient is lower than the Pu^{3+} coefficient in UO_{2-x} (with a very small deviation). It has been already understood in the previous section that the Pu^{3+} is more mobile in UO_{2-x} than that of Pu^{4+} in UO_{2-x} .

On the other hand, the Pu^{4+} diffusion (as well as the Pu diffusion) in UO_{2+x} increases gradually. Whereas, the Pu^{3+} diffusion in UO_{2+x} decreases gradually. Hence, the Pu diffusion reached its minimum value at the stoichiometry of $O/M \sim 2.00$. The concentration of U^{5+} increases in the UO_{2+x} gradually. As discussed in the previous section, the mobility of Pu^{4+} is high in the presence of U^{5+} (if compared to the presence of U^{4+} or U^{3+}) which explains the gradual increase of Pu^{4+} diffusion followed by the Pu diffusion in UO_{2+x} . Similarly, the mobility of Pu^{3+} is lower in the presence U^{5+} (than the Pu^{3+} mobility in the presence of U^{3+} or U^{4+}).

The Pu diffusion in hyper stoichiometric plutonia is reported in the figure 6.3. It has been already pointed out that plutonia does not possess a hyper-stoichiometric regime (as discussed in chapter – 2). Therefore, the results noted for the hyper-stoichiometric plutonia in the figure is purely an extrapolation and need not be considered in the discussion.

The Pu^{4+} diffusion is higher in PuO_{2-x} than the Pu^{3+} diffusion in PuO_{2-x} . The diffusion of Pu^{4+} (or Pu^{3+}) does not vary with the variation of stoichiometry as the mobility parameters are set to be same in the presence of any of the three plutonium cations, Pu^{3+} , Pu^{4+} and Pu^{5+} (as mentioned in section 6.2). However, with the decrease of stoichiometry, the Pu^{3+} concentration increases. This increase of the Pu^{3+} concentration then causes the decrease overall Pu diffusion with the decrease of stoichiometry (as Pu diffusion is an aggregation of Pu^{3+} diffusion and Pu^{4+} diffusion).

6.4. Pu diffusion in $(U, Pu)O_{2\pm x}$:

This section presents the calculated results of plutonium diffusion in MO_x with different plutonium contents. These results are compared with the selected experimental data of plutonium diffusion available in literature. These experimental data are already discussed in the chapter – 3.

The Figure – 6.4 represents the plutonium diffusion in $U_{0.85}Pu_{0.15}O_{2\pm x}$ (left) and in $U_{0.82}Pu_{0.18}O_{2\pm x}$ (right). The results are compared with the experimental measurements of Riemer & Scherff [4] and Matzke [5].

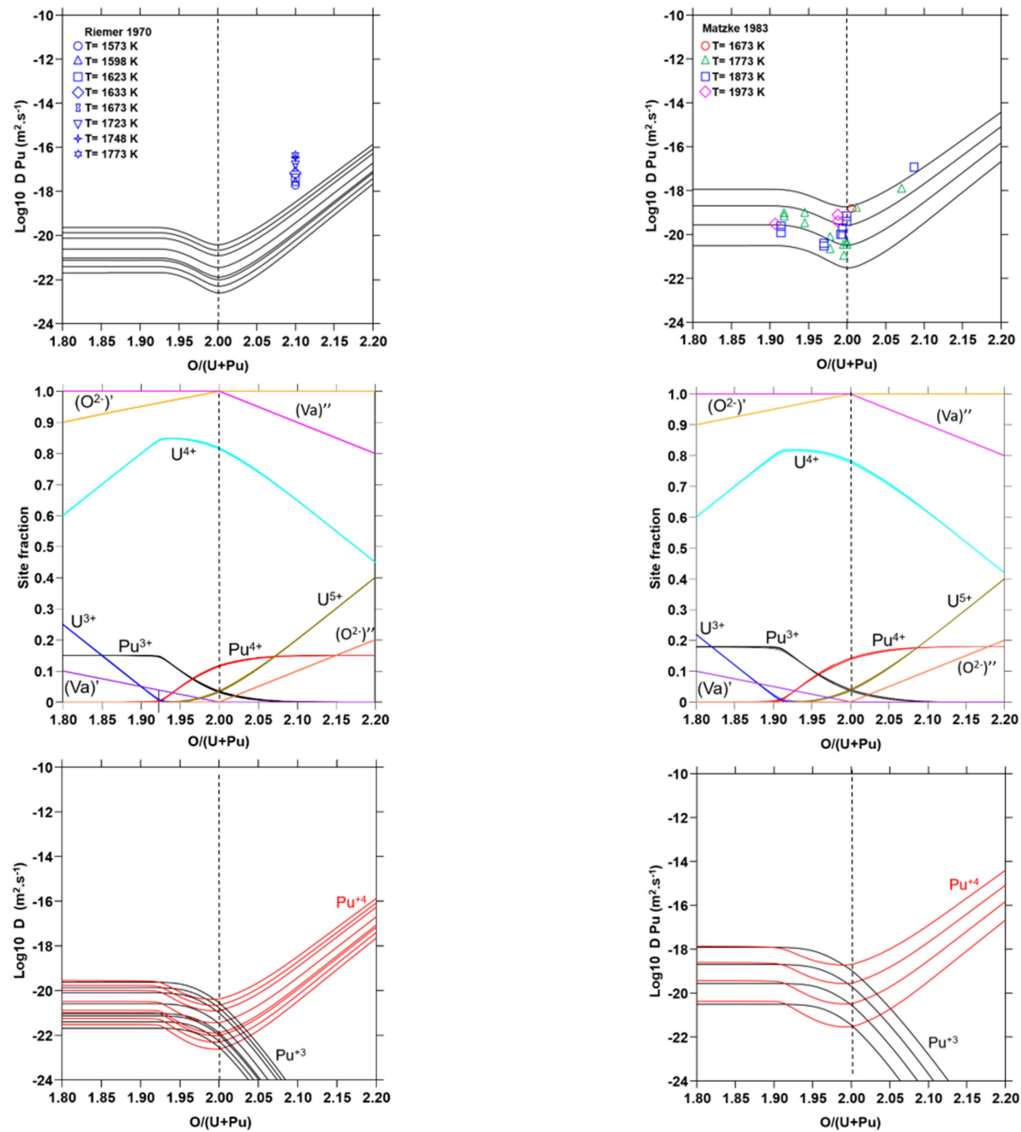


Figure 6.4: Plutonium diffusion in $U_{0.85}Pu_{0.15}O_{2\pm x}$ (left) and in $U_{0.82}Pu_{0.18}O_{2\pm x}$ (right)[6].

In the figure 6.4, the respective species concentration map (calculated with the thermodynamic CALPHAD model of Moore [7]) is also included. The figure also reports the diffusion coefficient of Pu^{3+} cation and Pu^{4+} cation separately.

Similarly, the figure 6.5 represents the Pu diffusion coefficient calculated by this model in $\text{U}_{0.8}\text{Pu}_{0.2}\text{O}_{2\pm x}$ and in $\text{U}_{0.55}\text{Pu}_{0.45}\text{O}_{2\pm x}$. The experimental results of Lambert [1] (for $\text{U}_{0.8}\text{Pu}_{0.2}\text{O}_{2\pm x}$) and of Noyau [8] (for $\text{U}_{0.55}\text{Pu}_{0.45}\text{O}_{2-x}$) are also compared with the calculated results. The respective species concentration maps are also reported. The diffusion coefficients of Pu^{3+} cation and Pu^{4+} cation are noted separately in this figure too.

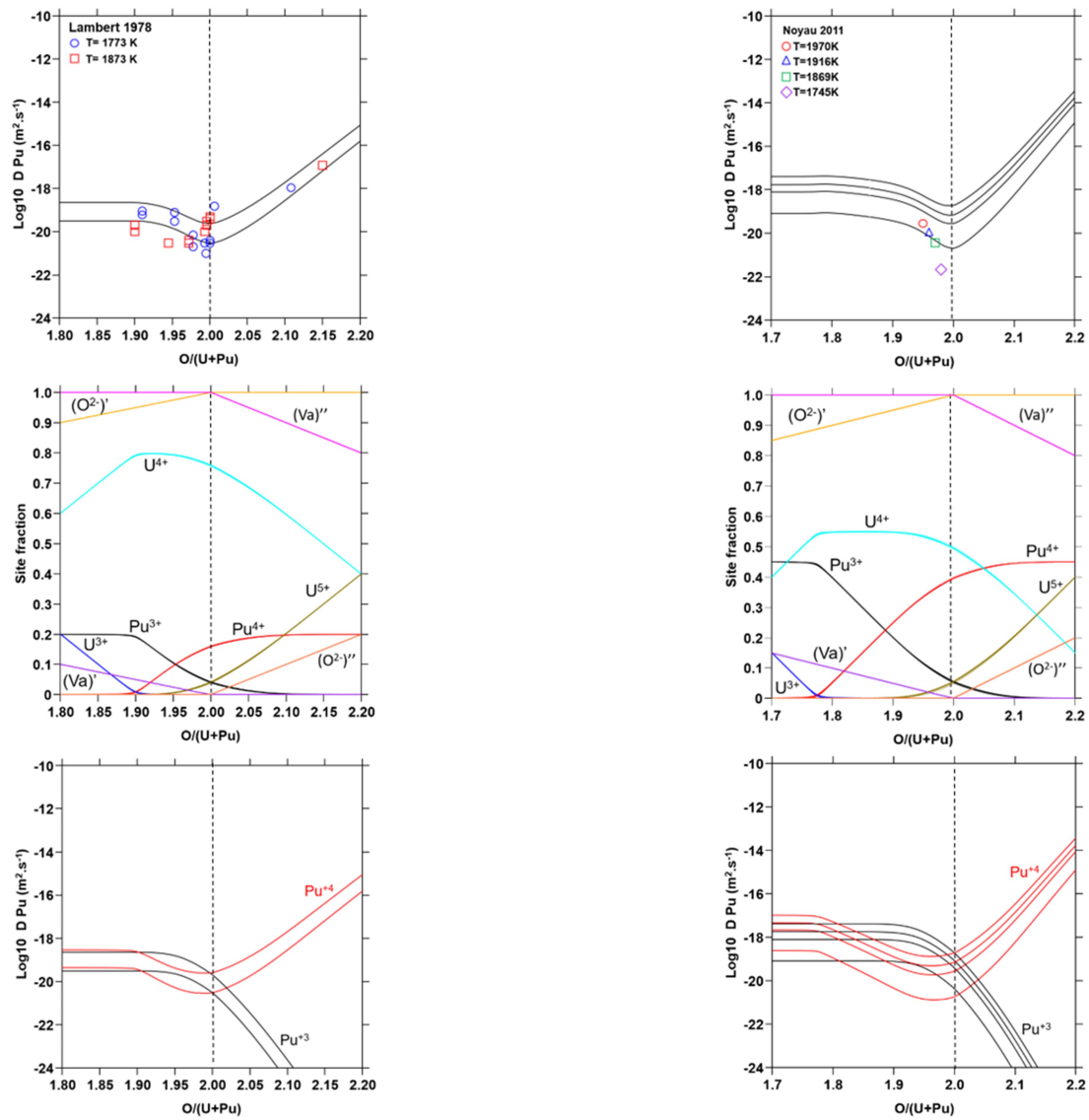


Figure 6.5: The Plutonium diffusion in $\text{U}_{0.8}\text{Pu}_{0.2}\text{O}_{2\pm x}$ (left) and in $\text{U}_{0.55}\text{Pu}_{0.45}\text{O}_{2\pm x}$ (right)[6].

From figure 6.4, it is evident that the experimental data of Pu diffusion in $U_{0.85}Pu_{0.15}O_{2.10}$ is not in accordance to the calculated diffusion coefficient in the hyper-stoichiometric mixed oxide. The Pu diffusion coefficient calculated using the model is in agreement with the experimental results in MOx with 18% Pu content [5] and 20% Pu content [1] for O/M higher than 2.00.

Therefore, one possible explanation for the disagreement between the calculated results and the data of Riemer [4] can be the inconsistency of the Riemer's data with the data of Lambert [1] and Matzke [5] as evidenced by the figure 3.6 of chapter – 3.

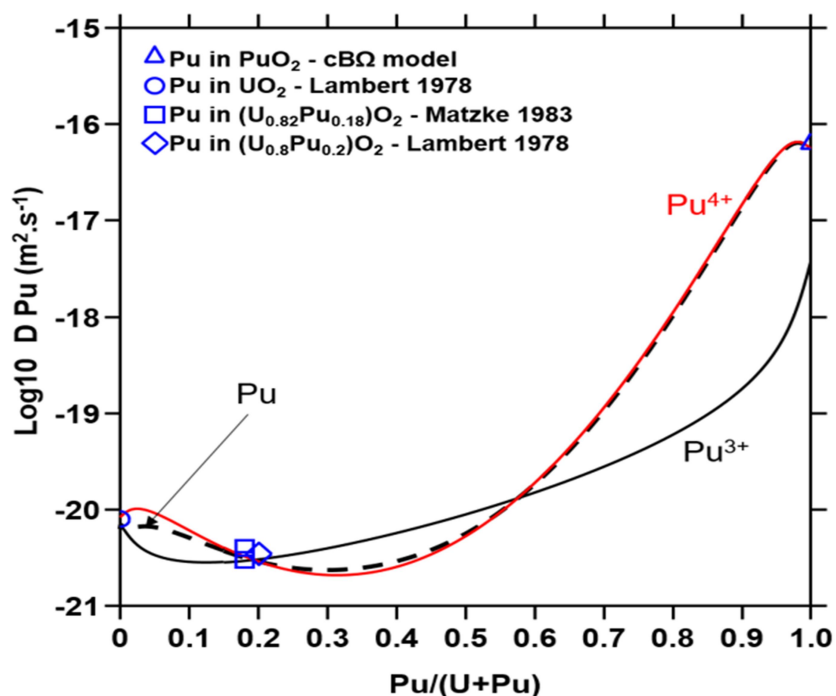


Figure 6.6: Pu, Pu³⁺ and Pu⁴⁺ diffusion in UO₂-PuO₂ for exact stoichiometry at 1773 K.

The over-estimation of the calculated data with respect to the results of Noyau is very evident in the figure 6.5. The results of Noyau also show a significant deprivation with respect to the results of Lambert [1] and Matzke [5], as shown in the figure 3.5. Therefore, in this study, we could not reach a better agreement with the results of Noyau. The disagreement is around two orders of magnitude.

The shape of the curve is well produced (as per figure 3.3) with our model. The minimum of the curve (for diffusion coefficient of Pu) is calculated at O/M~2. In literature it has been reported to exist at O/M~1.98 at $U_{0.82}Pu_{0.18}O_{2\pm x}$ [5]. The shift of the minimum towards O/M~2.00 is though noted in the Pu diffusion of MOx, the minimum diffusion coefficient of Pu⁴⁺ is noted at O/M~1.98. Therefore, the over-weightage given to Pu³⁺ diffusion in the stoichiometric ratio near 2.00 can be the possible explanation of this discrepancy.

The peculiar shift of minimum diffusion coefficient towards hypo-stoichiometry with the increase of temperature (as reported by Matzke [5]) could not be produced with this model as well. The reason can be the simplicity of the model as the model takes into account neither the metal vacancy nor the metal interstitial. However, similar phenomenon in iron oxide was successfully modelled using DICTRA code as well [10].

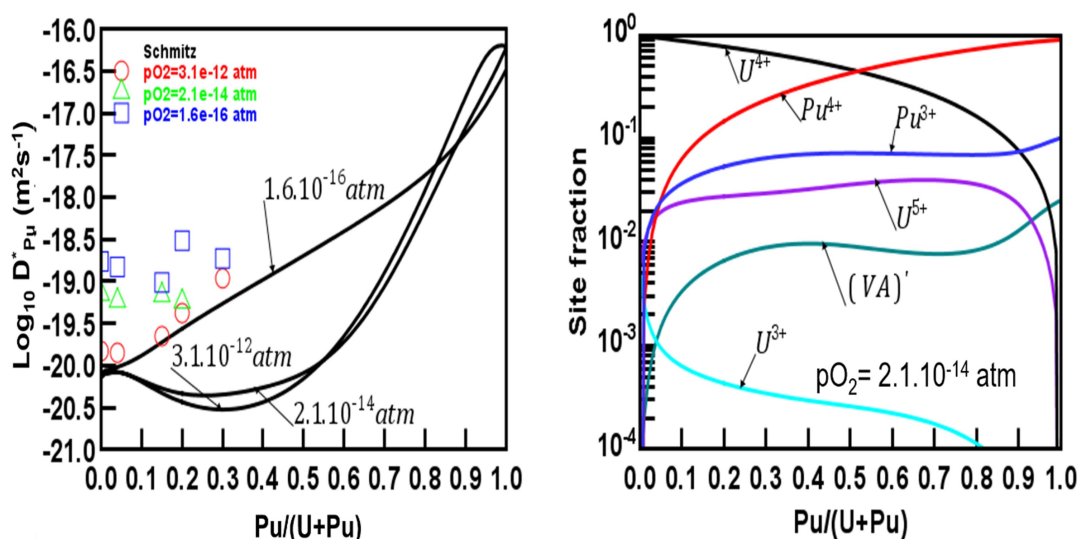


Figure 6.7: Pu diffusion in non-stoichiometric MOx with respect to the plutonium content at 1783 K (left). The respective stoichiometry for the $p\text{O}_2$ of $1.6 \cdot 10^{-16} \text{ atm}$, $2.1 \cdot 10^{-14} \text{ atm}$ and $3.1 \cdot 10^{-12} \text{ atm}$ are 1.99 (for urania) – 1.73 (for plutonia), 2.00 (for urania) – 1.95 (for plutonia) and 2.00 (for urania) – 1.98 (for plutonia). The site fraction of the species of MOx at $p\text{O}_2 = 2.1 \cdot 10^{-14} \text{ atm}$ and 1783 K (right). The experimental data are from [9].

We overall may divide the behavior of the diffusion coefficient in three distinct region, according to the relative contribution of Pu^{3+} and Pu^{4+} ;

- For low O/M ratio below ~ 1.9 (1.93 for 15% Pu content, 1.78 for 45 % Pu content), the Pu diffusion coefficient displays a plateau as suggested in the literature [1][5], where the mobility of Pu^{4+} and Pu^{3+} are constant with very close values. The existence of this plateau depends on the Pu^{3+} contribution that remains constant in this region, followed by a complete reduction of Pu^{4+} into Pu^{3+} .
- For O/M ratio near stoichiometric line which is ranged from $\text{O}/\text{M} \sim 1.9$ (1.93 for 15% Pu content, 1.78 for 45 % Pu content) and $\text{O}/\text{M} = 2.00$, the Pu diffusion coefficient decreases with the increase of O/M ratio due to significant decrease of Pu^{3+} diffusion rate. Pu diffusion exhibits a minimum value at a O/M ratio very close to 2 where the Pu^{4+} and Pu^{3+} mobilities are equal but Pu^{4+} diffusion coefficient exhibits a minimum at about $\text{O}/\text{M} = 1.98$ (and 1.97 for 45 % Pu content). The defect model is able to explain this variation: in this

region, Pu^{3+} diffuses faster than the Pu^{4+} . However, with the increase of stoichiometric ratio, fraction Pu^{3+} decreases up to a low value at $\text{O}/\text{M}=2$ whereas Pu^{4+} fraction increases.

- For O/M higher than 2, Pu^{4+} emerges as the major diffusing species, consistent with the thermodynamic model. The Pu diffusion coefficient increases with the O/M ratio.

We now turn to the Pu diffusion coefficient against $\text{Pu}/(\text{U}+\text{Pu})$ ratio as reported in figure 6.6. The figure reports the calculated Pu diffusion coefficient at the exact oxygen stoichiometry 2.00 at 1773 K. These results are compared with the available experimental data in UO_2 [1] and in MOx [1, 5]. The result at PuO_2 is also compared with the obtained result from $\text{cB}\Omega$ model (this work).

The figure 6.7 represents the calculated data for Pu diffusion at non-stoichiometric MOx with oxygen partial pressure of $3.1 \cdot 10^{-12}$ atm, $2.1 \cdot 10^{-14}$ atm and $1.6 \cdot 10^{-16}$ atm, at 1783 K. The results are compared with the experimental measurements of Schmitz and Marjofsky (up to 30% Pu MOx) [9].

The diffusion coefficient exhibits a U-shape in both figure 6.6 and 6.7, with a minimum at around 30% of plutonium in MOx , except one at $1.6 \cdot 10^{-16}$ atm. This U-shape with a minimum at $\sim 30\%$ MOx can be explained using the figure 6.7 (right) where we can observe that the concentration of U^{3+} reduces rapidly with the increase of plutonium content in the system. We already have discussed that the mobility of Pu^{3+} is significantly higher in the presence of U^{4+} and U^{3+} at first sublattice than the presence of U^{5+} at the first sublattice. So, the rapid decrease of U^{3+} concentration and a constant presence of U^{5+} reduces the overall Pu^{3+} mobility (hence the diffusion) and attains a minimum of diffusion rate at around 30% of Pu. But with further increase of plutonium content, the effect of Pu^{4+} diffusion becomes a major contributor and compensates for the reduction of Pu^{3+} diffusion. Eventually the Plutonium diffusion attains a higher value in pure plutonia than in the pure urania.

The Pu diffusion in MOx with $p\text{O}_2 = 1.6 \cdot 10^{-16}$ atm, at 1783 K shows a linear increase from UO_2 to PuO_2 . The explanation could be very low stoichiometry of the system. The stoichiometric ratio of urania is 1.99 and the stoichiometric ratio of plutonia is 1.73 at this partial pressure and temperature (as calculated by the thermodynamic model of Moore [7]). Hence, the stoichiometric ratio is very low compared to the other two conditions (as shown in the figure 2.6). In this very low stoichiometric ratio, the concentration of U^{3+} is significantly high and the variation is less (as the oxide is highly reduced). Therefore, the U-shaped variation of plutonium diffusion coefficient is not visible in this case.

The experimental data of both Lambert [1] and Matzke [5] are in accordance with the calculated results of this model. However, the results of calculation are under-estimated compared to the experimental data of Schmitz [9]. The results of Schmitz are already compared with the results of Matzke and Lambert [1, 5] in chapter – 3. The results of Schmitz are higher than that of Lambert and Matzke [1, 5]. This explains the reason behind the under estimation of Pu diffusion from our model with respect to the data of Schmitz et al [9].

6.5. Activation energy and prefactor of Pu diffusion:

We finally calculate the activation energy and prefactor of Pu diffusion in UO_2 , PuO_2 and $(\text{U, Pu})\text{O}_{2\pm x}$, in this section. The results are also compared with the estimations in literature. These results are reported in the table 6.2.

Compounds	Q_{act} (eV) DICTRA	Q_{act} (eV) exp. or calc.	D_0 (m^2s^{-1}) DICTRA	D_0 (m^2s^{-1}) exp. or calc.	Reference
PuO_2	4.0	4.0	$1.1 \cdot 10^{-5}$	$1.2 \cdot 10^{-5}$	cBΩ (This work)
UO_2	5.8	5.6	$1.9 \cdot 10^{-4}$	$6.5 \cdot 10^{-5}$	Lambert [1]
$(\text{U}_{0.85}\text{Pu}_{0.15})\text{O}_{2+x}$	5.5	3.8	$1.4 \cdot 10^{-3}$	$2.5 \cdot 10^{-6}$	Riemer [4]
$(\text{U}_{0.80}\text{Pu}_{0.20})\text{O}_{2\pm x}$	5.6 (O/M=1.9)	5.7 (I_{Pu}) [#]	$2.5 \cdot 10^{-4}$	-	Matzke [5]
	5.9 (O/M)=2	8.8 (S) [#]	$1.6 \cdot 10^{-4}$		
	5.5 (O/M=2.1)	3 (V_{Pu}) [#]	$1.9 \cdot 10^{-3}$		
$(\text{U}_{0.75}\text{Pu}_{0.25})\text{O}_2$	5.8	4.90 – 5.48* (V_{Pu}) 4.01** (I_{Pu})	$7.8 \cdot 10^{-5}$	-	Cheik Njifon [11]
$(\text{U}_{0.55}\text{Pu}_{0.45})\text{O}_{2-x}$	5.5	6.48	$1.7 \cdot 10^{-5}$	$1.1 \cdot 10^{-3}$	Noyau [8]

Table 6.2: Activation energy and Prefactor of Pu diffusion;

#This data is extracted from the figure 13 of the article [5].

*The migration energy is calculated for both neutral and formal charged Pu vacancy. The activation energy of the corresponding migration energies are 8.47 – 7.45 eV.

**The migration energy is calculated for neutral Pu interstitial. The corresponding activation energy is 11.2 eV.

The activation energy and prefactor of Pu diffusion in UO_2 , calculated from this model, are in accordance to the experimental results [1]. The same results of Pu diffusion in PuO_2 are compared with the cBΩ model. The results are in agreement to each other.

The activation energy of Pu diffusion in $\text{U}_{0.85}\text{Pu}_{0.15}\text{O}_{2+x}$ is over-estimated with our model than the estimation of Riemer [4]. The prefactor calculated with our model is also over-estimated from the data of Riemer [4]. The discrepancy of the diffusion coefficient calculated by our model and the value of Riemer has already been discussed in the previous section.

The activation energy deduced by Matzke [5] is in agreement with the results of our model for $O/M < 2.00$. However, the activation energy calculated by our model at stoichiometry $O/M = 2.00$ is an underestimation than that of Matzke. Similarly, the activation energy in hyper stoichiometry is again overestimated with our model. The highest activation energy is still at the perfect stoichiometry even with our model, similar to the results of Matzke.

The results calculated by the DFT computation (the results of Cheik Njifon) are calculated at 0 K with perfect crystal (having no defects) [11]. Therefore, the activation energy includes both the formation and migration energy of defects. Hence, the activation energy results are higher by a factor of two than the results we computed with our model but the migration energy results are in accordance to our computational results. The last results of the activation energy at $\text{U}_{0.55}\text{Pu}_{0.45}\text{O}_{2-x}$ are well fitted with the

results of our model. Although the prefactor is over estimated with our model, compared to the results of Noyau [7].

The results from our model are relevant, with comparison to the literature available, in the hypo-stoichiometric regime. Our model is too simple to describe the complexity of hyper-stoichiometry and would require the introduction of metal vacancy or oxygen cluster in order to explain the diffusion phenomenon in the hyper-stoichiometric region.

Considering this issue, we present a full thermo-kinetic model of plutonium diffusion in MO_x, for the first time for any plutonium content, stoichiometry or system temperature. In the next section we will discuss the variation of the diffusion coefficient with the variation of different system conditions, as predicted by our model.

6.6. Effect of temperature, plutonium content and stoichiometry on Pu diffusion:

In this section we will discuss the variation of the diffusion coefficient of plutonium with respect to the plutonium content and temperature, primarily, as predicted by our model. The data of the figure 6.8 and 6.9 are given in the Appendix – A.3.

6.6.1. Effect of temperature and stoichiometry:

In the figure 6.8, the diffusion coefficient of plutonium in $U_{0.8}Pu_{0.2}O_{2\pm x}$ is reported with the variation of stoichiometric ratio and the system temperature. The upper and lower boundaries of the phase (fluorite phase) are reported in the figure. The perfect stoichiometric ratio ($O/M=2.00$) is also denoted in the figure.

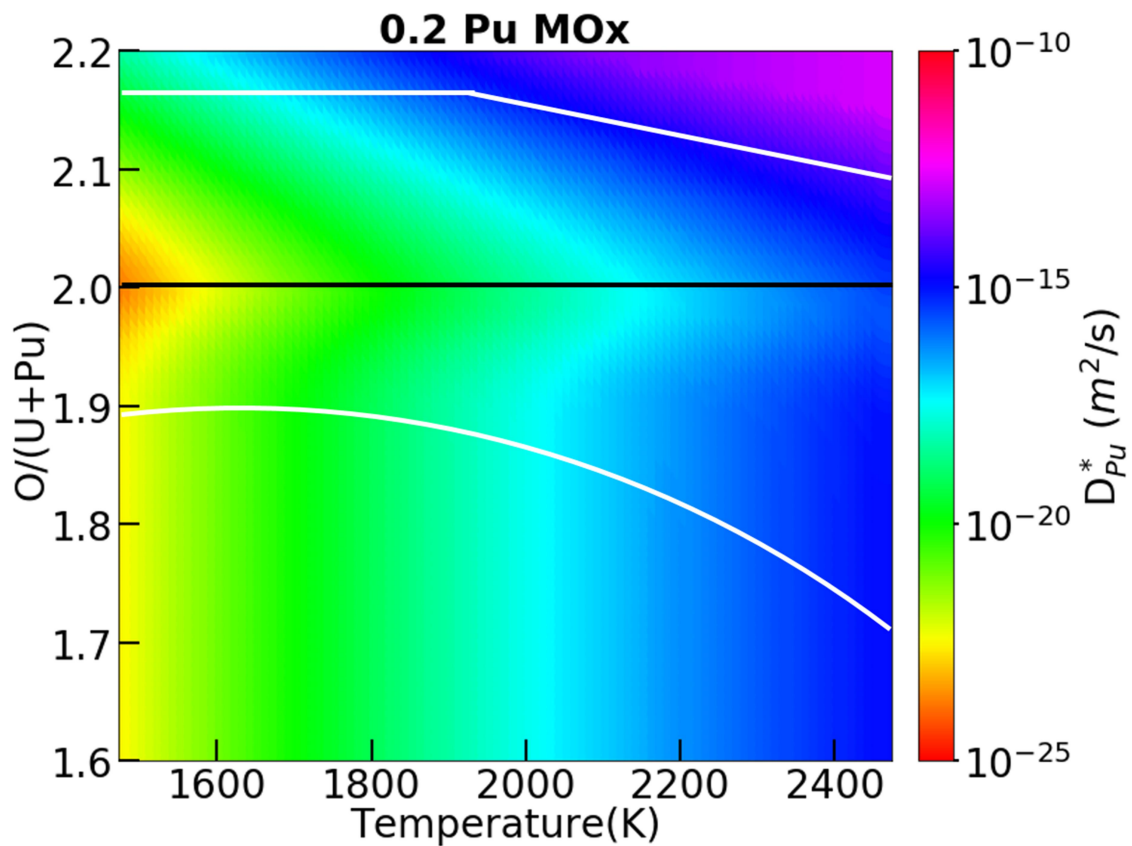


Figure 6.8: Pu diffusion variation with respect to temperature and stoichiometric ratio in $U_{0.8}Pu_{0.2}O_{2\pm x}$. White solid lines represent the phase boundaries of fluorite phase. Black solid line represents $O/M=2.00$.

The diffusion coefficient of plutonium rapidly increases with the increment of temperature (at a fixed stoichiometry) for both hypo and hyper stoichiometric MOx. The diffusion coefficient at a fixed temperature is always found to be minimum at $O/M= 2.00$. It does not correspond to the results of

previous studies [5]. However, it has been discussed that with our simplistic model, the variation of the positioning of plutonium diffusion coefficient with respect to temperature could not be reproduced. Although, the value of minimum diffusion coefficient increases with the increase of temperature, as the increase of temperature causes the increase of defect concentration in the system.

At a fixed temperature, the Pu diffusion coefficient varies more rapidly in hyper-stoichiometric MO_x than in hypo-stoichiometric MO_x, with respect to its stoichiometric ratio. Overall, the plutonium diffusion coefficient increases with increase of both stoichiometric deviation (deviation from O/M= 2.00) and system temperature, in both hypo and hyper stoichiometric MO_x.

6.6.2. Effect of plutonium content and stoichiometry:

In the figure 6.9, the coefficient of plutonium diffusion is reported with the variation of both stoichiometric ratio and plutonium content. These results are calculated at the temperature of 1773 K. The upper and lower boundary of the phase (fluorite phase) is reported which is already discussed in chapter- 2. The perfect stoichiometric ratio (O/M=2.00) is also denoted in the figure.

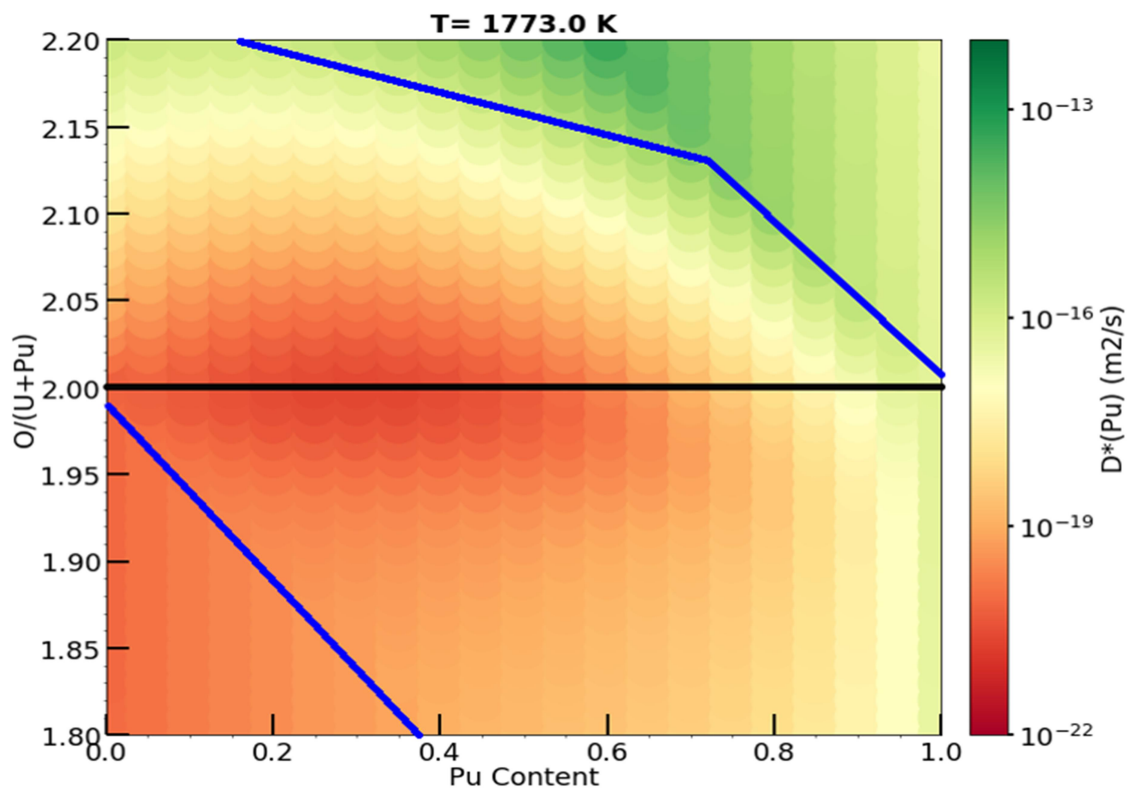


Figure 6.9: Pu diffusion variation with respect to plutonium content and stoichiometric ratio at 1773 K. Blue solid lines represent the phase boundary of fluorite phase. Black solid line represents O/M=2.00.

The results in the figure reports that the plutonium diffusion increases with the increase of plutonium content at a fixed stoichiometry in the hypo stoichiometric MOx. From the stoichiometric line, the diffusion coefficient increases with the decrease of stoichiometry at a fixed plutonium content, in the hypo-stoichiometric MOx. The plutonium diffusion coefficient does not vary significantly in hypo stoichiometric MOx with $O/M < 1.9$ and at a plutonium content ranging from 20% to 80%. However, the diffusion coefficient in hypo-stoichiometric MOx with $O/M > 1.9$ varies drastically with the change of stoichiometric ratio. In that range of stoichiometric ratio ($1.9 < O/M < 2.00$), the variation of Pu diffusion is not significant with respect to plutonium content up to 70% of plutonium in MOx. On contrary, in the hypo-stoichiometric MOx with Pu content more than 80%, the diffusion coefficient does not vary with the variation of stoichiometry at a fixed plutonium content, though the variation of diffusion coefficient with plutonium content, at a fixed stoichiometry, is significant.

In the hyper stoichiometric MOx with up to $O/M < 2.05$, the diffusion coefficient variation with the plutonium content (up to a plutonium content of 60%) is not significant, at a fixed stoichiometric ratio. In the hyper stoichiometry with $O/M > 2.05$, the diffusion coefficient rapidly increases with the increase of stoichiometric ratio, at a fixed plutonium content.

Reference:

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CHAPTER - VII

CONCLUSION AND PERSPECTIVE

This chapter summarises the work done under the scope of this thesis. The conclusive remarks are made based on the detailed study of both $cB\Omega$ model and the DICTRA-based plutonium diffusion model for $(U,Pu)O_2$ mixed oxide. The strengths and limitations of the models are highlighted. Finally, possible future developments of this work are proposed.

As mentioned before, the mixed oxide of uranium and plutonium $(U,Pu)O_{2\pm x}$ (MOx) is the fuel for the Sodium-cooled Fast Reactor (SFR) and some of the thermal Pressurized Water Reactors (PWR). One of the most important aspect of synthesis of MOx fuel is the controlled microstructure, desired plutonium content, oxygen stoichiometry and good homogeneity. In SFR reactors, the high thermal gradient experienced by the MOx pellet during the reactor operation causes the plutonium redistribution in the fuel pellet and leads to the formation of a central void. Therefore, a reliable thermo-kinetic understanding of the MOx fuel is important to both optimize the synthesis process and predict the in-pile behavior of the fuel. The aim of this work is the development of a mobility based diffusion model for the plutonium diffusion in mixed oxide of uranium and plutonium, using DICTRA code.

Existing diffusion models consider the point defect model to describe the thermodynamic aspect of the system. However, the application of CALPHAD approach and the possibility of combining both thermodynamic database and mobility database makes it possible to develop a model on both thermodynamic and kinetic properties. The previous works includes the development of the thermodynamic CALPHAD model by Guéneau et al (described in Chapter 2) and the oxygen mobility-based diffusion model in $(U, Pu)O_2$ by Moore et al.

In order to approach the modelling, we first analyzed the experimental data of plutonium diffusion and selected few of the data based on their self-consistency and reliability. We realized that there is no data for the plutonium diffusion in plutonium dioxide. Therefore, we applied the $cB\Omega$ model to determine the plutonium diffusion in PuO_2 . Using the selected experimental data and the results of $cB\Omega$ model, we then constructed a mobility database to develop the diffusion model with the DICTRA code.

A critical analysis of the existing literature data has been performed first, starting with the analysis of Pu diffusion in UO_2 and PuO_2 . This analysis enables us to point out that there is no data available for the plutonium diffusion in plutonium dioxide. Even the data available for the plutonium diffusion in mixed oxide are in the range of less than 45% plutonium content. Moreover the available experimental data in mixed oxide are not consistent. This inconsistency of the data are discussed in details in chapter – 3. The incoherent data causes the difficulty of selecting data for the mobility database. Hence, we have compared all the data based on different parameters, i.e. partial pressure of oxygen, plutonium content, and stoichiometric ratio. We have selected the data which are free from the grain boundary effect and coherent with the diffusion in single-crystalline mixed oxide.

The data of plutonium diffusion in plutonium dioxide is required in order to deduce the mobility parameter in mixed oxide with higher plutonium content. Therefore, we have used another diffusion

model – ‘cBΩ’ model (as discussed in Chapter – 4). The cBΩ model has already been applied in order to calculate the oxygen diffusion in transactinium binary oxides. To our knowledge, the use of this model to compute the metal diffusion in binary oxides has never yet been attempted.

The application of cBΩ model is based on the fit of a single parameter, c . The parameter can be fitted with even a single set of experimental data. The model is applied to determine the metal diffusion coefficients of UO₂ and ThO₂. The crystal structure of Li₂O is similar to the fluorite crystal except the lithium cations are arranged in a cube around an oxygen anion (anti-fluorite). Therefore, the diffusion of oxygen in Li₂O is also determined using the cBΩ model. In order to apply such model, the analysis of the experimental diffusion coefficient from the literature is essential but not enough. The analysis of other properties such as, lattice parameter, bulk modulus, Debye frequency etc. is required for these binary compounds. Based on this analysis the data are selected as an input for the model. The diffusion coefficients are computed with the variation of temperature.

The values of the fitted parameter c are posed into a linear relation to the ionic radius of diffusing ions and a linear fit is then deduced between the value of c and the ionic radius of the diffusing species. This linear relation is the key to extrapolate the diffusion coefficient of plutonium in PuO₂. The other properties of plutonium dioxide are then analyzed and the relevant value of c for plutonium diffusion in PuO₂ is extrapolated. It had led us to the first set of plutonium diffusion coefficient data in plutonium dioxide. As mentioned before, there is no plutonium diffusion coefficient data in PuO₂ available to verify our results however the activation energy of plutonium diffusion in PuO₂ was experimentally deduced before (which is mentioned in chapter – 3). Both the activation energies from literature and our calculations are in agreement.

The use of cBΩ model combined with the linear fit between c and ionic radius is a robust tool for calculations of diffusion data in such binary oxides with fluorite structure where data is not available at all. Therefore, the tool has been utilized in our work to extrapolate the metal diffusion in ceria and other minor actinide oxides (PaO₂, NpO₂, AmO₂, CmO₂, BkO₂ and CfO₂). In most of these cases, there is no available diffusion data. However, the activation energy of metal diffusion is available in CeO₂ and AmO₂. The activation energies calculated from our model are also in agreement with the activation energies coming from literature.

With the successful implementation of cBΩ model in order to compute the plutonium diffusion in PuO₂, and using the selected experimental data of Pu diffusion coefficient in UO₂ and (U, Pu)O₂, the mobility database has been finalized and the mobility parameters have been assessed. The assessment technique and the results are discussed in details in chapter – 5 and chapter – 6.

In the DICTRA-based model, the plutonium mobility is described as the linear combination of Pu³⁺ mobility and Pu⁴⁺ mobility. With the Compound Energy Formalism, also used for the thermodynamic

CALPHAD model, the mobility parameters of Pu^{3+} and Pu^{4+} are described in each end-member of the sublattice model (described in chapter – 2) containing a single cation in the first sublattice. The Pu mobility is then the combination of all the end-member parameters. Each end-member parameter has an effect on the variation of the plutonium cation mobility (either Pu^{3+} or Pu^{4+}) with the oxygen to metal ratio and plutonium content.

Due to incorporation of the effects of each end-members, the number of mobility parameters for assessment is initially very high (96 parameters). The parameters are reduced to 12 (not considering the interaction parameter) afterwards using reasonable assumptions and relations to decrease the degree of freedom of the model (discussed in chapter – 5). The aggregation of parameters of all the end-members, in the appropriate framework of compound energy formalism deduces the mobility of plutonium ions (either Pu^{3+} or Pu^{4+}).

The first set of mobility parameters are assessed for the plutonium diffusion in UO_2 and PuO_2 . In case of UO_2 , the assessed results are in good agreement with the available experimental data. There is no experimental data available for the case of PuO_2 . Thus, the assessed results are compared with the results of cB Ω model. A good agreement is also obtained.

In the next step, the plutonium mobility in ternary mixed oxide is assessed. The assessment of mobility parameters in UO_2 and PuO_2 makes it possible, through combination, to model the plutonium diffusion in ternary oxide with the addition of an interaction parameter. The description of the plutonium mobility in ternary oxide requires the assessment of an interaction term between U^{4+} and Pu^{4+} to be able to well reproduce the experimental data for mixed oxides with different plutonium contents and O/M=2. With this interaction term included in the exponential of mobility term, the activation energy of mobility is adjusted with the change in the plutonium composition. The magnitude of the interaction term indicates that an important interaction between U^{4+} and Pu^{4+} takes place in the first sublattice. As reported in the literature, the diffusion mechanism of plutonium is certainly impacted by the formation of cluster in mixed oxide. However, the effect of cluster formation is not taken into account in our model.

The mobility of each of Pu^{3+} and Pu^{4+} varies with the variation of uranium cation in first sublattice and oxygen defects in second and third sublattices (as the model considers the effect of each end-member). This variation of mobility helps to accommodate not only the change of plutonium content and temperature but also the oxygen stoichiometry of the system. This is one advantage of the model developed with DICTRA code over the cB Ω model.

The overall shape of the plutonium diffusion curve with the variation of oxygen stoichiometry is reproduced with our model. The curve consists of a plateau in hypo-stoichiometric region with O/M < 1.9 (due to the constant mobilities of both Pu^{3+} and Pu^{4+}), a minimum near stoichiometric ratio O/M= 2.00 (due to the synergic change of defects concentration) and a sharp increase in the hyper

stoichiometric region (due to the higher mobility and concentration of Pu^{4+}). A reasonable agreement is found with the calculated data (both in urania and MOx) and the literature data in view of their scarcity and inconsistencies. A comparison between the activation energy and prefactor of Pu diffusion in UO_2 and MOx are also presented for both calculated results and the literature data. Barring few inconsistencies, an overall agreement is also obtained (as discussed in chapter – 6).

The positioning of the minimum diffusion coefficient against oxygen stoichiometry changes with the variation of temperature, as reported in literature. However, our model cannot reproduce this peculiar phenomenon. The lack of consideration of cluster and metal vacancy is the possible reason of this limitation. Therefore, the model could be improved by including the oxygen cluster and the metal interstitials and vacancies. New experimental data of plutonium diffusion especially in PuO_{2-x} and $(\text{U,Pu})\text{O}_{2+x}$ will be very useful for improving the reliability of this model.

Despite the use on other oxides (Fe-O, Cr-O), the DICTRA code is here used for the first time on a ternary oxide system. The current model can calculate the plutonium diffusion in MOx at any temperature, plutonium content and oxygen stoichiometry. This newly developed model of plutonium diffusion is combined with the full CALPHAD model of Guéneau et al and the oxygen diffusion model developed by Moore et al. This is the first full and comprehensive thermo-kinetic model developed for the plutonium diffusion in ternary $(\text{U,Pu})\text{O}_2$ mixed oxide.

The ongoing and future works include the development of a similar model for uranium diffusion in mixed oxide in order to have a full model for the ternary $(\text{U,Pu})\text{O}_2$ oxide. The rarity of the uranium diffusion data in mixed oxide makes it extremely difficult to construct a mobility database. Therefore, further experiments and atomic scale calculations to determine uranium diffusion in mixed oxide will be very useful as well. More experimental data are also needed for plutonium diffusion in mixed oxide as well.

Even the implementation of $\text{cB}\Omega$ model in the non-stoichiometric oxide also can be an interesting step forward which may further be extrapolated into ternary mixed oxide regime. We have tried to implement it in the non-stoichiometric range for UO_2 but it could not be successfully applied.

In parallel, metal vacancies and interstitials could be introduced in the sublattice model to better describe the general shape and variation with temperature of the plutonium diffusion properties.

The current model for $(\text{U, Pu})\text{O}_2$ could be used with the DICTRA code to simulate diffusion couple experiments, reduction/oxidation heat treatments and for the prediction of the oxygen to metal ratio

variation during synthesis process of the fuel. The model could also be applied to model the thermal diffusion phenomenon within the MOx fuel pellet.

In addition, this existing model provides input data to be used in fuel performance codes to describe the plutonium redistribution during reactor operation. The model can also be used in other multiscale modelling to be a reference point for plutonium diffusion. It is indeed of interest to introduce the grain boundary effect in this model because the grain boundary diffusion has a significant impact on the plutonium diffusion in MOx.

The model could be extended by introducing a small amount of americium in the mixed oxide of uranium and plutonium.

Finally this approach combining DICTRA framework and cB Ω model could be applied to other materials and applications.

APPENDIX

A.1. Python Scripts for $cB\Omega$ calculations:

A.1.1. Python script for U diffusion in UO_2 :

```
#!/usr/bin/python
import numpy as numpy
from numpy import poly1d
from scipy import optimize
#####
##Bulk modulus & Lattice parameter##
a0=poly1d([5.45225]) #Lattice parameter at 0K in Angstrom
b0=poly1d([215.4]) #Bulk modulus at 0K in GPa
#####
#Initiation of data
cell=a0
bulk=b0
nu_D=50.4 #Debye Frequency at 0K in THz
#####
cell2=poly1d(numpy.polymul(cell,cell)) #Square of Lattice parameter at 0K
cell3=poly1d(numpy.polymul(cell,cell2)) #Cube of Lattice parameter at 0K
Omega=0.25*cell3 #Mean volume per atom of fcc lattice ( $\Omega_0$ ) at 0K
BOmega=100.*poly1d(numpy.polymul(Omega,bulk)) #product of bulk modulus  $B_0$  and  $\Omega_0$ 
BPrime=numpy.polyder(BOmega)
k=1.38064852 #value of Boltzmann constant in J/K
kb=8.617333262145e-5 #value of Boltzmann constant in eV/K
invkb=1/kb
invk=1/k
fcc=0.78146/60000. #fcc geometric lattice constant
D_0=fcc*nu_D*1e-8*cell2 #product of all the coefficient in prefactor ( $D'_0$ )
#####
#Loading Experimental Data Points from the data file
T, Log10D= numpy.loadtxt(['Matzke']UO2_T_Self-D.data', delimiter=' ', usecols=(0, 1), unpack=True)
#####
LnD= (numpy.log(10))*(Log10D) #Change of the Logarithmic Base for the Diffusion Coefficient
Ln_Coeff= numpy.log(D_0(T)) #Numerical Log of the product of all coefficient
B_Omega=BOmega(T)
lhs_2= (Ln_Coeff/B_Omega) #this term represents  $LnD'_0/B_0\Omega_0$ 
lhs_1= (LnD/B_Omega) #this term represents  $LnD^*/B_0\Omega_0$ 
Y_axis= (lhs_2-lhs_1)
kT= (k*T) #Denominator of the exponential term
X_axis= 1/(kT)
#####
#This function is to fit the parameter c;
def C_finder(X, C):
    return C*X
#####
c_calcul= optimize.curve_fit(C_finder, X_axis, Y_axis) #fitting step using Scipy-Library
c_fit= c_calcul[0][0] #Generating the value of c
numpy.savetxt('C_fitted_Value.txt', c_calcul) #Saving the value of c in an external file
#####
# Generate Diffusion coefficient with fitted c
C_fit=c_fit
T=numpy.arange(1000,3000,100) #Initiation of system temperature
invT=1/T*10000.
invkT=1/(T*8.617333262145e-5)
kT= (k*T) #Denominator of the exponential term
Q=-C_fit*BOmega(T)*invkbT #exponential term of  $cB\Omega$  equation
Log_D=(numpy.log(D_0(T))+Q)/numpy.log(10.)
Ln_D=numpy.log(D_0(T))+Q
# Output the results in an external file
numpy.savetxt('Out.txt',numpy.column_stack([T,invT,Log_D,invkT,Ln_D]), delimiter=' ')
```

A.1.2. Python Script for Th diffusion in ThO₂:

```
#!/usr/bin/python
import numpy as numpy
from numpy import poly1d
from scipy import optimize
#####
##Bulk modulus & Lattice parameter##
b0=poly1d([207.5]) #Bulk modulus at 0K in GPa
a0=poly1d([5.58348]) #Lattice parameter at 0K in Angstrom
#####
#Initiation of data
bulk=b0
cell=a0
nu_D= 5.14e+1 #Debye Frequency at 0K in THz
#####
cell2=poly1d(numpy.polymul(cell,cell)) #Square of Lattice parameter at 0K
cell3=poly1d(numpy.polymul(cell,cell2)) #Cube of Lattice parameter at 0K
Omega=cell3/4. #Mean volume per atom of fcc lattice ( $\Omega_0$ ) at 0K
BOmega=100.*poly1d(numpy.polymul(Omega,bulk)) #product of bulk modulus  $B_0$  and  $\Omega_0$ 
k=1.38064852 #value of Boltzmann constant in J/K
kb=8.617333262145e-5 #value of Boltzmann constant in eV/K
invkb=1/kb
invk=1/k
fcc=0.78146/60000. #fcc geometric lattice constant
D_0=fcc*nu_D*1e-8*cell2 #product of all the coefficient in prefactor ( $D'_0$ )
#####
#Loading Experimental Data Points from the data file
T, Log10D= numpy.loadtxt('ThO2_T_Self-D.dat', delimiter=' ', usecols=(0, 1), unpack=True)
#####
LnD= (numpy.log(10))*(Log10D) #Change of the Logarithmic Base for the Diffusion Coefficient
Ln_Coeff= numpy.log(D_0(T)) #Numerical Log of the product of all coefficient
B_Omega=BOmega(T)
lhs_2= (Ln_Coeff/B_Omega) #this term represents  $LnD'_0/B_0\Omega_0$ 
lhs_1= (LnD/B_Omega) #this term represents  $LnD^*/B_0\Omega_0$ 
Y_axis= (lhs_2-lhs_1)
kT= (k*T) #Denominator of the exponential term
X_axis= 1/(kT)
#####
# This function is to fit the parameter c;
def C_finder(X, C):
    return C*X
#####
c_calcul= optimize.curve_fit(C_finder, X_axis, Y_axis) #fitting step using Scipy-Library
c_fit= c_calcul[0][0] #Generating the value of c
numpy.savetxt('C_fitted_Value.txt', c_calcul) #Saving the value of c in an external file
#####
# Generate Diffusion coefficient with fitted c
C_fit=c_fit
T=numpy.arange(1000,3000,100) #Initiation of system temperature
invkbT=1./(k*T)
invT=1/T*10000.
invkT=1/(T*8.617333262145e-5)
kT= (k*T) #Denominator of the exponential term
Q=-C_fit*BOmega(T)*invkbT #exponential term of  $cB\Omega$  equation
Log_D=(numpy.log(D_0(T))+Q)/numpy.log(10.)
Ln_D=numpy.log(D_0(T))+Q
# Output the results in an external file
numpy.savetxt('Out.txt',numpy.column_stack([T,invT,Log_D,invkT,Ln_D]), delimiter=' ')
```

A.1.3. Python Script for Ox diffusion in Li_2O :

```
#!/usr/bin/python
import numpy as numpy
from numpy import poly1d
from scipy import optimize
#####
##Bulk modulus & Lattice parameter##
b0=poly1d([84.5051403837])           #Bulk modulus at 0K in GPa
a0=poly1d([4.572721654])           #Lattice parameter at 0K in Angstrom
#####
#Initiation of data
bulk=b0
cell=a0
nu_D= 1.415e+2                      #Debye Frequency at 0K in THz
#####
cell2=poly1d(numpy.polymul(cell,cell)) #Square of Lattice parameter at 0K
cell3=poly1d(numpy.polymul(cell,cell2)) #Cube of Lattice parameter at 0K
Omega=cell3/4.                      #Mean volume per atom of fcc lattice ( $\Omega_0$ ) at 0K
BOmega=100.*poly1d(numpy.polymul(Omega,bulk))
k=1.38064852                         #value of Boltzmann constant in J/K
kb=8.617333262145e-5                #value of Boltzmann constant in eV/K
invkb=1/kb
invk=1/k
fcc=0.78146/60000.                  #fcc geometric lattice constant
D_0=fcc*nu_D*1e-8*cell2              #product of all the coefficient in prefactor ( $D'_0$ )
#####
#Loading Experimental Data Points from the files
T, Log10D= numpy.loadtxt('Low_T]Li2O_T_Self-D.data', delimiter=' ', usecols=(0, 1), unpack=True)
#####
LnD= (numpy.log(10))*(Log10D)        #Change of the Logarithmic Base for the Diffusion Coefficient
Ln_Coeff= numpy.log(D_0(T))          #Numerical Log of the product of all coefficient
B_Omega=BOmega(T)
lhs_2= (Ln_Coeff/B_Omega)            #this term represents  $\text{Ln}D'_0/B_0\Omega_0$ 
lhs_1= (LnD/B_Omega)                 #this term represents  $\text{Ln}D^*/B_0\Omega_0$ 
Y_axis= (lhs_2-lhs_1)
kT= (k*T)                             #Denominator of the exponential term
X_axis= 1/(kT)
#####
# This function is to fit the parameter c;
def C_finder(X, C):
    return C*X
#####
c_calcul= optimize.curve_fit(C_finder, X_axis, Y_axis) #fitting step using Scipy-Library
c_fit= c_calcul[0][0]                               #Generating the value of c
numpy.savetxt('C_fitted_Value.txt', c_calcul)       #Saving the value of c in an external file
#####
# Generate Diffusion coefficient with fitted c
C_fit=c_fit
T=numpy.arange(1000,3000,100)                    #Initiation of system temperature
invkbT=1./(k*T)
invT=1/T*10000.
invkT=1/(T*8.617333262145e-5)
kT= (k*T)                                         #Denominator of the exponential term
Q=-C_fit*BOmega(T)*invkbT                        #exponential term of  $cB\Omega$  equation
Log_D=(numpy.log(D_0(T))+Q)/numpy.log(10.)
Ln_D=numpy.log(D_0(T))+Q
# Output the results in an external file
numpy.savetxt('Out.txt',numpy.column_stack([T,invT,Log_D,invkT,Ln_D]), delimiter=' ')
```


A.1.4. Python Script for Pu diffusion in PuO₂:

```

#!/usr/bin/python
import numpy as numpy
from numpy import poly1d
#####
##Bulk modulus & Lattice parameter##
b0=poly1d([220.8]) #Bulk modulus at 0K in GPa
a0=poly1d([5.38147]) #Lattice parameter at 0K in Angstrom
#####
#Initiation of data
bulk=b0
cell=a0
nu_D= 5.4434e+1 #Debye Frequency at 0K in THz
#####
cell2=poly1d(numpy.polymul(cell,cell)) #Square of Lattice parameter at 0K
cell3=poly1d(numpy.polymul(cell,cell2)) #Cube of Lattice parameter at 0K
Omega=cell3/4. #Mean volume per atom of fcc lattice ( $\Omega_0$ ) at 0K
BOmega=100.*poly1d(numpy.polymul(Omega,bulk))
k=1.38064852 #value of Boltzmann constant in J/K
kb=8.617333262145e-5 #value of Boltzmann constant in eV/K
invkb=1/kb
invk=1/k
fcc=0.78146/60000. #fcc geometric lattice constant
D_0=fcc*nu_D*1e-8*cell2 # product of all the coefficient in prefactor ( $D_0'$ )
#####
#Calculated value of c from ionic radius
ri= 0.96 #ionic radius of Pu4+ in Angstrom
C_fit=(0.2762*ri)-0.1792 #calculation of c from linear fit with ionic radius
#####
# Generate Diffusion coefficient with fitted c
T=numpy.arange(1000,3000,100) #Initiation of system temperature
invkbT=1./(k*T)
invT=1/T*10000.
invkT=1/(T*8.617333262145e-5)
kT=(k*T) #Denominator of the exponential term
Q=-C_fit*BOmega(T)*invkbT #exponential term of cB $\Omega$  equation
Log_D=(numpy.log(D_0(T))+Q)/numpy.log(10.)
Ln_D=numpy.log(D_0(T))+Q
# Output the results in an external file
numpy.savetxt('Out.txt',numpy.column_stack([T,invT,Log_D,invkT,Ln_D]), delimiter=' ')

```

A.2. Pu self diffusion data in (U, Pu)O_{2+x}:

A.2.1. (U_{0.9}Pu_{0.1})O_{2+x}:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∞] _{Pu} (m ² /s)
1273	0.1	1.9500	-2.61966E+01
1273	0.1	1.9510	-2.61935E+01
1273	0.1	1.9520	-2.61911E+01
1273	0.1	1.9530	-2.61902E+01
1273	0.1	1.9540	-2.61909E+01
1273	0.1	1.9550	-2.61930E+01
1273	0.1	1.9560	-2.61964E+01
1273	0.1	1.9570	-2.62010E+01
1273	0.1	1.9580	-2.62067E+01
1273	0.1	1.9590	-2.62134E+01
1273	0.1	1.9600	-2.62212E+01
1273	0.1	1.9610	-2.62298E+01
1273	0.1	1.9620	-2.62394E+01
1273	0.1	1.9630	-2.62498E+01
1273	0.1	1.9640	-2.62609E+01
1273	0.1	1.9650	-2.62729E+01
1273	0.1	1.9660	-2.62856E+01
1273	0.1	1.9670	-2.62991E+01
1273	0.1	1.9680	-2.63133E+01
1273	0.1	1.9690	-2.63282E+01
1273	0.1	1.9700	-2.63439E+01
1273	0.1	1.9710	-2.63602E+01
1273	0.1	1.9720	-2.63772E+01
1273	0.1	1.9730	-2.63949E+01
1273	0.1	1.9740	-2.64133E+01
1273	0.1	1.9750	-2.64322E+01
1273	0.1	1.9760	-2.64518E+01
1273	0.1	1.9770	-2.64720E+01
1273	0.1	1.9780	-2.64927E+01
1273	0.1	1.9790	-2.65140E+01
1273	0.1	1.9800	-2.65357E+01
1273	0.1	1.9810	-2.65578E+01
1273	0.1	1.9820	-2.65802E+01
1273	0.1	1.9830	-2.66030E+01
1273	0.1	1.9840	-2.66259E+01
1273	0.1	1.9850	-2.66490E+01
1273	0.1	1.9860	-2.66721E+01
1273	0.1	1.9870	-2.66952E+01
1273	0.1	1.9880	-2.67180E+01
1273	0.1	1.9890	-2.67406E+01
1273	0.1	1.9900	-2.67628E+01
1273	0.1	1.9910	-2.67844E+01
1273	0.1	1.9920	-2.68054E+01
1273	0.1	1.9930	-2.68256E+01
1273	0.1	1.9940	-2.68449E+01
1273	0.1	1.9950	-2.68632E+01
1273	0.1	1.9960	-2.68803E+01
1273	0.1	1.9970	-2.68962E+01
1273	0.1	1.9980	-2.69106E+01
1273	0.1	1.9990	-2.69236E+01
1273	0.1	2.0000	-2.69351E+01
1273	0.1	2.0010	-2.69409E+01
1273	0.1	2.0020	-2.69446E+01
1273	0.1	2.0030	-2.69462E+01
1273	0.1	2.0040	-2.69459E+01
1273	0.1	2.0050	-2.69435E+01
1273	0.1	2.0060	-2.69394E+01
1273	0.1	2.0070	-2.69334E+01
1273	0.1	2.0080	-2.69259E+01
1273	0.1	2.0090	-2.69168E+01
1273	0.1	2.0100	-2.69062E+01
1273	0.1	2.0110	-2.68944E+01
1273	0.1	2.0120	-2.68814E+01
1273	0.1	2.0130	-2.68672E+01
1273	0.1	2.0140	-2.68520E+01
1273	0.1	2.0150	-2.68359E+01
1273	0.1	2.0160	-2.68189E+01
1273	0.1	2.0170	-2.68012E+01
1273	0.1	2.0180	-2.67827E+01
1273	0.1	2.0190	-2.67635E+01
1273	0.1	2.0200	-2.67437E+01
1273	0.1	2.0210	-2.67234E+01
1273	0.1	2.0220	-2.67025E+01
1273	0.1	2.0230	-2.66811E+01
1273	0.1	2.0240	-2.66592E+01
1273	0.1	2.0250	-2.66369E+01
1273	0.1	2.0260	-2.66142E+01
1273	0.1	2.0270	-2.65911E+01
1273	0.1	2.0280	-2.65676E+01
1273	0.1	2.0290	-2.65437E+01
1273	0.1	2.0300	-2.65195E+01
1273	0.1	2.0310	-2.64950E+01
1273	0.1	2.0320	-2.64702E+01
1273	0.1	2.0330	-2.64450E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∞] _{Pu} (m ² /s)
1273	0.1	2.0340	-2.64196E+01
1273	0.1	2.0350	-2.63939E+01
1273	0.1	2.0360	-2.63680E+01
1273	0.1	2.0370	-2.63418E+01
1273	0.1	2.0380	-2.63153E+01
1273	0.1	2.0390	-2.62886E+01
1273	0.1	2.0400	-2.62617E+01
1273	0.1	2.0410	-2.62346E+01
1273	0.1	2.0420	-2.62073E+01
1273	0.1	2.0430	-2.61798E+01
1273	0.1	2.0440	-2.61521E+01
1273	0.1	2.0450	-2.61242E+01
1273	0.1	2.0460	-2.60961E+01
1273	0.1	2.0470	-2.60679E+01
1273	0.1	2.0480	-2.60396E+01
1273	0.1	2.0490	-2.60110E+01
1273	0.1	2.0500	-2.59824E+01
1273	0.1	2.0510	-2.59536E+01
1273	0.1	2.0520	-2.59247E+01
1273	0.1	2.0530	-2.58956E+01
1273	0.1	2.0540	-2.58665E+01
1273	0.1	2.0550	-2.58372E+01
1273	0.1	2.0560	-2.58078E+01
1273	0.1	2.0570	-2.57784E+01
1273	0.1	2.0580	-2.57488E+01
1273	0.1	2.0590	-2.57191E+01
1273	0.1	2.0600	-2.56894E+01
1273	0.1	2.0610	-2.56596E+01
1273	0.1	2.0620	-2.56297E+01
1273	0.1	2.0630	-2.55997E+01
1273	0.1	2.0640	-2.55697E+01
1273	0.1	2.0650	-2.55396E+01
1273	0.1	2.0660	-2.55095E+01
1273	0.1	2.0670	-2.54793E+01
1273	0.1	2.0680	-2.54491E+01
1273	0.1	2.0690	-2.54188E+01
1273	0.1	2.0700	-2.53884E+01
1273	0.1	2.0710	-2.53580E+01
1273	0.1	2.0720	-2.53276E+01
1273	0.1	2.0730	-2.52971E+01
1273	0.1	2.0740	-2.52666E+01
1273	0.1	2.0750	-2.52361E+01
1273	0.1	2.0760	-2.52056E+01
1273	0.1	2.0770	-2.51750E+01
1273	0.1	2.0780	-2.51444E+01
1273	0.1	2.0790	-2.51137E+01
1273	0.1	2.0800	-2.50831E+01
1273	0.1	2.0810	-2.50524E+01
1273	0.1	2.0820	-2.50217E+01
1273	0.1	2.0830	-2.49910E+01
1273	0.1	2.0840	-2.49602E+01
1273	0.1	2.0850	-2.49295E+01
1273	0.1	2.0860	-2.48987E+01
1273	0.1	2.0870	-2.48680E+01
1273	0.1	2.0880	-2.48372E+01
1273	0.1	2.0890	-2.48064E+01
1273	0.1	2.0900	-2.47756E+01
1273	0.1	2.0910	-2.47448E+01
1273	0.1	2.0920	-2.47139E+01
1273	0.1	2.0930	-2.46831E+01
1273	0.1	2.0940	-2.46523E+01
1273	0.1	2.0950	-2.46214E+01
1273	0.1	2.0960	-2.45906E+01
1273	0.1	2.0970	-2.45597E+01
1273	0.1	2.0980	-2.45289E+01
1273	0.1	2.0990	-2.44980E+01
1273	0.1	2.1000	-2.44672E+01
1273	0.1	2.1010	-2.44363E+01
1273	0.1	2.1020	-2.44055E+01
1273	0.1	2.1030	-2.43746E+01
1273	0.1	2.1040	-2.43438E+01
1273	0.1	2.1050	-2.43129E+01
1273	0.1	2.1060	-2.42821E+01
1273	0.1	2.1070	-2.42512E+01
1273	0.1	2.1080	-2.42204E+01
1273	0.1	2.1090	-2.41895E+01
1273	0.1	2.1100	-2.41587E+01
1273	0.1	2.1110	-2.41278E+01
1273	0.1	2.1120	-2.40970E+01
1273	0.1	2.1130	-2.40661E+01
1273	0.1	2.1140	-2.40353E+01
1273	0.1	2.1150	-2.40045E+01
1273	0.1	2.1160	-2.39736E+01
1273	0.1	2.1170	-2.39428E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∞] _{Pu} (m ² /s)
1273	0.1	2.1180	-2.39120E+01
1273	0.1	2.1190	-2.38812E+01
1273	0.1	2.1200	-2.38504E+01
1273	0.1	2.1210	-2.38196E+01
1273	0.1	2.1220	-2.37888E+01
1273	0.1	2.1230	-2.37580E+01
1273	0.1	2.1240	-2.37272E+01
1273	0.1	2.1250	-2.36964E+01
1273	0.1	2.1260	-2.36656E+01
1273	0.1	2.1270	-2.36348E+01
1273	0.1	2.1280	-2.36040E+01
1273	0.1	2.1290	-2.35733E+01
1273	0.1	2.1300	-2.35425E+01
1273	0.1	2.1310	-2.35118E+01
1273	0.1	2.1320	-2.34810E+01
1273	0.1	2.1330	-2.34503E+01
1273	0.1	2.1340	-2.34195E+01
1273	0.1	2.1350	-2.33888E+01
1273	0.1	2.1360	-2.33581E+01
1273	0.1	2.1370	-2.33274E+01
1273	0.1	2.1380	-2.32967E+01
1273	0.1	2.1390	-2.32660E+01
1273	0.1	2.1400	-2.32353E+01
1273	0.1	2.1410	-2.32046E+01
1273	0.1	2.1420	-2.31739E+01
1273	0.1	2.1430	-2.31432E+01
1273	0.1	2.1440	-2.31125E+01
1273	0.1	2.1450	-2.30819E+01
1273	0.1	2.1460	-2.30512E+01
1273	0.1	2.1470	-2.30206E+01
1273	0.1	2.1480	-2.29899E+01
1273	0.1	2.1490	-2.29593E+01
1273	0.1	2.1500	-2.29287E+01
1273	0.1	2.1510	-2.28980E+01
1273	0.1	2.1520	-2.28674E+01
1273	0.1	2.1530	-2.28368E+01
1273	0.1	2.1540	-2.28062E+01
1273	0.1	2.1550	-2.27756E+01
1273	0.1	2.1560	-2.27450E+01
1273	0.1	2.1570	-2.27145E+01
1273	0.1	2.1580	-2.26839E+01
1273	0.1	2.1590	-2.26533E+01
1273	0.1	2.1600	-2.26228E+01
1273	0.1	2.1610	-2.25922E+01
1273	0.1	2.1620	-2.25617E+01
1273	0.1	2.1630	-2.25311E+01
1273	0.1	2.1640	-2.25006E+01
1273	0.1	2.1650	-2.24701E+01
1273	0.1	2.1660	-2.24396E+01
1273	0.1	2.1670	-2.24090E+01
1273	0.1	2.1680	-2.23785E+01
1273	0.1	2.1690	-2.23480E+01
1273	0.1	2.1700	-2.23176E+01
1273	0.1	2.1710	-2.22871E+01
1273	0.1	2.1720	-2.22566E+01
1273	0.1	2.1730	-2.22261E+01
1273	0.1	2.1740	-2.21957E+01
1273	0.1	2.1750	-2.21652E+01
1273	0.1	2.1760	-2.21348E+01
1273	0.1	2.1770	-2.21043E+01
1273	0.1	2.1780	-2.20739E+01
1273	0.1	2.1790	-2.20435E+01
1273	0.1	2.1800	-2.20131E+01
1273	0.1	2.1810	-2.19827E+01
1273	0.1	2.1820	-2.19523E+01
1273	0.1	2.1830	-2.19219E+01
1273	0.1	2.1840	-2.18915E+01
1273	0.1	2.1850	-2.18611E+01
1273	0.1	2.1860	-2.18307E+01
1273	0.1	2.1870	-2.18004E+01
1273	0.1	2.1880	-2.17700E+01
1273	0.1	2.1890	-2.17397E+01
1273	0.1	2.1900	-2.17093E+01
1273	0.1	2.1910	-2.16790E+01
1273	0		

1773	0.1	1.9210	-1.97695E+01
1773	0.1	1.9220	-1.97695E+01
1773	0.1	1.9230	-1.97696E+01
1773	0.1	1.9240	-1.97696E+01
1773	0.1	1.9250	-1.97697E+01
1773	0.1	1.9260	-1.97697E+01
1773	0.1	1.9270	-1.97698E+01
1773	0.1	1.9280	-1.97699E+01
1773	0.1	1.9290	-1.97699E+01
1773	0.1	1.9300	-1.97700E+01
1773	0.1	1.9310	-1.97701E+01
1773	0.1	1.9320	-1.97702E+01
1773	0.1	1.9330	-1.97703E+01
1773	0.1	1.9340	-1.97705E+01
1773	0.1	1.9350	-1.97706E+01
1773	0.1	1.9360	-1.97708E+01
1773	0.1	1.9370	-1.97710E+01
1773	0.1	1.9380	-1.97712E+01
1773	0.1	1.9390	-1.97714E+01
1773	0.1	1.9400	-1.97717E+01
1773	0.1	1.9410	-1.97721E+01
1773	0.1	1.9420	-1.97725E+01
1773	0.1	1.9430	-1.97730E+01
1773	0.1	1.9440	-1.97736E+01
1773	0.1	1.9450	-1.97744E+01
1773	0.1	1.9460	-1.97754E+01
1773	0.1	1.9470	-1.97767E+01
1773	0.1	1.9480	-1.97783E+01
1773	0.1	1.9490	-1.97803E+01
1773	0.1	1.9500	-1.97829E+01
1773	0.1	1.9510	-1.97862E+01
1773	0.1	1.9520	-1.97901E+01
1773	0.1	1.9530	-1.97949E+01
1773	0.1	1.9540	-1.98004E+01
1773	0.1	1.9550	-1.98067E+01
1773	0.1	1.9560	-1.98138E+01
1773	0.1	1.9570	-1.98216E+01
1773	0.1	1.9580	-1.98301E+01
1773	0.1	1.9590	-1.98393E+01
1773	0.1	1.9600	-1.98492E+01
1773	0.1	1.9610	-1.98597E+01
1773	0.1	1.9620	-1.98708E+01
1773	0.1	1.9630	-1.98824E+01
1773	0.1	1.9640	-1.98946E+01
1773	0.1	1.9650	-1.99072E+01
1773	0.1	1.9660	-1.99202E+01
1773	0.1	1.9670	-1.99337E+01
1773	0.1	1.9680	-1.99475E+01
1773	0.1	1.9690	-1.99617E+01
1773	0.1	1.9700	-1.99761E+01
1773	0.1	1.9710	-1.99907E+01
1773	0.1	1.9720	-2.00056E+01
1773	0.1	1.9730	-2.00205E+01
1773	0.1	1.9740	-2.00356E+01
1773	0.1	1.9750	-2.00507E+01
1773	0.1	1.9760	-2.00658E+01
1773	0.1	1.9770	-2.00808E+01
1773	0.1	1.9780	-2.00957E+01
1773	0.1	1.9790	-2.01104E+01
1773	0.1	1.9800	-2.01249E+01
1773	0.1	1.9810	-2.01391E+01
1773	0.1	1.9820	-2.01529E+01
1773	0.1	1.9830	-2.01663E+01
1773	0.1	1.9840	-2.01793E+01
1773	0.1	1.9850	-2.01918E+01
1773	0.1	1.9860	-2.02037E+01
1773	0.1	1.9870	-2.02150E+01
1773	0.1	1.9880	-2.02256E+01
1773	0.1	1.9890	-2.02356E+01
1773	0.1	1.9900	-2.02448E+01
1773	0.1	1.9910	-2.02532E+01
1773	0.1	1.9920	-2.02608E+01
1773	0.1	1.9930	-2.02677E+01
1773	0.1	1.9940	-2.02737E+01
1773	0.1	1.9950	-2.02788E+01
1773	0.1	1.9960	-2.02831E+01
1773	0.1	1.9970	-2.02865E+01
1773	0.1	1.9980	-2.02890E+01
1773	0.1	1.9990	-2.02906E+01
1773	0.1	2.0000	-2.02910E+01
1773	0.1	2.0010	-2.02885E+01
1773	0.1	2.0020	-2.02845E+01
1773	0.1	2.0030	-2.02794E+01
1773	0.1	2.0040	-2.02735E+01
1773	0.1	2.0050	-2.02666E+01
1773	0.1	2.0060	-2.02589E+01
1773	0.1	2.0070	-2.02504E+01
1773	0.1	2.0080	-2.02411E+01
1773	0.1	2.0090	-2.02311E+01
1773	0.1	2.0100	-2.02205E+01
1773	0.1	2.0110	-2.02093E+01
1773	0.1	2.0120	-2.01974E+01

1773	0.1	2.0130	-2.01851E+01
1773	0.1	2.0140	-2.01723E+01
1773	0.1	2.0150	-2.01590E+01
1773	0.1	2.0160	-2.01452E+01
1773	0.1	2.0170	-2.01311E+01
1773	0.1	2.0180	-2.01166E+01
1773	0.1	2.0190	-2.01017E+01
1773	0.1	2.0200	-2.00865E+01
1773	0.1	2.0210	-2.00710E+01
1773	0.1	2.0220	-2.00552E+01
1773	0.1	2.0230	-2.00391E+01
1773	0.1	2.0240	-2.00227E+01
1773	0.1	2.0250	-2.00061E+01
1773	0.1	2.0260	-1.99892E+01
1773	0.1	2.0270	-1.99721E+01
1773	0.1	2.0280	-1.99547E+01
1773	0.1	2.0290	-1.99372E+01
1773	0.1	2.0300	-1.99195E+01
1773	0.1	2.0310	-1.99015E+01
1773	0.1	2.0320	-1.98834E+01
1773	0.1	2.0330	-1.98650E+01
1773	0.1	2.0340	-1.98465E+01
1773	0.1	2.0350	-1.98278E+01
1773	0.1	2.0360	-1.98099E+01
1773	0.1	2.0370	-1.97919E+01
1773	0.1	2.0380	-1.97737E+01
1773	0.1	2.0390	-1.97553E+01
1773	0.1	2.0400	-1.97371E+01
1773	0.1	2.0410	-1.97181E+01
1773	0.1	2.0420	-1.96992E+01
1773	0.1	2.0430	-1.96802E+01
1773	0.1	2.0440	-1.96612E+01
1773	0.1	2.0450	-1.96421E+01
1773	0.1	2.0460	-1.96230E+01
1773	0.1	2.0470	-1.96038E+01
1773	0.1	2.0480	-1.95846E+01
1773	0.1	2.0490	-1.95654E+01
1773	0.1	2.0500	-1.95462E+01
1773	0.1	2.0510	-1.95270E+01
1773	0.1	2.0520	-1.95078E+01
1773	0.1	2.0530	-1.94886E+01
1773	0.1	2.0540	-1.94694E+01
1773	0.1	2.0550	-1.94502E+01
1773	0.1	2.0560	-1.94310E+01
1773	0.1	2.0570	-1.94118E+01
1773	0.1	2.0580	-1.93926E+01
1773	0.1	2.0590	-1.93734E+01
1773	0.1	2.0600	-1.93542E+01
1773	0.1	2.0610	-1.93350E+01
1773	0.1	2.0620	-1.93158E+01
1773	0.1	2.0630	-1.92966E+01
1773	0.1	2.0640	-1.92774E+01
1773	0.1	2.0650	-1.92582E+01
1773	0.1	2.0660	-1.92390E+01
1773	0.1	2.0670	-1.92198E+01
1773	0.1	2.0680	-1.92006E+01
1773	0.1	2.0690	-1.91814E+01
1773	0.1	2.0700	-1.91622E+01
1773	0.1	2.0710	-1.91430E+01
1773	0.1	2.0720	-1.91238E+01
1773	0.1	2.0730	-1.91046E+01
1773	0.1	2.0740	-1.90854E+01
1773	0.1	2.0750	-1.90662E+01
1773	0.1	2.0760	-1.90470E+01
1773	0.1	2.0770	-1.90278E+01
1773	0.1	2.0780	-1.90086E+01
1773	0.1	2.0790	-1.89894E+01
1773	0.1	2.0800	-1.89702E+01
1773	0.1	2.0810	-1.89510E+01
1773	0.1	2.0820	-1.89318E+01
1773	0.1	2.0830	-1.89126E+01
1773	0.1	2.0840	-1.88934E+01
1773	0.1	2.0850	-1.88742E+01
1773	0.1	2.0860	-1.88550E+01
1773	0.1	2.0870	-1.88358E+01
1773	0.1	2.0880	-1.88166E+01
1773	0.1	2.0890	-1.87974E+01
1773	0.1	2.0900	-1.87782E+01
1773	0.1	2.0910	-1.87590E+01
1773	0.1	2.0920	-1.87398E+01
1773	0.1	2.0930	-1.87206E+01
1773	0.1	2.0940	-1.87014E+01
1773	0.1	2.0950	-1.86822E+01
1773	0.1	2.0960	-1.86630E+01
1773	0.1	2.0970	-1.86438E+01
1773	0.1	2.0980	-1.86246E+01
1773	0.1	2.0990	-1.86054E+01
1773	0.1	2.1000	-1.85862E+01
1773	0.1	2.1010	-1.85670E+01
1773	0.1	2.1020	-1.85478E+01
1773	0.1	2.1030	-1.85286E+01
1773	0.1	2.1040	-1.85094E+01

1773	0.1	2.1050	-1.82435E+01
1773	0.1	2.1060	-1.82188E+01
1773	0.1	2.1070	-1.81941E+01
1773	0.1	2.1080	-1.81694E+01
1773	0.1	2.1090	-1.81447E+01
1773	0.1	2.1100	-1.81199E+01
1773	0.1	2.1110	-1.80952E+01
1773	0.1	2.1120	-1.80704E+01
1773	0.1	2.1130	-1.80456E+01
1773	0.1	2.1140	-1.80208E+01
1773	0.1	2.1150	-1.79960E+01
1773	0.1	2.1160	-1.79712E+01
1773	0.1	2.1170	-1.79464E+01
1773	0.1	2.1180	-1.79215E+01
1773	0.1	2.1190	-1.78967E+01
1773	0.1	2.1200	-1.78718E+01
1773	0.1	2.1210	-1.78470E+01
1773	0.1	2.1220	-1.78221E+01
1773	0.1	2.1230	-1.77972E+01
1773	0.1	2.1240	-1.77723E+01
1773	0.1	2.1250	-1.77475E+01
1773	0.1	2.1260	-1.77226E+01
1773	0.1	2.1270	-1.76977E+01
1773	0.1	2.1280	-1.76728E+01
1773	0.1	2.1290	-1.76478E+01
1773	0.1	2.1300	-1.76229E+01
1773	0.1	2.1310	-1.75980E+01
1773	0.1	2.1320	-1.75731E+01
1773	0.1	2.1330	-1.75482E+01
1773	0.1	2.1340	-1.75233E+01
1773	0.1	2.1350	-1.74983E+01
1773	0.1	2.1360	-1.74734E+01
1773	0.1	2.1370	-1.74485E+01
1773	0.1	2.1380	-1.74235E+01
1773	0.1	2.1390	-1.73986E+01
1773	0.1	2.1400	-1.73737E+01
1773	0.1	2.1410	-1.73487E+01
1773	0.1	2.1420	-1.73238E+01
1773	0.1	2.1430	-1.72989E+01
1773	0.1	2.1440	-1.72739E+01
1773	0.1	2.1450	-1.72490E+01
1773	0.1	2.1460	-1.72241E+01
1773	0.1	2.1470	-1.71992E+01
1773	0.1	2.1480	-1.71742E+01
1773	0.1	2.1490	-1.71493E+01
1773	0.1	2.1500	-1.71244E+01
1773	0.1	2.1510	-1.70995E+01
1773	0.1	2.1520	-1.70745E+01
1773	0.1	2.1530	-1.70496E+01
1773	0.1	2.1540	-1.70247E+01
1773	0.1	2.1550	-1.69998E+01
1773	0.1	2.1560	-1.69749E+01
1773	0.1	2.1570	-1.69499E+01
1773	0.1	2.1580	-1.69250E+01
1773	0.1	2.1590	-1.69001E+01
1773	0.1	2.1600	-1.68752E+01
1773	0.1	2.1610	-1.68503E+01
1773	0.1	2.1620	-1.68254E+01
1773	0.1	2.1630	-1.68005E+01
1773	0.1	2.1640	-1.67756E+01
1773	0.1	2.1650	-1.67507E+01
1773	0.1	2.1660	-1.67259E+01
1773	0.1	2.1670	-1.67010E+01
1773	0.1	2.1680	-1.66761E+01
1773	0.1	2.1690	-1.66512E+01
1773	0.1	2.1700	-1.66264E+01
1773	0.1		

1773	0.1	2.1970	-1.59564E+01
1773	0.1	2.1980	-1.59316E+01
1773	0.1	2.1990	-1.59069E+01
1773	0.1	2.2000	-1.58822E+01
2273	0.1	1.8000	-1.61472E+01
2273	0.1	1.8010	-1.61472E+01
2273	0.1	1.8020	-1.61473E+01
2273	0.1	1.8030	-1.61473E+01
2273	0.1	1.8040	-1.61474E+01
2273	0.1	1.8050	-1.61474E+01
2273	0.1	1.8060	-1.61475E+01
2273	0.1	1.8070	-1.61475E+01
2273	0.1	1.8080	-1.61476E+01
2273	0.1	1.8090	-1.61477E+01
2273	0.1	1.8100	-1.61477E+01
2273	0.1	1.8110	-1.61478E+01
2273	0.1	1.8120	-1.61478E+01
2273	0.1	1.8130	-1.61479E+01
2273	0.1	1.8140	-1.61480E+01
2273	0.1	1.8150	-1.61480E+01
2273	0.1	1.8160	-1.61481E+01
2273	0.1	1.8170	-1.61481E+01
2273	0.1	1.8180	-1.61482E+01
2273	0.1	1.8190	-1.61483E+01
2273	0.1	1.8200	-1.61483E+01
2273	0.1	1.8210	-1.61484E+01
2273	0.1	1.8220	-1.61485E+01
2273	0.1	1.8230	-1.61486E+01
2273	0.1	1.8240	-1.61486E+01
2273	0.1	1.8250	-1.61487E+01
2273	0.1	1.8260	-1.61488E+01
2273	0.1	1.8270	-1.61488E+01
2273	0.1	1.8280	-1.61489E+01
2273	0.1	1.8290	-1.61490E+01
2273	0.1	1.8300	-1.61491E+01
2273	0.1	1.8310	-1.61491E+01
2273	0.1	1.8320	-1.61492E+01
2273	0.1	1.8330	-1.61493E+01
2273	0.1	1.8340	-1.61494E+01
2273	0.1	1.8350	-1.61495E+01
2273	0.1	1.8360	-1.61495E+01
2273	0.1	1.8370	-1.61496E+01
2273	0.1	1.8380	-1.61497E+01
2273	0.1	1.8390	-1.61498E+01
2273	0.1	1.8400	-1.61499E+01
2273	0.1	1.8410	-1.61500E+01
2273	0.1	1.8420	-1.61501E+01
2273	0.1	1.8430	-1.61502E+01
2273	0.1	1.8440	-1.61502E+01
2273	0.1	1.8450	-1.61503E+01
2273	0.1	1.8460	-1.61504E+01
2273	0.1	1.8470	-1.61505E+01
2273	0.1	1.8480	-1.61506E+01
2273	0.1	1.8490	-1.61507E+01
2273	0.1	1.8500	-1.61508E+01
2273	0.1	1.8510	-1.61510E+01
2273	0.1	1.8520	-1.61511E+01
2273	0.1	1.8530	-1.61512E+01
2273	0.1	1.8540	-1.61513E+01
2273	0.1	1.8550	-1.61514E+01
2273	0.1	1.8560	-1.61515E+01
2273	0.1	1.8570	-1.61516E+01
2273	0.1	1.8580	-1.61518E+01
2273	0.1	1.8590	-1.61519E+01
2273	0.1	1.8600	-1.61520E+01
2273	0.1	1.8610	-1.61521E+01
2273	0.1	1.8620	-1.61523E+01
2273	0.1	1.8630	-1.61524E+01
2273	0.1	1.8640	-1.61525E+01
2273	0.1	1.8650	-1.61527E+01
2273	0.1	1.8660	-1.61528E+01
2273	0.1	1.8670	-1.61530E+01
2273	0.1	1.8680	-1.61531E+01
2273	0.1	1.8690	-1.61533E+01
2273	0.1	1.8700	-1.61534E+01
2273	0.1	1.8710	-1.61536E+01
2273	0.1	1.8720	-1.61538E+01
2273	0.1	1.8730	-1.61539E+01
2273	0.1	1.8740	-1.61541E+01
2273	0.1	1.8750	-1.61543E+01
2273	0.1	1.8760	-1.61544E+01
2273	0.1	1.8770	-1.61546E+01
2273	0.1	1.8780	-1.61548E+01
2273	0.1	1.8790	-1.61550E+01
2273	0.1	1.8800	-1.61552E+01
2273	0.1	1.8810	-1.61554E+01
2273	0.1	1.8820	-1.61556E+01
2273	0.1	1.8830	-1.61559E+01
2273	0.1	1.8840	-1.61561E+01
2273	0.1	1.8850	-1.61563E+01
2273	0.1	1.8860	-1.61566E+01
2273	0.1	1.8870	-1.61568E+01

2273	0.1	1.8880	-1.61571E+01
2273	0.1	1.8890	-1.61573E+01
2273	0.1	1.8900	-1.61576E+01
2273	0.1	1.8910	-1.61579E+01
2273	0.1	1.8920	-1.61581E+01
2273	0.1	1.8930	-1.61584E+01
2273	0.1	1.8940	-1.61587E+01
2273	0.1	1.8950	-1.61591E+01
2273	0.1	1.8960	-1.61594E+01
2273	0.1	1.8970	-1.61597E+01
2273	0.1	1.8980	-1.61601E+01
2273	0.1	1.8990	-1.61604E+01
2273	0.1	1.9000	-1.61608E+01
2273	0.1	1.9010	-1.61612E+01
2273	0.1	1.9020	-1.61616E+01
2273	0.1	1.9030	-1.61620E+01
2273	0.1	1.9040	-1.61625E+01
2273	0.1	1.9050	-1.61629E+01
2273	0.1	1.9060	-1.61634E+01
2273	0.1	1.9070	-1.61639E+01
2273	0.1	1.9080	-1.61644E+01
2273	0.1	1.9090	-1.61650E+01
2273	0.1	1.9100	-1.61655E+01
2273	0.1	1.9110	-1.61661E+01
2273	0.1	1.9120	-1.61667E+01
2273	0.1	1.9130	-1.61674E+01
2273	0.1	1.9140	-1.61680E+01
2273	0.1	1.9150	-1.61688E+01
2273	0.1	1.9160	-1.61695E+01
2273	0.1	1.9170	-1.61703E+01
2273	0.1	1.9180	-1.61711E+01
2273	0.1	1.9190	-1.61720E+01
2273	0.1	1.9200	-1.61729E+01
2273	0.1	1.9210	-1.61738E+01
2273	0.1	1.9220	-1.61749E+01
2273	0.1	1.9230	-1.61759E+01
2273	0.1	1.9240	-1.61771E+01
2273	0.1	1.9250	-1.61783E+01
2273	0.1	1.9260	-1.61796E+01
2273	0.1	1.9270	-1.61809E+01
2273	0.1	1.9280	-1.61824E+01
2273	0.1	1.9290	-1.61839E+01
2273	0.1	1.9300	-1.61856E+01
2273	0.1	1.9310	-1.61873E+01
2273	0.1	1.9320	-1.61892E+01
2273	0.1	1.9330	-1.61912E+01
2273	0.1	1.9340	-1.61934E+01
2273	0.1	1.9350	-1.61957E+01
2273	0.1	1.9360	-1.61981E+01
2273	0.1	1.9370	-1.62008E+01
2273	0.1	1.9380	-1.62036E+01
2273	0.1	1.9390	-1.62066E+01
2273	0.1	1.9400	-1.62099E+01
2273	0.1	1.9410	-1.62134E+01
2273	0.1	1.9420	-1.62172E+01
2273	0.1	1.9430	-1.62212E+01
2273	0.1	1.9440	-1.62256E+01
2273	0.1	1.9450	-1.62302E+01
2273	0.1	1.9460	-1.62352E+01
2273	0.1	1.9470	-1.62405E+01
2273	0.1	1.9480	-1.62462E+01
2273	0.1	1.9490	-1.62522E+01
2273	0.1	1.9500	-1.62586E+01
2273	0.1	1.9510	-1.62653E+01
2273	0.1	1.9520	-1.62725E+01
2273	0.1	1.9530	-1.62800E+01
2273	0.1	1.9540	-1.62879E+01
2273	0.1	1.9550	-1.62961E+01
2273	0.1	1.9560	-1.63047E+01
2273	0.1	1.9570	-1.63136E+01
2273	0.1	1.9580	-1.63228E+01
2273	0.1	1.9590	-1.63323E+01
2273	0.1	1.9600	-1.63421E+01
2273	0.1	1.9610	-1.63521E+01
2273	0.1	1.9620	-1.63623E+01
2273	0.1	1.9630	-1.63727E+01
2273	0.1	1.9640	-1.63832E+01
2273	0.1	1.9650	-1.63938E+01
2273	0.1	1.9660	-1.64044E+01
2273	0.1	1.9670	-1.64151E+01
2273	0.1	1.9680	-1.64257E+01
2273	0.1	1.9690	-1.64362E+01
2273	0.1	1.9700	-1.64467E+01
2273	0.1	1.9710	-1.64570E+01
2273	0.1	1.9720	-1.64671E+01
2273	0.1	1.9730	-1.64770E+01
2273	0.1	1.9740	-1.64866E+01
2273	0.1	1.9750	-1.64959E+01
2273	0.1	1.9760	-1.65048E+01
2273	0.1	1.9770	-1.65133E+01
2273	0.1	1.9780	-1.65215E+01
2273	0.1	1.9790	-1.65291E+01

2273	0.1	1.9800	-1.65363E+01
2273	0.1	1.9810	-1.65430E+01
2273	0.1	1.9820	-1.65491E+01
2273	0.1	1.9830	-1.65546E+01
2273	0.1	1.9840	-1.65596E+01
2273	0.1	1.9850	-1.65640E+01
2273	0.1	1.9860	-1.65677E+01
2273	0.1	1.9870	-1.65709E+01
2273	0.1	1.9880	-1.65734E+01
2273	0.1	1.9890	-1.65753E+01
2273	0.1	1.9900	-1.65765E+01
2273	0.1	1.9910	-1.65771E+01
2273	0.1	1.9920	-1.65771E+01
2273	0.1	1.9930	-1.65765E+01
2273	0.1	1.9940	-1.65752E+01
2273	0.1	1.9950	-1.65734E+01
2273	0.1	1.9960	-1.65709E+01
2273	0.1	1.9970	-1.65677E+01
2273	0.1	1.9980	-1.65639E+01
2273	0.1	1.9990	-1.65594E+01
2273	0.1	2.0000	-1.65540E+01
2273	0.1	2.0010	-1.65476E+01
2273	0.1	2.0020	-1.65404E+01
2273	0.1	2.0030	-1.65323E+01
2273	0.1	2.0040	-1.65237E+01
2273	0.1	2.0050	-1.65145E+01
2273	0.1	2.0060	-1.65047E+01
2273	0.1	2.0070	-1.64945E+01
2273	0.1	2.0080	-1.64839E+01
2273	0.1	2.0090	-1.64729E+01
2273	0.1	2.0100	-1.64615E+01
2273	0.1	2.0110	-1.64497E+01
2273	0.1	2.0120	-1.64377E+01
2273	0.1	2.0130	-1.64253E+01
2273	0.1	2.0140	-1.64126E+01
2273	0.1	2.0150	-1.63997E+01
2273	0.1	2.0160	-1.63865E+01
2273	0.1	2.0170	-1.63731E+01
2273	0.1	2.0180	-1.63595E+01
2273	0.1	2.0190	-1.63457E+01
2273	0.1	2.0200	-1.63317E+01
2273	0.1	2.0210	-1.63174E+01
2273	0.1	2.0220	-1.63031E+01
2273	0.1	2.0230	-1.62885E+01
2273	0.1	2.0240	-1.62738E+01
2273	0.1	2.0250	-1.62589E+01
2273	0.1	2.0260	-1.62439E+01
2273	0.1	2.0270	-1.62287E+01
2273	0.1	2.0280	-1.62134E+01
2273	0.1	2.0290	-1.61980E+01
2273	0.1	2.0300	-1.61825E+01
2273	0.1	2.0310	-1.61668E+01
2273	0.1	2.0320	-1.61510E+01
2273	0.1	2.0330	-1.61351E+01
2273	0.1	2.0340	-1.61191E+01
2273	0.1	2.0350	-1.61029E+01
2273	0.1	2.0360	-1.60867E+01
2273	0.1	2.0370	-1.60704E+01
2273	0.1	2.0380	-1.60539E+01
2273	0.1	2.0390	-1.60374E+01
2273	0.1	2.0400	-1.60207E+01
2273	0.1	2.0410	-1.60040E+01
2273	0.1	2.0420	-1.59871E+01
2273	0.1	2.0430	-1.59702E+01
2273	0.1	2.0440	-1.59532E+01
2273	0.1	2.0450	-1.59361E+01
2273	0.1		

2273	0.1	2.0720	-1.54439E+01
2273	0.1	2.0730	-1.54247E+01
2273	0.1	2.0740	-1.54054E+01
2273	0.1	2.0750	-1.53861E+01
2273	0.1	2.0760	-1.53667E+01
2273	0.1	2.0770	-1.53473E+01
2273	0.1	2.0780	-1.53278E+01
2273	0.1	2.0790	-1.53083E+01
2273	0.1	2.0800	-1.52886E+01
2273	0.1	2.0810	-1.52690E+01
2273	0.1	2.0820	-1.52493E+01
2273	0.1	2.0830	-1.52295E+01
2273	0.1	2.0840	-1.52097E+01
2273	0.1	2.0850	-1.51899E+01
2273	0.1	2.0860	-1.51700E+01
2273	0.1	2.0870	-1.51500E+01
2273	0.1	2.0880	-1.51300E+01
2273	0.1	2.0890	-1.51100E+01
2273	0.1	2.0900	-1.50899E+01
2273	0.1	2.0910	-1.50698E+01
2273	0.1	2.0920	-1.50496E+01
2273	0.1	2.0930	-1.50294E+01
2273	0.1	2.0940	-1.50091E+01
2273	0.1	2.0950	-1.49888E+01
2273	0.1	2.0960	-1.49685E+01
2273	0.1	2.0970	-1.49481E+01
2273	0.1	2.0980	-1.49277E+01
2273	0.1	2.0990	-1.49073E+01
2273	0.1	2.1000	-1.48868E+01
2273	0.1	2.1010	-1.48663E+01
2273	0.1	2.1020	-1.48458E+01

2273	0.1	2.1030	-1.48252E+01
2273	0.1	2.1040	-1.48046E+01
2273	0.1	2.1050	-1.47840E+01
2273	0.1	2.1060	-1.47634E+01
2273	0.1	2.1070	-1.47427E+01
2273	0.1	2.1080	-1.47220E+01
2273	0.1	2.1090	-1.47012E+01
2273	0.1	2.1100	-1.46805E+01
2273	0.1	2.1110	-1.46597E+01
2273	0.1	2.1120	-1.46389E+01
2273	0.1	2.1130	-1.46180E+01
2273	0.1	2.1140	-1.45972E+01
2273	0.1	2.1150	-1.45763E+01
2273	0.1	2.1160	-1.45554E+01
2273	0.1	2.1170	-1.45345E+01
2273	0.1	2.1180	-1.45135E+01
2273	0.1	2.1190	-1.44925E+01
2273	0.1	2.1200	-1.44716E+01
2273	0.1	2.1210	-1.44506E+01
2273	0.1	2.1220	-1.44295E+01
2273	0.1	2.1230	-1.44085E+01
2273	0.1	2.1240	-1.43875E+01
2273	0.1	2.1250	-1.43664E+01
2273	0.1	2.1260	-1.43453E+01
2273	0.1	2.1270	-1.43242E+01
2273	0.1	2.1280	-1.43031E+01
2273	0.1	2.1290	-1.42820E+01
2273	0.1	2.1300	-1.42608E+01
2273	0.1	2.1310	-1.42397E+01
2273	0.1	2.1320	-1.42185E+01
2273	0.1	2.1330	-1.41973E+01

2273	0.1	2.1340	-1.41761E+01
2273	0.1	2.1350	-1.41549E+01
2273	0.1	2.1360	-1.41337E+01
2273	0.1	2.1370	-1.41125E+01
2273	0.1	2.1380	-1.40913E+01
2273	0.1	2.1390	-1.40700E+01
2273	0.1	2.1400	-1.40488E+01
2273	0.1	2.1410	-1.40275E+01
2273	0.1	2.1420	-1.40062E+01
2273	0.1	2.1430	-1.39850E+01
2273	0.1	2.1440	-1.39637E+01
2273	0.1	2.1450	-1.39424E+01
2273	0.1	2.1460	-1.39211E+01
2273	0.1	2.1470	-1.38998E+01
2273	0.1	2.1480	-1.38785E+01
2273	0.1	2.1490	-1.38571E+01
2273	0.1	2.1500	-1.38358E+01
2273	0.1	2.1510	-1.38145E+01
2273	0.1	2.1520	-1.37932E+01
2273	0.1	2.1530	-1.37718E+01
2273	0.1	2.1540	-1.37505E+01
2273	0.1	2.1550	-1.37291E+01
2273	0.1	2.1560	-1.37078E+01
2273	0.1	2.1570	-1.36864E+01
2273	0.1	2.1580	-1.36650E+01
2273	0.1	2.1590	-1.36437E+01
2273	0.1	2.1600	-1.36223E+01

A.2.2. $(U_{0.8}Pu_{0.2})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∗] _{Pu} (m ² /s)
1273	0.2	1.9000	-2.57434E+01
1273	0.2	1.9010	-2.57400E+01
1273	0.2	1.9020	-2.57364E+01
1273	0.2	1.9030	-2.57336E+01
1273	0.2	1.9040	-2.57317E+01
1273	0.2	1.9050	-2.57306E+01
1273	0.2	1.9060	-2.57302E+01
1273	0.2	1.9070	-2.57306E+01
1273	0.2	1.9080	-2.57317E+01
1273	0.2	1.9090	-2.57333E+01
1273	0.2	1.9100	-2.57355E+01
1273	0.2	1.9110	-2.57381E+01
1273	0.2	1.9120	-2.57412E+01
1273	0.2	1.9130	-2.57447E+01
1273	0.2	1.9140	-2.57486E+01
1273	0.2	1.9150	-2.57529E+01
1273	0.2	1.9160	-2.57574E+01
1273	0.2	1.9170	-2.57623E+01
1273	0.2	1.9180	-2.57675E+01
1273	0.2	1.9190	-2.57729E+01
1273	0.2	1.9200	-2.57785E+01
1273	0.2	1.9210	-2.57844E+01
1273	0.2	1.9220	-2.57905E+01
1273	0.2	1.9230	-2.57968E+01
1273	0.2	1.9240	-2.58033E+01
1273	0.2	1.9250	-2.58100E+01
1273	0.2	1.9260	-2.58169E+01
1273	0.2	1.9270	-2.58239E+01
1273	0.2	1.9280	-2.58311E+01
1273	0.2	1.9290	-2.58385E+01
1273	0.2	1.9300	-2.58460E+01
1273	0.2	1.9310	-2.58537E+01
1273	0.2	1.9320	-2.58616E+01
1273	0.2	1.9330	-2.58696E+01
1273	0.2	1.9340	-2.58778E+01
1273	0.2	1.9350	-2.58861E+01
1273	0.2	1.9360	-2.58946E+01
1273	0.2	1.9370	-2.59033E+01
1273	0.2	1.9380	-2.59122E+01
1273	0.2	1.9390	-2.59212E+01
1273	0.2	1.9400	-2.59305E+01
1273	0.2	1.9410	-2.59399E+01
1273	0.2	1.9420	-2.59495E+01
1273	0.2	1.9430	-2.59594E+01
1273	0.2	1.9440	-2.59695E+01
1273	0.2	1.9450	-2.59798E+01
1273	0.2	1.9460	-2.59904E+01
1273	0.2	1.9470	-2.60013E+01
1273	0.2	1.9480	-2.60124E+01
1273	0.2	1.9490	-2.60238E+01
1273	0.2	1.9500	-2.60355E+01
1273	0.2	1.9510	-2.60476E+01
1273	0.2	1.9520	-2.60600E+01
1273	0.2	1.9530	-2.60728E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∗] _{Pu} (m ² /s)
1273	0.2	1.9540	-2.60859E+01
1273	0.2	1.9550	-2.60995E+01
1273	0.2	1.9560	-2.61134E+01
1273	0.2	1.9570	-2.61278E+01
1273	0.2	1.9580	-2.61426E+01
1273	0.2	1.9590	-2.61580E+01
1273	0.2	1.9600	-2.61738E+01
1273	0.2	1.9610	-2.61901E+01
1273	0.2	1.9620	-2.62069E+01
1273	0.2	1.9630	-2.62243E+01
1273	0.2	1.9640	-2.62422E+01
1273	0.2	1.9650	-2.62607E+01
1273	0.2	1.9660	-2.62798E+01
1273	0.2	1.9670	-2.62995E+01
1273	0.2	1.9680	-2.63197E+01
1273	0.2	1.9690	-2.63406E+01
1273	0.2	1.9700	-2.63621E+01
1273	0.2	1.9710	-2.63842E+01
1273	0.2	1.9720	-2.64069E+01
1273	0.2	1.9730	-2.64302E+01
1273	0.2	1.9740	-2.64541E+01
1273	0.2	1.9750	-2.64785E+01
1273	0.2	1.9760	-2.65036E+01
1273	0.2	1.9770	-2.65292E+01
1273	0.2	1.9780	-2.65554E+01
1273	0.2	1.9790	-2.65821E+01
1273	0.2	1.9800	-2.66094E+01
1273	0.2	1.9810	-2.66370E+01
1273	0.2	1.9820	-2.66652E+01
1273	0.2	1.9830	-2.66937E+01
1273	0.2	1.9840	-2.67227E+01
1273	0.2	1.9850	-2.67519E+01
1273	0.2	1.9860	-2.67814E+01
1273	0.2	1.9870	-2.68112E+01
1273	0.2	1.9880	-2.68411E+01
1273	0.2	1.9890	-2.68711E+01
1273	0.2	1.9900	-2.69011E+01
1273	0.2	1.9910	-2.69311E+01
1273	0.2	1.9920	-2.69610E+01
1273	0.2	1.9930	-2.69906E+01
1273	0.2	1.9940	-2.70198E+01
1273	0.2	1.9950	-2.70486E+01
1273	0.2	1.9960	-2.70769E+01
1273	0.2	1.9970	-2.71044E+01
1273	0.2	1.9980	-2.71312E+01
1273	0.2	1.9990	-2.71570E+01
1273	0.2	2.0000	-2.71817E+01
1273	0.2	2.0010	-2.72023E+01
1273	0.2	2.0020	-2.72208E+01
1273	0.2	2.0030	-2.72369E+01
1273	0.2	2.0040	-2.72507E+01
1273	0.2	2.0050	-2.72619E+01
1273	0.2	2.0060	-2.72706E+01
1273	0.2	2.0070	-2.72768E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D [∗] _{Pu} (m ² /s)
1273	0.2	2.0080	-2.72805E+01
1273	0.2	2.0090	-2.72818E+01
1273	0.2	2.0100	-2.72807E+01
1273	0.2	2.0110	-2.72773E+01
1273	0.2	2.0120	-2.72718E+01
1273	0.2	2.0130	-2.72644E+01
1273	0.2	2.0140	-2.72550E+01
1273	0.2	2.0150	-2.72440E+01
1273	0.2	2.0160	-2.72314E+01
1273	0.2	2.0170	-2.72173E+01
1273	0.2	2.0180	-2.72020E+01
1273	0.2	2.0190	-2.71854E+01
1273	0.2	2.0200	-2.71678E+01
1273	0.2	2.0210	-2.71492E+01
1273	0.2	2.0220	-2.71297E+01
1273	0.2	2.0230	-2.71095E+01
1273	0.2	2.0240	-2.70884E+01
1273	0.2	2.0250	-2.70667E+01
1273	0.2	2.0260	-2.70444E+01
1273	0.2	2.0270	-2.70215E+01
1273	0.2	2.0280	-2.69981E+01
1273	0.2	2.0290	-2.69741E+01
1273	0.2	2.0300	-2.69497E+01
1273	0.2	2.0310	-2.69249E+01
1273	0.2	2.0320	-2.68997E+01
1273	0.2	2.0330	-2.68740E+01
1273	0.2	2.0340	-2.68480E+01
1273	0.2	2.0350	-2.68216E+01
1273	0.2	2.0360	-2.67949E+01
1273	0.2	2.0370	-2.67679E+01
1273	0.2	2.0380	-2.67405E+01
1273	0.2	2.0390	-2.67128E+01
1273	0.2	2.0400	-2.66848E+01
1273	0.2	2.0410	-2.66566E+01
1273	0.2	2.0420	-2.66280E+01
1273	0.2	2.0430	-2.65992E+01
1273	0.2	2.0440	-2.65701E+01
1273	0.2	2.0450	-2.65407E+01
1273	0.2	2.0460	-2.65111E+01
1273	0.2	2.0470	-2.64813E+01
1273	0.2	2.0480	-2.64512E+01
1273	0.2	2.0490	-2.64209E+01
1273	0.2	2.0500	-2.63904E+01
1273	0.2	2.0510	-2.63596E+01
1273			

1273	0.2	2.0620	-2.60091E+01
1273	0.2	2.0630	-2.59762E+01
1273	0.2	2.0640	-2.59433E+01
1273	0.2	2.0650	-2.59102E+01
1273	0.2	2.0660	-2.58770E+01
1273	0.2	2.0670	-2.58437E+01
1273	0.2	2.0680	-2.58103E+01
1273	0.2	2.0690	-2.57768E+01
1273	0.2	2.0700	-2.57432E+01
1273	0.2	2.0710	-2.57095E+01
1273	0.2	2.0720	-2.56757E+01
1273	0.2	2.0730	-2.56418E+01
1273	0.2	2.0740	-2.56079E+01
1273	0.2	2.0750	-2.55739E+01
1273	0.2	2.0760	-2.55398E+01
1273	0.2	2.0770	-2.55056E+01
1273	0.2	2.0780	-2.54714E+01
1273	0.2	2.0790	-2.54371E+01
1273	0.2	2.0800	-2.54028E+01
1273	0.2	2.0810	-2.53684E+01
1273	0.2	2.0820	-2.53339E+01
1273	0.2	2.0830	-2.52995E+01
1273	0.2	2.0840	-2.52649E+01
1273	0.2	2.0850	-2.52304E+01
1273	0.2	2.0860	-2.51958E+01
1273	0.2	2.0870	-2.51612E+01
1273	0.2	2.0880	-2.51265E+01
1273	0.2	2.0890	-2.50918E+01
1273	0.2	2.0900	-2.50571E+01
1273	0.2	2.0910	-2.50224E+01
1273	0.2	2.0920	-2.49876E+01
1273	0.2	2.0930	-2.49529E+01
1273	0.2	2.0940	-2.49181E+01
1273	0.2	2.0950	-2.48833E+01
1273	0.2	2.0960	-2.48484E+01
1273	0.2	2.0970	-2.48136E+01
1273	0.2	2.0980	-2.47788E+01
1273	0.2	2.0990	-2.47439E+01
1273	0.2	2.1000	-2.47090E+01
1273	0.2	2.1010	-2.46742E+01
1273	0.2	2.1020	-2.46393E+01
1273	0.2	2.1030	-2.46044E+01
1273	0.2	2.1040	-2.45695E+01
1273	0.2	2.1050	-2.45346E+01
1273	0.2	2.1060	-2.44997E+01
1273	0.2	2.1070	-2.44648E+01
1273	0.2	2.1080	-2.44300E+01
1273	0.2	2.1090	-2.43951E+01
1273	0.2	2.1100	-2.43602E+01
1273	0.2	2.1110	-2.43253E+01
1273	0.2	2.1120	-2.42904E+01
1273	0.2	2.1130	-2.42555E+01
1273	0.2	2.1140	-2.42206E+01
1273	0.2	2.1150	-2.41858E+01
1273	0.2	2.1160	-2.41509E+01
1273	0.2	2.1170	-2.41160E+01
1273	0.2	2.1180	-2.40812E+01
1273	0.2	2.1190	-2.40463E+01
1273	0.2	2.1200	-2.40115E+01
1273	0.2	2.1210	-2.39767E+01
1273	0.2	2.1220	-2.39419E+01
1273	0.2	2.1230	-2.39070E+01
1273	0.2	2.1240	-2.38722E+01
1273	0.2	2.1250	-2.38374E+01
1273	0.2	2.1260	-2.38026E+01
1273	0.2	2.1270	-2.37679E+01
1273	0.2	2.1280	-2.37331E+01
1273	0.2	2.1290	-2.36983E+01
1273	0.2	2.1300	-2.36636E+01
1273	0.2	2.1310	-2.36289E+01
1273	0.2	2.1320	-2.35941E+01
1273	0.2	2.1330	-2.35594E+01
1273	0.2	2.1340	-2.35247E+01
1273	0.2	2.1350	-2.34900E+01
1273	0.2	2.1360	-2.34554E+01
1273	0.2	2.1370	-2.34207E+01
1273	0.2	2.1380	-2.33860E+01
1273	0.2	2.1390	-2.33514E+01
1273	0.2	2.1400	-2.33168E+01
1273	0.2	2.1410	-2.32822E+01
1273	0.2	2.1420	-2.32476E+01
1273	0.2	2.1430	-2.32130E+01
1273	0.2	2.1440	-2.31784E+01
1273	0.2	2.1450	-2.31438E+01
1273	0.2	2.1460	-2.31093E+01
1273	0.2	2.1470	-2.30747E+01
1273	0.2	2.1480	-2.30402E+01
1273	0.2	2.1490	-2.30057E+01
1273	0.2	2.1500	-2.29712E+01
1273	0.2	2.1510	-2.29367E+01
1273	0.2	2.1520	-2.29022E+01
1273	0.2	2.1530	-2.28678E+01

1273	0.2	2.1540	-2.28333E+01
1273	0.2	2.1550	-2.27989E+01
1273	0.2	2.1560	-2.27645E+01
1273	0.2	2.1570	-2.27301E+01
1273	0.2	2.1580	-2.26957E+01
1273	0.2	2.1590	-2.26613E+01
1273	0.2	2.1600	-2.26270E+01
1273	0.2	2.1610	-2.25926E+01
1273	0.2	2.1620	-2.25583E+01
1273	0.2	2.1630	-2.25240E+01
1273	0.2	2.1640	-2.24897E+01
1273	0.2	2.1650	-2.24554E+01
1273	0.2	2.1660	-2.24211E+01
1273	0.2	2.1670	-2.23869E+01
1273	0.2	2.1680	-2.23526E+01
1273	0.2	2.1690	-2.23184E+01
1273	0.2	2.1700	-2.22842E+01
1273	0.2	2.1710	-2.22500E+01
1273	0.2	2.1720	-2.22158E+01
1273	0.2	2.1730	-2.21816E+01
1273	0.2	2.1740	-2.21474E+01
1273	0.2	2.1750	-2.21133E+01
1273	0.2	2.1760	-2.20792E+01
1273	0.2	2.1770	-2.20450E+01
1273	0.2	2.1780	-2.20109E+01
1273	0.2	2.1790	-2.19769E+01
1273	0.2	2.1800	-2.19428E+01
1273	0.2	1.8700	-1.95073E+01
1273	0.2	1.8710	-1.95073E+01
1273	0.2	1.8720	-1.95073E+01
1273	0.2	1.8730	-1.95073E+01
1273	0.2	1.8740	-1.95072E+01
1273	0.2	1.8750	-1.95072E+01
1273	0.2	1.8760	-1.95072E+01
1273	0.2	1.8770	-1.95072E+01
1273	0.2	1.8780	-1.95071E+01
1273	0.2	1.8790	-1.95071E+01
1273	0.2	1.8800	-1.95071E+01
1273	0.2	1.8810	-1.95070E+01
1273	0.2	1.8820	-1.95070E+01
1273	0.2	1.8830	-1.95069E+01
1273	0.2	1.8840	-1.95069E+01
1273	0.2	1.8850	-1.95068E+01
1273	0.2	1.8860	-1.95068E+01
1273	0.2	1.8870	-1.95067E+01
1273	0.2	1.8880	-1.95067E+01
1273	0.2	1.8890	-1.95066E+01
1273	0.2	1.8900	-1.95065E+01
1273	0.2	1.8910	-1.95064E+01
1273	0.2	1.8920	-1.95063E+01
1273	0.2	1.8930	-1.95062E+01
1273	0.2	1.8940	-1.95061E+01
1273	0.2	1.8950	-1.95060E+01
1273	0.2	1.8960	-1.95060E+01
1273	0.2	1.8970	-1.95059E+01
1273	0.2	1.8980	-1.95059E+01
1273	0.2	1.8990	-1.95059E+01
1273	0.2	1.8990	-1.95060E+01
1273	0.2	1.9000	-1.95061E+01
1273	0.2	1.9010	-1.95064E+01
1273	0.2	1.9020	-1.95069E+01
1273	0.2	1.9030	-1.95076E+01
1273	0.2	1.9040	-1.95085E+01
1273	0.2	1.9050	-1.95097E+01
1273	0.2	1.9060	-1.95112E+01
1273	0.2	1.9070	-1.95130E+01
1273	0.2	1.9080	-1.95151E+01
1273	0.2	1.9090	-1.95175E+01
1273	0.2	1.9100	-1.95202E+01
1273	0.2	1.9110	-1.95232E+01
1273	0.2	1.9120	-1.95264E+01
1273	0.2	1.9130	-1.95300E+01
1273	0.2	1.9140	-1.95338E+01
1273	0.2	1.9150	-1.95379E+01
1273	0.2	1.9160	-1.95423E+01
1273	0.2	1.9170	-1.95469E+01
1273	0.2	1.9180	-1.95517E+01
1273	0.2	1.9190	-1.95568E+01
1273	0.2	1.9200	-1.95622E+01
1273	0.2	1.9210	-1.95678E+01
1273	0.2	1.9220	-1.95736E+01
1273	0.2	1.9230	-1.95797E+01
1273	0.2	1.9240	-1.95860E+01
1273	0.2	1.9250	-1.95926E+01
1273	0.2	1.9260	-1.95994E+01
1273	0.2	1.9270	-1.96064E+01
1273	0.2	1.9280	-1.96137E+01
1273	0.2	1.9290	-1.96212E+01
1273	0.2	1.9300	-1.96290E+01
1273	0.2	1.9310	-1.96370E+01
1273	0.2	1.9320	-1.96453E+01
1273	0.2	1.9330	-1.96538E+01
1273	0.2	1.9340	-1.96626E+01

1773	0.2	1.9350	-1.96716E+01
1773	0.2	1.9360	-1.96809E+01
1773	0.2	1.9370	-1.96905E+01
1773	0.2	1.9380	-1.97003E+01
1773	0.2	1.9390	-1.97104E+01
1773	0.2	1.9400	-1.97208E+01
1773	0.2	1.9410	-1.97315E+01
1773	0.2	1.9420	-1.97425E+01
1773	0.2	1.9430	-1.97538E+01
1773	0.2	1.9440	-1.97653E+01
1773	0.2	1.9450	-1.97772E+01
1773	0.2	1.9460	-1.97893E+01
1773	0.2	1.9470	-1.98017E+01
1773	0.2	1.9480	-1.98145E+01
1773	0.2	1.9490	-1.98275E+01
1773	0.2	1.9500	-1.98408E+01
1773	0.2	1.9510	-1.98545E+01
1773	0.2	1.9520	-1.98684E+01
1773	0.2	1.9530	-1.98826E+01
1773	0.2	1.9540	-1.98970E+01
1773	0.2	1.9550	-1.99118E+01
1773	0.2	1.9560	-1.99268E+01
1773	0.2	1.9570	-1.99421E+01
1773	0.2	1.9580	-1.99577E+01
1773	0.2	1.9590	-1.99734E+01
1773	0.2	1.9600	-1.99894E+01
1773	0.2	1.9610	-2.00057E+01
1773	0.2	1.9620	-2.00221E+01
1773	0.2	1.9630	-2.00387E+01
1773	0.2	1.9640	-2.00555E+01
1773	0.2	1.9650	-2.00725E+01
1773	0.2	1.9660	-2.00895E+01
1773	0.2	1.9670	-2.01067E+01
1773	0.2	1.9680	-2.01240E+01
1773	0.2	1.9690	-2.01413E+01
1773	0.2	1.9700	-2.01587E+01
1773	0.2	1.9710	-2.01761E+01
1773	0.2	1.9720	-2.01934E+01
1773	0.2	1.9730	-2.02107E+01
1773	0.2	1.9740	-2.02280E+01
1773	0.2	1.9750	-2.02451E+01
1773	0.2	1.9760	-2.02621E+01
1773	0.2	1.9770	-2.02797E+01
1773	0.2	1.9780	-2.02955E+01
1773	0.2	1.9790	-2.03118E+01
1773	0.2	1.9800	-2.03279E+01
1773	0.2	1.9810	-2.03436E+01
1773	0.2	1.9820	-2.03590E+01
1773	0.2	1.9830	-2.03739E+01
1773	0.2	1.9840	-2.03884E+01
1773	0.2	1.9850	-2.04025E+01
1773	0.2	1.9860	-2.04160E+01
1773	0.2	1.9870	-2.04290E+01
1773	0.2	1.9880	-2.04413E+01
1773	0.2	1.9890	-2.04531E+01
1773	0.2	1.9900	-2.04642E+01
1773	0.2	1.9910	-2.04747E+01
1773	0.2	1.9920	-2.04844E+01
1773	0.2	1.9930	-2.04935E+01
1773	0.2	1.9940	-2.05017E+01
1773	0.2	1.9950	-2.05093E+01
1773	0.2	1.9960	-2.05160E+01
1773	0.2	1.9970	-2.05220E+01
1773	0.2	1.9980	-2.05271E+01
1773	0.2	1.9990	-2.05315E+01
1773	0.2		

1773	0.2	2.0270	-2.02336E+01
1773	0.2	2.0280	-2.02163E+01
1773	0.2	2.0290	-2.01988E+01
1773	0.2	2.0300	-2.01810E+01
1773	0.2	2.0310	-2.01630E+01
1773	0.2	2.0320	-2.01448E+01
1773	0.2	2.0330	-2.01264E+01
1773	0.2	2.0340	-2.01077E+01
1773	0.2	2.0350	-2.00889E+01
1773	0.2	2.0360	-2.00699E+01
1773	0.2	2.0370	-2.00507E+01
1773	0.2	2.0380	-2.00313E+01
1773	0.2	2.0390	-2.00117E+01
1773	0.2	2.0400	-1.99919E+01
1773	0.2	2.0410	-1.99720E+01
1773	0.2	2.0420	-1.99518E+01
1773	0.2	2.0430	-1.99315E+01
1773	0.2	2.0440	-1.99111E+01
1773	0.2	2.0450	-1.98904E+01
1773	0.2	2.0460	-1.98696E+01
1773	0.2	2.0470	-1.98487E+01
1773	0.2	2.0480	-1.98276E+01
1773	0.2	2.0490	-1.98063E+01
1773	0.2	2.0500	-1.97848E+01
1773	0.2	2.0510	-1.97632E+01
1773	0.2	2.0520	-1.97415E+01
1773	0.2	2.0530	-1.97196E+01
1773	0.2	2.0540	-1.96975E+01
1773	0.2	2.0550	-1.96753E+01
1773	0.2	2.0560	-1.96529E+01
1773	0.2	2.0570	-1.96304E+01
1773	0.2	2.0580	-1.96078E+01
1773	0.2	2.0590	-1.95850E+01
1773	0.2	2.0600	-1.95621E+01
1773	0.2	2.0610	-1.95390E+01
1773	0.2	2.0620	-1.95158E+01
1773	0.2	2.0630	-1.94924E+01
1773	0.2	2.0640	-1.94690E+01
1773	0.2	2.0650	-1.94454E+01
1773	0.2	2.0660	-1.94216E+01
1773	0.2	2.0670	-1.93978E+01
1773	0.2	2.0680	-1.93738E+01
1773	0.2	2.0690	-1.93497E+01
1773	0.2	2.0700	-1.93255E+01
1773	0.2	2.0710	-1.93011E+01
1773	0.2	2.0720	-1.92767E+01
1773	0.2	2.0730	-1.92521E+01
1773	0.2	2.0740	-1.92274E+01
1773	0.2	2.0750	-1.92026E+01
1773	0.2	2.0760	-1.91777E+01
1773	0.2	2.0770	-1.91527E+01
1773	0.2	2.0780	-1.91276E+01
1773	0.2	2.0790	-1.91024E+01
1773	0.2	2.0800	-1.90771E+01
1773	0.2	2.0810	-1.90517E+01
1773	0.2	2.0820	-1.90262E+01
1773	0.2	2.0830	-1.90006E+01
1773	0.2	2.0840	-1.89750E+01
1773	0.2	2.0850	-1.89492E+01
1773	0.2	2.0860	-1.89234E+01
1773	0.2	2.0870	-1.88975E+01
1773	0.2	2.0880	-1.88715E+01
1773	0.2	2.0890	-1.88454E+01
1773	0.2	2.0900	-1.88193E+01
1773	0.2	2.0910	-1.87930E+01
1773	0.2	2.0920	-1.87668E+01
1773	0.2	2.0930	-1.87404E+01
1773	0.2	2.0940	-1.87140E+01
1773	0.2	2.0950	-1.86875E+01
1773	0.2	2.0960	-1.86610E+01
1773	0.2	2.0970	-1.86344E+01
1773	0.2	2.0980	-1.86078E+01
1773	0.2	2.0990	-1.85811E+01
1773	0.2	2.1000	-1.85543E+01
1773	0.2	2.1010	-1.85275E+01
1773	0.2	2.1020	-1.85007E+01
1773	0.2	2.1030	-1.84738E+01
1773	0.2	2.1040	-1.84469E+01
1773	0.2	2.1050	-1.84199E+01
1773	0.2	2.1060	-1.83929E+01
1773	0.2	2.1070	-1.83658E+01
1773	0.2	2.1080	-1.83387E+01
1773	0.2	2.1090	-1.83116E+01
1773	0.2	2.1100	-1.82845E+01
1773	0.2	2.1110	-1.82573E+01
1773	0.2	2.1120	-1.82300E+01
1773	0.2	2.1130	-1.82028E+01
1773	0.2	2.1140	-1.81755E+01
1773	0.2	2.1150	-1.81482E+01
1773	0.2	2.1160	-1.81209E+01
1773	0.2	2.1170	-1.80936E+01
1773	0.2	2.1180	-1.80662E+01

1773	0.2	2.1190	-1.80388E+01
1773	0.2	2.1200	-1.80114E+01
1773	0.2	2.1210	-1.79840E+01
1773	0.2	2.1220	-1.79565E+01
1773	0.2	2.1230	-1.79291E+01
1773	0.2	2.1240	-1.79016E+01
1773	0.2	2.1250	-1.78741E+01
1773	0.2	2.1260	-1.78466E+01
1773	0.2	2.1270	-1.78191E+01
1773	0.2	2.1280	-1.77915E+01
1773	0.2	2.1290	-1.77640E+01
1773	0.2	2.1300	-1.77365E+01
1773	0.2	2.1310	-1.77089E+01
1773	0.2	2.1320	-1.76813E+01
1773	0.2	2.1330	-1.76538E+01
1773	0.2	2.1340	-1.76262E+01
1773	0.2	2.1350	-1.75986E+01
1773	0.2	2.1360	-1.75710E+01
1773	0.2	2.1370	-1.75434E+01
1773	0.2	2.1380	-1.75158E+01
1773	0.2	2.1390	-1.74882E+01
1773	0.2	2.1400	-1.74606E+01
1773	0.2	2.1410	-1.74330E+01
1773	0.2	2.1420	-1.74054E+01
1773	0.2	2.1430	-1.73778E+01
1773	0.2	2.1440	-1.73502E+01
1773	0.2	2.1450	-1.73226E+01
1773	0.2	2.1460	-1.72950E+01
1773	0.2	2.1470	-1.72674E+01
1773	0.2	2.1480	-1.72398E+01
1773	0.2	2.1490	-1.72122E+01
1773	0.2	2.1500	-1.71846E+01
1773	0.2	2.1510	-1.71570E+01
1773	0.2	2.1520	-1.71294E+01
1773	0.2	2.1530	-1.71018E+01
1773	0.2	2.1540	-1.70742E+01
1773	0.2	2.1550	-1.70466E+01
1773	0.2	2.1560	-1.70190E+01
1773	0.2	2.1570	-1.69914E+01
1773	0.2	2.1580	-1.69639E+01
1773	0.2	2.1590	-1.69363E+01
1773	0.2	2.1600	-1.69087E+01
1773	0.2	2.1610	-1.68812E+01
1773	0.2	2.1620	-1.68536E+01
1773	0.2	2.1630	-1.68261E+01
1773	0.2	2.1640	-1.67985E+01
1773	0.2	2.1650	-1.67710E+01
1773	0.2	2.1660	-1.67435E+01
1773	0.2	2.1670	-1.67159E+01
1773	0.2	2.1680	-1.66884E+01
1773	0.2	2.1690	-1.66609E+01
1773	0.2	2.1700	-1.66334E+01
1773	0.2	2.1710	-1.66059E+01
1773	0.2	2.1720	-1.65784E+01
1773	0.2	2.1730	-1.65509E+01
1773	0.2	2.1740	-1.65234E+01
1773	0.2	2.1750	-1.64960E+01
1773	0.2	2.1760	-1.64685E+01
1773	0.2	2.1770	-1.64411E+01
1773	0.2	2.1780	-1.64136E+01
1773	0.2	2.1790	-1.63862E+01
1773	0.2	2.1800	-1.63587E+01
2273	0.2	1.8000	-1.59880E+01
2273	0.2	1.8010	-1.59880E+01
2273	0.2	1.8020	-1.59880E+01
2273	0.2	1.8030	-1.59880E+01
2273	0.2	1.8040	-1.59880E+01
2273	0.2	1.8050	-1.59881E+01
2273	0.2	1.8060	-1.59881E+01
2273	0.2	1.8070	-1.59881E+01
2273	0.2	1.8080	-1.59881E+01
2273	0.2	1.8090	-1.59881E+01
2273	0.2	1.8100	-1.59882E+01
2273	0.2	1.8110	-1.59882E+01
2273	0.2	1.8120	-1.59882E+01
2273	0.2	1.8130	-1.59882E+01
2273	0.2	1.8140	-1.59882E+01
2273	0.2	1.8150	-1.59883E+01
2273	0.2	1.8160	-1.59883E+01
2273	0.2	1.8170	-1.59883E+01
2273	0.2	1.8180	-1.59883E+01
2273	0.2	1.8190	-1.59884E+01
2273	0.2	1.8200	-1.59884E+01
2273	0.2	1.8210	-1.59884E+01
2273	0.2	1.8220	-1.59884E+01
2273	0.2	1.8230	-1.59885E+01
2273	0.2	1.8240	-1.59885E+01
2273	0.2	1.8250	-1.59885E+01
2273	0.2	1.8260	-1.59886E+01
2273	0.2	1.8270	-1.59886E+01
2273	0.2	1.8280	-1.59886E+01
2273	0.2	1.8290	-1.59887E+01

2273	0.2	1.8300	-1.59887E+01
2273	0.2	1.8310	-1.59887E+01
2273	0.2	1.8320	-1.59888E+01
2273	0.2	1.8330	-1.59888E+01
2273	0.2	1.8340	-1.59889E+01
2273	0.2	1.8350	-1.59889E+01
2273	0.2	1.8360	-1.59890E+01
2273	0.2	1.8370	-1.59890E+01
2273	0.2	1.8380	-1.59890E+01
2273	0.2	1.8390	-1.59891E+01
2273	0.2	1.8400	-1.59891E+01
2273	0.2	1.8410	-1.59892E+01
2273	0.2	1.8420	-1.59892E+01
2273	0.2	1.8430	-1.59893E+01
2273	0.2	1.8440	-1.59893E+01
2273	0.2	1.8450	-1.59894E+01
2273	0.2	1.8460	-1.59894E+01
2273	0.2	1.8470	-1.59895E+01
2273	0.2	1.8480	-1.59896E+01
2273	0.2	1.8490	-1.59896E+01
2273	0.2	1.8500	-1.59897E+01
2273	0.2	1.8510	-1.59898E+01
2273	0.2	1.8520	-1.59899E+01
2273	0.2	1.8530	-1.59900E+01
2273	0.2	1.8540	-1.59900E+01
2273	0.2	1.8550	-1.59901E+01
2273	0.2	1.8560	-1.59902E+01
2273	0.2	1.8570	-1.59903E+01
2273	0.2	1.8580	-1.59904E+01
2273	0.2	1.8590	-1.59905E+01
2273	0.2	1.8600	-1.59906E+01
2273	0.2	1.8610	-1.59908E+01
2273	0.2	1.8620	-1.59909E+01
2273	0.2	1.8630	-1.59910E+01
2273	0.2	1.8640	-1.59912E+01
2273	0.2	1.8650	-1.59913E+01
2273	0.2	1.8660	-1.59915E+01
2273	0.2	1.8670	-1.59916E+01
2273	0.2	1.8680	-1.59918E+01
2273	0.2	1.8690	-1.59920E+01
2273	0.2	1.8700	-1.59922E+01
2273	0.2	1.8710	-1.59924E+01
2273	0.2	1.8720	-1.59927E+01
2273	0.2	1.8730	-1.59929E+01
2273	0.2	1.8740	-1.59932E+01
2273	0.2	1.8750	-1.59934E+01
2273	0.2	1.8760	-1.59937E+01
2273	0.2	1.8770	-1.59941E+01
2273	0.2	1.8780	-1.59944E+01
2273	0.2	1.8790	-1.59948E+01
2273	0.2	1.8800	-1.59952E+01
2273	0.2	1.8810	-1.59956E+01
2273	0.2	1.8820	-1.59961E+01
2273	0.2	1.8830	-1.59966E+01
2273	0.2	1.8840	-1.59971E+01
2273	0.2	1.8850	-1.59977E+01
2273	0.2	1.8860	-1.59983E+01
2273	0.2	1.8870	-1.59990E+01
2273	0.2	1.8880	-1.59998E+01
2273	0.2	1.8890	-1.60006E+01
2273	0.2	1.8900	-1.60015E+01
2273	0.2	1.8910	-1.60024E+01
2273	0.2	1.8920	-1.60035E+01
2273	0.2	1.8930	-1.60046E+01
2273	0.2	1.8940	-1.60058E+01
2273	0.2	1.8950	-1.60071E+01
2273	0.2		

2273	0.2	1.9220	-1.61086E+01
2273	0.2	1.9230	-1.61154E+01
2273	0.2	1.9240	-1.61224E+01
2273	0.2	1.9250	-1.61297E+01
2273	0.2	1.9260	-1.61372E+01
2273	0.2	1.9270	-1.61449E+01
2273	0.2	1.9280	-1.61529E+01
2273	0.2	1.9290	-1.61611E+01
2273	0.2	1.9300	-1.61695E+01
2273	0.2	1.9310	-1.61781E+01
2273	0.2	1.9320	-1.61870E+01
2273	0.2	1.9330	-1.61961E+01
2273	0.2	1.9340	-1.62054E+01
2273	0.2	1.9350	-1.62149E+01
2273	0.2	1.9360	-1.62247E+01
2273	0.2	1.9370	-1.62346E+01
2273	0.2	1.9380	-1.62448E+01
2273	0.2	1.9390	-1.62551E+01
2273	0.2	1.9400	-1.62656E+01
2273	0.2	1.9410	-1.62763E+01
2273	0.2	1.9420	-1.62872E+01
2273	0.2	1.9430	-1.62983E+01
2273	0.2	1.9440	-1.63095E+01
2273	0.2	1.9450	-1.63208E+01
2273	0.2	1.9460	-1.63323E+01
2273	0.2	1.9470	-1.63440E+01
2273	0.2	1.9480	-1.63557E+01
2273	0.2	1.9490	-1.63675E+01
2273	0.2	1.9500	-1.63795E+01
2273	0.2	1.9510	-1.63915E+01
2273	0.2	1.9520	-1.64036E+01
2273	0.2	1.9530	-1.64157E+01
2273	0.2	1.9540	-1.64279E+01
2273	0.2	1.9550	-1.64400E+01
2273	0.2	1.9560	-1.64522E+01
2273	0.2	1.9570	-1.64644E+01
2273	0.2	1.9580	-1.64765E+01
2273	0.2	1.9590	-1.64886E+01
2273	0.2	1.9600	-1.65006E+01
2273	0.2	1.9610	-1.65125E+01
2273	0.2	1.9620	-1.65243E+01
2273	0.2	1.9630	-1.65360E+01
2273	0.2	1.9640	-1.65475E+01
2273	0.2	1.9650	-1.65588E+01
2273	0.2	1.9660	-1.65700E+01
2273	0.2	1.9670	-1.65809E+01
2273	0.2	1.9680	-1.65916E+01
2273	0.2	1.9690	-1.66020E+01
2273	0.2	1.9700	-1.66121E+01
2273	0.2	1.9710	-1.66220E+01
2273	0.2	1.9720	-1.66315E+01
2273	0.2	1.9730	-1.66407E+01
2273	0.2	1.9740	-1.66495E+01
2273	0.2	1.9750	-1.66580E+01
2273	0.2	1.9760	-1.66661E+01
2273	0.2	1.9770	-1.66737E+01
2273	0.2	1.9780	-1.66809E+01
2273	0.2	1.9790	-1.66877E+01
2273	0.2	1.9800	-1.66941E+01
2273	0.2	1.9810	-1.66999E+01
2273	0.2	1.9820	-1.67053E+01
2273	0.2	1.9830	-1.67103E+01
2273	0.2	1.9840	-1.67147E+01
2273	0.2	1.9850	-1.67187E+01
2273	0.2	1.9860	-1.67221E+01
2273	0.2	1.9870	-1.67251E+01
2273	0.2	1.9880	-1.67275E+01
2273	0.2	1.9890	-1.67295E+01
2273	0.2	1.9900	-1.67310E+01
2273	0.2	1.9910	-1.67319E+01

2273	0.2	1.9920	-1.67324E+01
2273	0.2	1.9930	-1.67323E+01
2273	0.2	1.9940	-1.67317E+01
2273	0.2	1.9950	-1.67307E+01
2273	0.2	1.9960	-1.67290E+01
2273	0.2	1.9970	-1.67268E+01
2273	0.2	1.9980	-1.67240E+01
2273	0.2	1.9990	-1.67203E+01
2273	0.2	2.0000	-1.67156E+01
2273	0.2	2.0010	-1.67098E+01
2273	0.2	2.0020	-1.67030E+01
2273	0.2	2.0030	-1.66953E+01
2273	0.2	2.0040	-1.66869E+01
2273	0.2	2.0050	-1.66780E+01
2273	0.2	2.0060	-1.66686E+01
2273	0.2	2.0070	-1.66587E+01
2273	0.2	2.0080	-1.66484E+01
2273	0.2	2.0090	-1.66378E+01
2273	0.2	2.0100	-1.66268E+01
2273	0.2	2.0110	-1.66154E+01
2273	0.2	2.0120	-1.66038E+01
2273	0.2	2.0130	-1.65918E+01
2273	0.2	2.0140	-1.65796E+01
2273	0.2	2.0150	-1.65672E+01
2273	0.2	2.0160	-1.65545E+01
2273	0.2	2.0170	-1.65415E+01
2273	0.2	2.0180	-1.65284E+01
2273	0.2	2.0190	-1.65150E+01
2273	0.2	2.0200	-1.65014E+01
2273	0.2	2.0210	-1.64876E+01
2273	0.2	2.0220	-1.64737E+01
2273	0.2	2.0230	-1.64595E+01
2273	0.2	2.0240	-1.64452E+01
2273	0.2	2.0250	-1.64308E+01
2273	0.2	2.0260	-1.64161E+01
2273	0.2	2.0270	-1.64014E+01
2273	0.2	2.0280	-1.63864E+01
2273	0.2	2.0290	-1.63713E+01
2273	0.2	2.0300	-1.63561E+01
2273	0.2	2.0310	-1.63408E+01
2273	0.2	2.0320	-1.63253E+01
2273	0.2	2.0330	-1.63096E+01
2273	0.2	2.0340	-1.62939E+01
2273	0.2	2.0350	-1.62780E+01
2273	0.2	2.0360	-1.62620E+01
2273	0.2	2.0370	-1.62459E+01
2273	0.2	2.0380	-1.62296E+01
2273	0.2	2.0390	-1.62133E+01
2273	0.2	2.0400	-1.61968E+01
2273	0.2	2.0410	-1.61802E+01
2273	0.2	2.0420	-1.61635E+01
2273	0.2	2.0430	-1.61467E+01
2273	0.2	2.0440	-1.61298E+01
2273	0.2	2.0450	-1.61127E+01
2273	0.2	2.0460	-1.60956E+01
2273	0.2	2.0470	-1.60784E+01
2273	0.2	2.0480	-1.60610E+01
2273	0.2	2.0490	-1.60436E+01
2273	0.2	2.0500	-1.60260E+01
2273	0.2	2.0510	-1.60083E+01
2273	0.2	2.0520	-1.59906E+01
2273	0.2	2.0530	-1.59727E+01
2273	0.2	2.0540	-1.59547E+01
2273	0.2	2.0550	-1.59367E+01
2273	0.2	2.0560	-1.59185E+01
2273	0.2	2.0570	-1.59003E+01
2273	0.2	2.0580	-1.58819E+01
2273	0.2	2.0590	-1.58635E+01
2273	0.2	2.0600	-1.58449E+01
2273	0.2	2.0610	-1.58263E+01

2273	0.2	2.0620	-1.58076E+01
2273	0.2	2.0630	-1.57987E+01
2273	0.2	2.0640	-1.57698E+01
2273	0.2	2.0650	-1.57508E+01
2273	0.2	2.0660	-1.57317E+01
2273	0.2	2.0670	-1.57125E+01
2273	0.2	2.0680	-1.56933E+01
2273	0.2	2.0690	-1.56739E+01
2273	0.2	2.0700	-1.56545E+01
2273	0.2	2.0710	-1.56349E+01
2273	0.2	2.0720	-1.56153E+01
2273	0.2	2.0730	-1.55956E+01
2273	0.2	2.0740	-1.55758E+01
2273	0.2	2.0750	-1.55559E+01
2273	0.2	2.0760	-1.55360E+01
2273	0.2	2.0770	-1.55160E+01
2273	0.2	2.0780	-1.54958E+01
2273	0.2	2.0790	-1.54756E+01
2273	0.2	2.0800	-1.54554E+01
2273	0.2	2.0810	-1.54350E+01
2273	0.2	2.0820	-1.54146E+01
2273	0.2	2.0830	-1.53941E+01
2273	0.2	2.0840	-1.53735E+01
2273	0.2	2.0850	-1.53529E+01
2273	0.2	2.0860	-1.53322E+01
2273	0.2	2.0870	-1.53114E+01
2273	0.2	2.0880	-1.52905E+01
2273	0.2	2.0890	-1.52696E+01
2273	0.2	2.0900	-1.52486E+01
2273	0.2	2.0910	-1.52275E+01
2273	0.2	2.0920	-1.52064E+01
2273	0.2	2.0930	-1.51852E+01
2273	0.2	2.0940	-1.51639E+01
2273	0.2	2.0950	-1.51426E+01
2273	0.2	2.0960	-1.51212E+01
2273	0.2	2.0970	-1.50998E+01
2273	0.2	2.0980	-1.50783E+01
2273	0.2	2.0990	-1.50567E+01
2273	0.2	2.1000	-1.50351E+01
2273	0.2	2.1010	-1.50134E+01
2273	0.2	2.1020	-1.49917E+01
2273	0.2	2.1030	-1.49699E+01
2273	0.2	2.1040	-1.49481E+01
2273	0.2	2.1050	-1.49262E+01
2273	0.2	2.1060	-1.49043E+01
2273	0.2	2.1070	-1.48823E+01
2273	0.2	2.1080	-1.48602E+01
2273	0.2	2.1090	-1.48382E+01
2273	0.2	2.1100	-1.48160E+01
2273	0.2	2.1110	-1.47939E+01
2273	0.2	2.1120	-1.47716E+01
2273	0.2	2.1130	-1.47494E+01
2273	0.2	2.1140	-1.47271E+01
2273	0.2	2.1150	-1.47047E+01
2273	0.2	2.1160	-1.46824E+01
2273	0.2	2.1170	-1.46599E+01
2273	0.2	2.1180	-1.46375E+01
2273	0.2	2.1190	-1.46150E+01
2273	0.2	2.1200	-1.45925E+01

A.2.3. $(U_{0.7}Pu_{0.3})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{pu} _{pu} (m ² /s)
1273	0.3	1.8500	-2.52904E+01
1273	0.3	1.8510	-2.52865E+01
1273	0.3	1.8520	-2.52822E+01
1273	0.3	1.8530	-2.52783E+01
1273	0.3	1.8540	-2.52751E+01
1273	0.3	1.8550	-2.52726E+01
1273	0.3	1.8560	-2.52708E+01
1273	0.3	1.8570	-2.52695E+01
1273	0.3	1.8580	-2.52688E+01
1273	0.3	1.8590	-2.52686E+01
1273	0.3	1.8600	-2.52688E+01
1273	0.3	1.8610	-2.52695E+01
1273	0.3	1.8620	-2.52705E+01
1273	0.3	1.8630	-2.52719E+01
1273	0.3	1.8640	-2.52736E+01
1273	0.3	1.8650	-2.52756E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{pu} _{pu} (m ² /s)
1273	0.3	1.8660	-2.52778E+01
1273	0.3	1.8670	-2.52804E+01
1273	0.3	1.8680	-2.52831E+01
1273	0.3	1.8690	-2.52861E+01
1273	0.3	1.8700	-2.52892E+01
1273	0.3	1.8710	-2.52926E+01
1273	0.3	1.8720	-2.52961E+01
1273	0.3	1.8730	-2.52998E+01
1273	0.3	1.8740	-2.53036E+01
1273	0.3	1.8750	-2.53075E+01
1273	0.3	1.8760	-2.53116E+01
1273	0.3	1.8770	-2.53158E+01
1273	0.3	1.8780	-2.53200E+01
1273	0.3	1.8790	-2.53244E+01
1273	0.3	1.8800	-2.53289E+01
1273	0.3	1.8810	-2.53334E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{pu} _{pu} (m ² /s)
1273	0.3	1.8820	-2.53381E+01
1273	0.3	1.8830	-2.53428E+01
1273	0.3	1.8840	-2.53475E+01
1273	0.3	1.8850	-2.53524E+01
1273	0.3	1.8860	-2.53573E+01
1273	0.3	1.8870	-2.53622E+01
1273	0.3	1.8880	-2.53672E+01
1273	0.3	1.8890	-2.53723E+01
1273	0.3	1.8900	-2.53774E+01
1273	0.3	1.8910	-2.53825E+01
1273	0.		

1273	0.3	1.8980	-2.54196E+01
1273	0.3	1.8990	-2.54251E+01
1273	0.3	1.9000	-2.54305E+01
1273	0.3	1.9010	-2.54361E+01
1273	0.3	1.9020	-2.54416E+01
1273	0.3	1.9030	-2.54472E+01
1273	0.3	1.9040	-2.54529E+01
1273	0.3	1.9050	-2.54586E+01
1273	0.3	1.9060	-2.54643E+01
1273	0.3	1.9070	-2.54700E+01
1273	0.3	1.9080	-2.54759E+01
1273	0.3	1.9090	-2.54817E+01
1273	0.3	1.9100	-2.54876E+01
1273	0.3	1.9110	-2.54936E+01
1273	0.3	1.9120	-2.54996E+01
1273	0.3	1.9130	-2.55056E+01
1273	0.3	1.9140	-2.55118E+01
1273	0.3	1.9150	-2.55180E+01
1273	0.3	1.9160	-2.55242E+01
1273	0.3	1.9170	-2.55305E+01
1273	0.3	1.9180	-2.55369E+01
1273	0.3	1.9190	-2.55434E+01
1273	0.3	1.9200	-2.55500E+01
1273	0.3	1.9210	-2.55566E+01
1273	0.3	1.9220	-2.55634E+01
1273	0.3	1.9230	-2.55702E+01
1273	0.3	1.9240	-2.55771E+01
1273	0.3	1.9250	-2.55842E+01
1273	0.3	1.9260	-2.55914E+01
1273	0.3	1.9270	-2.55987E+01
1273	0.3	1.9280	-2.56061E+01
1273	0.3	1.9290	-2.56136E+01
1273	0.3	1.9300	-2.56213E+01
1273	0.3	1.9310	-2.56292E+01
1273	0.3	1.9320	-2.56372E+01
1273	0.3	1.9330	-2.56455E+01
1273	0.3	1.9340	-2.56538E+01
1273	0.3	1.9350	-2.56624E+01
1273	0.3	1.9360	-2.56712E+01
1273	0.3	1.9370	-2.56802E+01
1273	0.3	1.9380	-2.56895E+01
1273	0.3	1.9390	-2.56990E+01
1273	0.3	1.9400	-2.57087E+01
1273	0.3	1.9410	-2.57188E+01
1273	0.3	1.9420	-2.57291E+01
1273	0.3	1.9430	-2.57397E+01
1273	0.3	1.9440	-2.57506E+01
1273	0.3	1.9450	-2.57618E+01
1273	0.3	1.9460	-2.57734E+01
1273	0.3	1.9470	-2.57854E+01
1273	0.3	1.9480	-2.57977E+01
1273	0.3	1.9490	-2.58105E+01
1273	0.3	1.9500	-2.58236E+01
1273	0.3	1.9510	-2.58372E+01
1273	0.3	1.9520	-2.58512E+01
1273	0.3	1.9530	-2.58657E+01
1273	0.3	1.9540	-2.58806E+01
1273	0.3	1.9550	-2.58961E+01
1273	0.3	1.9560	-2.59120E+01
1273	0.3	1.9570	-2.59285E+01
1273	0.3	1.9580	-2.59455E+01
1273	0.3	1.9590	-2.59630E+01
1273	0.3	1.9600	-2.59810E+01
1273	0.3	1.9610	-2.59997E+01
1273	0.3	1.9620	-2.60189E+01
1273	0.3	1.9630	-2.60386E+01
1273	0.3	1.9640	-2.60590E+01
1273	0.3	1.9650	-2.60799E+01
1273	0.3	1.9660	-2.61014E+01
1273	0.3	1.9670	-2.61235E+01
1273	0.3	1.9680	-2.61462E+01
1273	0.3	1.9690	-2.61695E+01
1273	0.3	1.9700	-2.61934E+01
1273	0.3	1.9710	-2.62178E+01
1273	0.3	1.9720	-2.62429E+01
1273	0.3	1.9730	-2.62685E+01
1273	0.3	1.9740	-2.62947E+01
1273	0.3	1.9750	-2.63214E+01
1273	0.3	1.9760	-2.63487E+01
1273	0.3	1.9770	-2.63765E+01
1273	0.3	1.9780	-2.64049E+01
1273	0.3	1.9790	-2.64338E+01
1273	0.3	1.9800	-2.64632E+01
1273	0.3	1.9810	-2.64931E+01
1273	0.3	1.9820	-2.65234E+01
1273	0.3	1.9830	-2.65542E+01
1273	0.3	1.9840	-2.65855E+01
1273	0.3	1.9850	-2.66171E+01
1273	0.3	1.9860	-2.66491E+01
1273	0.3	1.9870	-2.66814E+01
1273	0.3	1.9880	-2.67141E+01
1273	0.3	1.9890	-2.67470E+01

1273	0.3	1.9900	-2.67802E+01
1273	0.3	1.9910	-2.68135E+01
1273	0.3	1.9920	-2.68469E+01
1273	0.3	1.9930	-2.68805E+01
1273	0.3	1.9940	-2.69140E+01
1273	0.3	1.9950	-2.69475E+01
1273	0.3	1.9960	-2.69808E+01
1273	0.3	1.9970	-2.70139E+01
1273	0.3	1.9980	-2.70466E+01
1273	0.3	1.9990	-2.70789E+01
1273	0.3	2.0000	-2.71106E+01
1273	0.3	2.0010	-2.71410E+01
1273	0.3	2.0020	-2.71696E+01
1273	0.3	2.0030	-2.71965E+01
1273	0.3	2.0040	-2.72212E+01
1273	0.3	2.0050	-2.72437E+01
1273	0.3	2.0060	-2.72636E+01
1273	0.3	2.0070	-2.72810E+01
1273	0.3	2.0080	-2.72956E+01
1273	0.3	2.0090	-2.73074E+01
1273	0.3	2.0100	-2.73163E+01
1273	0.3	2.0110	-2.73223E+01
1273	0.3	2.0120	-2.73254E+01
1273	0.3	2.0130	-2.73258E+01
1273	0.3	2.0140	-2.73234E+01
1273	0.3	2.0150	-2.73184E+01
1273	0.3	2.0160	-2.73110E+01
1273	0.3	2.0170	-2.73014E+01
1273	0.3	2.0180	-2.72897E+01
1273	0.3	2.0190	-2.72761E+01
1273	0.3	2.0200	-2.72608E+01
1273	0.3	2.0210	-2.72439E+01
1273	0.3	2.0220	-2.72256E+01
1273	0.3	2.0230	-2.72060E+01
1273	0.3	2.0240	-2.71853E+01
1273	0.3	2.0250	-2.71635E+01
1273	0.3	2.0260	-2.71409E+01
1273	0.3	2.0270	-2.71174E+01
1273	0.3	2.0280	-2.70932E+01
1273	0.3	2.0290	-2.70682E+01
1273	0.3	2.0300	-2.70427E+01
1273	0.3	2.0310	-2.70166E+01
1273	0.3	2.0320	-2.69900E+01
1273	0.3	2.0330	-2.69630E+01
1273	0.3	2.0340	-2.69354E+01
1273	0.3	2.0350	-2.69075E+01
1273	0.3	2.0360	-2.68791E+01
1273	0.3	2.0370	-2.68504E+01
1273	0.3	2.0380	-2.68214E+01
1273	0.3	2.0390	-2.67919E+01
1273	0.3	2.0400	-2.67622E+01
1273	0.3	2.0410	-2.67321E+01
1273	0.3	2.0420	-2.67017E+01
1273	0.3	2.0430	-2.66711E+01
1273	0.3	2.0440	-2.66401E+01
1273	0.3	2.0450	-2.66088E+01
1273	0.3	2.0460	-2.65773E+01
1273	0.3	2.0470	-2.65455E+01
1273	0.3	2.0480	-2.65134E+01
1273	0.3	2.0490	-2.64811E+01
1273	0.3	2.0500	-2.64485E+01
1273	0.3	2.0510	-2.64157E+01
1273	0.3	2.0520	-2.63826E+01
1273	0.3	2.0530	-2.63493E+01
1273	0.3	2.0540	-2.63157E+01
1273	0.3	2.0550	-2.62820E+01
1273	0.3	2.0560	-2.62480E+01
1273	0.3	2.0570	-2.62138E+01
1273	0.3	2.0580	-2.61793E+01
1273	0.3	2.0590	-2.61447E+01
1273	0.3	2.0600	-2.61099E+01
1273	0.3	2.0610	-2.60749E+01
1273	0.3	2.0620	-2.60397E+01
1273	0.3	2.0630	-2.60043E+01
1273	0.3	2.0640	-2.59687E+01
1273	0.3	2.0650	-2.59330E+01
1273	0.3	2.0660	-2.58971E+01
1273	0.3	2.0670	-2.58610E+01
1273	0.3	2.0680	-2.58248E+01
1273	0.3	2.0690	-2.57885E+01
1273	0.3	2.0700	-2.57520E+01
1273	0.3	2.0710	-2.57154E+01
1273	0.3	2.0720	-2.56787E+01
1273	0.3	2.0730	-2.56418E+01
1273	0.3	2.0740	-2.56048E+01
1273	0.3	2.0750	-2.55677E+01
1273	0.3	2.0760	-2.55305E+01
1273	0.3	2.0770	-2.54932E+01
1273	0.3	2.0780	-2.54558E+01
1273	0.3	2.0790	-2.54184E+01
1273	0.3	2.0800	-2.53808E+01
1273	0.3	2.0810	-2.53432E+01

1273	0.3	2.0820	-2.53054E+01
1273	0.3	2.0830	-2.52676E+01
1273	0.3	2.0840	-2.52298E+01
1273	0.3	2.0850	-2.51919E+01
1273	0.3	2.0860	-2.51539E+01
1273	0.3	2.0870	-2.51158E+01
1273	0.3	2.0880	-2.50777E+01
1273	0.3	2.0890	-2.50396E+01
1273	0.3	2.0900	-2.50014E+01
1273	0.3	2.0910	-2.49632E+01
1273	0.3	2.0920	-2.49249E+01
1273	0.3	2.0930	-2.48866E+01
1273	0.3	2.0940	-2.48483E+01
1273	0.3	2.0950	-2.48100E+01
1273	0.3	2.0960	-2.47716E+01
1273	0.3	2.0970	-2.47332E+01
1273	0.3	2.0980	-2.46947E+01
1273	0.3	2.0990	-2.46563E+01
1273	0.3	2.1000	-2.46178E+01
1273	0.3	2.1010	-2.45794E+01
1273	0.3	2.1020	-2.45409E+01
1273	0.3	2.1030	-2.45024E+01
1273	0.3	2.1040	-2.44638E+01
1273	0.3	2.1050	-2.44253E+01
1273	0.3	2.1060	-2.43868E+01
1273	0.3	2.1070	-2.43483E+01
1273	0.3	2.1080	-2.43097E+01
1273	0.3	2.1090	-2.42712E+01
1273	0.3	2.1100	-2.42326E+01
1273	0.3	2.1110	-2.41941E+01
1273	0.3	2.1120	-2.41556E+01
1273	0.3	2.1130	-2.41170E+01
1273	0.3	2.1140	-2.40785E+01
1273	0.3	2.1150	-2.40400E+01
1273	0.3	2.1160	-2.40015E+01
1273	0.3	2.1170	-2.39630E+01
1273	0.3	2.1180	-2.39245E+01
1273	0.3	2.1190	-2.38860E+01
1273	0.3	2.1200	-2.38475E+01
1273	0.3	2.1210	-2.38090E+01
1273	0.3	2.1220	-2.37705E+01
1273	0.3	2.1230	-2.37321E+01
1273	0.3	2.1240	-2.36937E+01
1273	0.3	2.1250	-2.36552E+01
1273	0.3	2.1260	-2.36168E+01
1273	0.3	2.1270	-2.35784E+01
1273	0.3	2.1280	-2.35400E+01
1273	0.3	2.1290	-2.35017E+01
1273	0.3	2.1300	-2.34633E+01
1273	0.3	2.1310	-2.34250E+01
1273	0.3	2.1320	-2.33866E+01
1273	0.3	2.1330	-2.33483E+01
1273	0.3	2.1340	-2.33100E+01
1273	0.3	2.1350	-2.32718E+01
1273	0.3	2.1360	-2.32335E+01
1273	0.3	2.1370	-2.31953E+01
1273	0.3	2.1380	-2.31570E+01
1273	0.3	2.1390	-2.31188E+01
1273	0.3	2.1400	-2.30806E+01
1273	0.3	2.1410	-2.30425E+01
1273	0.3	2.1420	-2.30043E+01
1273	0.3	2.1430	-2.29662E+01
1273	0.3	2.1440	-2.29281E+01
1273	0.3	2.1450	-2.28900E+01
1273	0.3	2.1460	-2.28519E+01
1273	0.3	2.1470	-2.28139E+01
1273	0.3		

1773	0.3	1.8430	-1.92440E+01
1773	0.3	1.8440	-1.92437E+01
1773	0.3	1.8450	-1.92434E+01
1773	0.3	1.8460	-1.92430E+01
1773	0.3	1.8470	-1.92425E+01
1773	0.3	1.8480	-1.92420E+01
1773	0.3	1.8490	-1.92415E+01
1773	0.3	1.8500	-1.92410E+01
1773	0.3	1.8510	-1.92405E+01
1773	0.3	1.8520	-1.92401E+01
1773	0.3	1.8530	-1.92398E+01
1773	0.3	1.8540	-1.92395E+01
1773	0.3	1.8550	-1.92394E+01
1773	0.3	1.8560	-1.92395E+01
1773	0.3	1.8570	-1.92398E+01
1773	0.3	1.8580	-1.92402E+01
1773	0.3	1.8590	-1.92408E+01
1773	0.3	1.8600	-1.92417E+01
1773	0.3	1.8610	-1.92427E+01
1773	0.3	1.8620	-1.92439E+01
1773	0.3	1.8630	-1.92452E+01
1773	0.3	1.8640	-1.92468E+01
1773	0.3	1.8650	-1.92485E+01
1773	0.3	1.8660	-1.92504E+01
1773	0.3	1.8670	-1.92525E+01
1773	0.3	1.8680	-1.92547E+01
1773	0.3	1.8690	-1.92570E+01
1773	0.3	1.8700	-1.92595E+01
1773	0.3	1.8710	-1.92621E+01
1773	0.3	1.8720	-1.92649E+01
1773	0.3	1.8730	-1.92678E+01
1773	0.3	1.8740	-1.92708E+01
1773	0.3	1.8750	-1.92739E+01
1773	0.3	1.8760	-1.92771E+01
1773	0.3	1.8770	-1.92805E+01
1773	0.3	1.8780	-1.92839E+01
1773	0.3	1.8790	-1.92875E+01
1773	0.3	1.8800	-1.92912E+01
1773	0.3	1.8810	-1.92949E+01
1773	0.3	1.8820	-1.92988E+01
1773	0.3	1.8830	-1.93028E+01
1773	0.3	1.8840	-1.93068E+01
1773	0.3	1.8850	-1.93109E+01
1773	0.3	1.8860	-1.93152E+01
1773	0.3	1.8870	-1.93195E+01
1773	0.3	1.8880	-1.93239E+01
1773	0.3	1.8890	-1.93284E+01
1773	0.3	1.8900	-1.93330E+01
1773	0.3	1.8910	-1.93376E+01
1773	0.3	1.8920	-1.93424E+01
1773	0.3	1.8930	-1.93472E+01
1773	0.3	1.8940	-1.93521E+01
1773	0.3	1.8950	-1.93571E+01
1773	0.3	1.8960	-1.93622E+01
1773	0.3	1.8970	-1.93674E+01
1773	0.3	1.8980	-1.93727E+01
1773	0.3	1.8990	-1.93781E+01
1773	0.3	1.9000	-1.93835E+01
1773	0.3	1.9010	-1.93891E+01
1773	0.3	1.9020	-1.93947E+01
1773	0.3	1.9030	-1.94005E+01
1773	0.3	1.9040	-1.94064E+01
1773	0.3	1.9050	-1.94123E+01
1773	0.3	1.9060	-1.94184E+01
1773	0.3	1.9070	-1.94246E+01
1773	0.3	1.9080	-1.94309E+01
1773	0.3	1.9090	-1.94373E+01
1773	0.3	1.9100	-1.94438E+01
1773	0.3	1.9110	-1.94505E+01
1773	0.3	1.9120	-1.94573E+01
1773	0.3	1.9130	-1.94642E+01
1773	0.3	1.9140	-1.94712E+01
1773	0.3	1.9150	-1.94785E+01
1773	0.3	1.9160	-1.94858E+01
1773	0.3	1.9170	-1.94933E+01
1773	0.3	1.9180	-1.95010E+01
1773	0.3	1.9190	-1.95088E+01
1773	0.3	1.9200	-1.95168E+01
1773	0.3	1.9210	-1.95250E+01
1773	0.3	1.9220	-1.95334E+01
1773	0.3	1.9230	-1.95419E+01
1773	0.3	1.9240	-1.95507E+01
1773	0.3	1.9250	-1.95596E+01
1773	0.3	1.9260	-1.95688E+01
1773	0.3	1.9270	-1.95781E+01
1773	0.3	1.9280	-1.95877E+01
1773	0.3	1.9290	-1.95975E+01
1773	0.3	1.9300	-1.96075E+01
1773	0.3	1.9310	-1.96178E+01
1773	0.3	1.9320	-1.96283E+01
1773	0.3	1.9330	-1.96391E+01
1773	0.3	1.9340	-1.96501E+01

1773	0.3	1.9350	-1.96613E+01
1773	0.3	1.9360	-1.96728E+01
1773	0.3	1.9370	-1.96846E+01
1773	0.3	1.9380	-1.96967E+01
1773	0.3	1.9390	-1.97090E+01
1773	0.3	1.9400	-1.97216E+01
1773	0.3	1.9410	-1.97344E+01
1773	0.3	1.9420	-1.97476E+01
1773	0.3	1.9430	-1.97610E+01
1773	0.3	1.9440	-1.97747E+01
1773	0.3	1.9450	-1.97887E+01
1773	0.3	1.9460	-1.98029E+01
1773	0.3	1.9470	-1.98175E+01
1773	0.3	1.9480	-1.98323E+01
1773	0.3	1.9490	-1.98474E+01
1773	0.3	1.9500	-1.98627E+01
1773	0.3	1.9510	-1.98783E+01
1773	0.3	1.9520	-1.98942E+01
1773	0.3	1.9530	-1.99104E+01
1773	0.3	1.9540	-1.99268E+01
1773	0.3	1.9550	-1.99434E+01
1773	0.3	1.9560	-1.99602E+01
1773	0.3	1.9570	-1.99773E+01
1773	0.3	1.9580	-1.99946E+01
1773	0.3	1.9590	-2.00121E+01
1773	0.3	1.9600	-2.00298E+01
1773	0.3	1.9610	-2.00477E+01
1773	0.3	1.9620	-2.00657E+01
1773	0.3	1.9630	-2.00839E+01
1773	0.3	1.9640	-2.01023E+01
1773	0.3	1.9650	-2.01207E+01
1773	0.3	1.9660	-2.01392E+01
1773	0.3	1.9670	-2.01578E+01
1773	0.3	1.9680	-2.01765E+01
1773	0.3	1.9690	-2.01952E+01
1773	0.3	1.9700	-2.02139E+01
1773	0.3	1.9710	-2.02326E+01
1773	0.3	1.9720	-2.02513E+01
1773	0.3	1.9730	-2.02699E+01
1773	0.3	1.9740	-2.02884E+01
1773	0.3	1.9750	-2.03068E+01
1773	0.3	1.9760	-2.03250E+01
1773	0.3	1.9770	-2.03430E+01
1773	0.3	1.9780	-2.03608E+01
1773	0.3	1.9790	-2.03783E+01
1773	0.3	1.9800	-2.03956E+01
1773	0.3	1.9810	-2.04125E+01
1773	0.3	1.9820	-2.04290E+01
1773	0.3	1.9830	-2.04452E+01
1773	0.3	1.9840	-2.04609E+01
1773	0.3	1.9850	-2.04761E+01
1773	0.3	1.9860	-2.04908E+01
1773	0.3	1.9870	-2.05049E+01
1773	0.3	1.9880	-2.05185E+01
1773	0.3	1.9890	-2.05314E+01
1773	0.3	1.9900	-2.05437E+01
1773	0.3	1.9910	-2.05552E+01
1773	0.3	1.9920	-2.05661E+01
1773	0.3	1.9930	-2.05762E+01
1773	0.3	1.9940	-2.05856E+01
1773	0.3	1.9950	-2.05942E+01
1773	0.3	1.9960	-2.06019E+01
1773	0.3	1.9970	-2.06089E+01
1773	0.3	1.9980	-2.06150E+01
1773	0.3	1.9990	-2.06202E+01
1773	0.3	2.0000	-2.06239E+01
1773	0.3	2.0010	-2.06234E+01
1773	0.3	2.0020	-2.06210E+01
1773	0.3	2.0030	-2.06174E+01
1773	0.3	2.0040	-2.06126E+01
1773	0.3	2.0050	-2.06068E+01
1773	0.3	2.0060	-2.05999E+01
1773	0.3	2.0070	-2.05920E+01
1773	0.3	2.0080	-2.05832E+01
1773	0.3	2.0090	-2.05735E+01
1773	0.3	2.0100	-2.05630E+01
1773	0.3	2.0110	-2.05517E+01
1773	0.3	2.0120	-2.05397E+01
1773	0.3	2.0130	-2.05270E+01
1773	0.3	2.0140	-2.05138E+01
1773	0.3	2.0150	-2.04999E+01
1773	0.3	2.0160	-2.04855E+01
1773	0.3	2.0170	-2.04706E+01
1773	0.3	2.0180	-2.04553E+01
1773	0.3	2.0190	-2.04395E+01
1773	0.3	2.0200	-2.04232E+01
1773	0.3	2.0210	-2.04067E+01
1773	0.3	2.0220	-2.03897E+01
1773	0.3	2.0230	-2.03724E+01
1773	0.3	2.0240	-2.03548E+01
1773	0.3	2.0250	-2.03369E+01
1773	0.3	2.0260	-2.03187E+01

1773	0.3	2.0270	-2.03003E+01
1773	0.3	2.0280	-2.02816E+01
1773	0.3	2.0290	-2.02626E+01
1773	0.3	2.0300	-2.02435E+01
1773	0.3	2.0310	-2.02240E+01
1773	0.3	2.0320	-2.02044E+01
1773	0.3	2.0330	-2.01846E+01
1773	0.3	2.0340	-2.01645E+01
1773	0.3	2.0350	-2.01443E+01
1773	0.3	2.0360	-2.01239E+01
1773	0.3	2.0370	-2.01033E+01
1773	0.3	2.0380	-2.00824E+01
1773	0.3	2.0390	-2.00615E+01
1773	0.3	2.0400	-2.00403E+01
1773	0.3	2.0410	-2.00190E+01
1773	0.3	2.0420	-1.99974E+01
1773	0.3	2.0430	-1.99758E+01
1773	0.3	2.0440	-1.99539E+01
1773	0.3	2.0450	-1.99319E+01
1773	0.3	2.0460	-1.99097E+01
1773	0.3	2.0470	-1.98874E+01
1773	0.3	2.0480	-1.98649E+01
1773	0.3	2.0490	-1.98422E+01
1773	0.3	2.0500	-1.98194E+01
1773	0.3	2.0510	-1.97964E+01
1773	0.3	2.0520	-1.97733E+01
1773	0.3	2.0530	-1.97500E+01
1773	0.3	2.0540	-1.97265E+01
1773	0.3	2.0550	-1.97029E+01
1773	0.3	2.0560	-1.96792E+01
1773	0.3	2.0570	-1.96553E+01
1773	0.3	2.0580	-1.96312E+01
1773	0.3	2.0590	-1.96070E+01
1773	0.3	2.0600	-1.95827E+01
1773	0.3	2.0610	-1.95582E+01
1773	0.3	2.0620	-1.95335E+01
1773	0.3	2.0630	-1.95087E+01
1773	0.3	2.0640	-1.94838E+01
1773	0.3	2.0650	-1.94587E+01
1773	0.3	2.0660	-1.94335E+01
1773	0.3	2.0670	-1.94082E+01
1773	0.3	2.0680	-1.93827E+01
1773	0.3	2.0690	-1.93571E+01
1773	0.3	2.0700	-1.93313E+01
1773	0.3	2.0710	-1.93054E+01
1773	0.3	2.0720	-1.92794E+01
1773	0.3	2.0730	-1.92533E+01
1773	0.3	2.0740	-1.92270E+01
1773	0.3	2.0750	-1.92006E+01
1773	0.3	2.0760	-1.91741E+01
1773	0.3	2.0770	-1.91475E+01
1773	0.3	2.0780	-1.91207E+01
1773	0.3	2.0790	-1.90938E+01
1773	0.3	2.0800	-1.90668E+01
1773	0.3	2.0810	-1.90397E+01
1773	0.3	2.0820	-1.90125E+01
1773	0.3	2.0830	-1.89852E+01
1773	0.3	2.0840	-1.89577E+01
1773	0.3	2.0850	-1.89302E+01
1773	0.3	2.0860	-1.89025E+01
1773	0.3	2.0870	-1.88748E+01
1773	0.3	2.0880	-1.88470E+01
1773	0.3	2.0890	-1.88190E+01
1773	0.3	2.0900	-1.87910E+01
1773	0.3	2.0910	-1.87629E+01
1773	0.3	2.0920	-1.87347E+01
1773	0.3		

1773	0.3	2.1190	-1.79485E+01
1773	0.3	2.1200	-1.79188E+01
1773	0.3	2.1210	-1.78890E+01
1773	0.3	2.1220	-1.78592E+01
1773	0.3	2.1230	-1.78294E+01
1773	0.3	2.1240	-1.77996E+01
1773	0.3	2.1250	-1.77697E+01
1773	0.3	2.1260	-1.77398E+01
1773	0.3	2.1270	-1.77099E+01
1773	0.3	2.1280	-1.76800E+01
1773	0.3	2.1290	-1.76501E+01
1773	0.3	2.1300	-1.76201E+01
1773	0.3	2.1310	-1.75902E+01
1773	0.3	2.1320	-1.75602E+01
1773	0.3	2.1330	-1.75302E+01
1773	0.3	2.1340	-1.75003E+01
1773	0.3	2.1350	-1.74703E+01
1773	0.3	2.1360	-1.74403E+01
1773	0.3	2.1370	-1.74102E+01
1773	0.3	2.1380	-1.73802E+01
1773	0.3	2.1390	-1.73502E+01
1773	0.3	2.1400	-1.73202E+01
1773	0.3	2.1410	-1.72902E+01
1773	0.3	2.1420	-1.72601E+01
1773	0.3	2.1430	-1.72301E+01
1773	0.3	2.1440	-1.72001E+01
1773	0.3	2.1450	-1.71700E+01
1773	0.3	2.1460	-1.71400E+01
1773	0.3	2.1470	-1.71099E+01
1773	0.3	2.1480	-1.70799E+01
1773	0.3	2.1490	-1.70499E+01
1773	0.3	2.1500	-1.70199E+01
2273	0.3	1.7600	-1.58330E+01
2273	0.3	1.7610	-1.58330E+01
2273	0.3	1.7620	-1.58330E+01
2273	0.3	1.7630	-1.58330E+01
2273	0.3	1.7640	-1.58330E+01
2273	0.3	1.7650	-1.58329E+01
2273	0.3	1.7660	-1.58329E+01
2273	0.3	1.7670	-1.58329E+01
2273	0.3	1.7680	-1.58329E+01
2273	0.3	1.7690	-1.58329E+01
2273	0.3	1.7700	-1.58329E+01
2273	0.3	1.7710	-1.58329E+01
2273	0.3	1.7720	-1.58329E+01
2273	0.3	1.7730	-1.58329E+01
2273	0.3	1.7740	-1.58328E+01
2273	0.3	1.7750	-1.58328E+01
2273	0.3	1.7760	-1.58328E+01
2273	0.3	1.7770	-1.58328E+01
2273	0.3	1.7780	-1.58328E+01
2273	0.3	1.7790	-1.58328E+01
2273	0.3	1.7800	-1.58328E+01
2273	0.3	1.7810	-1.58328E+01
2273	0.3	1.7820	-1.58327E+01
2273	0.3	1.7830	-1.58327E+01
2273	0.3	1.7840	-1.58327E+01
2273	0.3	1.7850	-1.58327E+01
2273	0.3	1.7860	-1.58327E+01
2273	0.3	1.7870	-1.58327E+01
2273	0.3	1.7880	-1.58327E+01
2273	0.3	1.7890	-1.58326E+01
2273	0.3	1.7900	-1.58326E+01
2273	0.3	1.7910	-1.58326E+01
2273	0.3	1.7920	-1.58326E+01
2273	0.3	1.7930	-1.58326E+01
2273	0.3	1.7940	-1.58326E+01
2273	0.3	1.7950	-1.58325E+01
2273	0.3	1.7960	-1.58325E+01
2273	0.3	1.7970	-1.58325E+01
2273	0.3	1.7980	-1.58325E+01
2273	0.3	1.7990	-1.58325E+01
2273	0.3	1.8000	-1.58325E+01
2273	0.3	1.8010	-1.58324E+01
2273	0.3	1.8020	-1.58324E+01
2273	0.3	1.8030	-1.58324E+01
2273	0.3	1.8040	-1.58324E+01
2273	0.3	1.8050	-1.58324E+01
2273	0.3	1.8060	-1.58324E+01
2273	0.3	1.8070	-1.58323E+01
2273	0.3	1.8080	-1.58323E+01
2273	0.3	1.8090	-1.58323E+01
2273	0.3	1.8100	-1.58323E+01
2273	0.3	1.8110	-1.58323E+01
2273	0.3	1.8120	-1.58323E+01
2273	0.3	1.8130	-1.58322E+01
2273	0.3	1.8140	-1.58322E+01
2273	0.3	1.8150	-1.58322E+01
2273	0.3	1.8160	-1.58322E+01
2273	0.3	1.8170	-1.58322E+01
2273	0.3	1.8180	-1.58322E+01
2273	0.3	1.8190	-1.58322E+01

2273	0.3	1.8200	-1.58322E+01
2273	0.3	1.8210	-1.58322E+01
2273	0.3	1.8220	-1.58322E+01
2273	0.3	1.8230	-1.58322E+01
2273	0.3	1.8240	-1.58322E+01
2273	0.3	1.8250	-1.58322E+01
2273	0.3	1.8260	-1.58322E+01
2273	0.3	1.8270	-1.58322E+01
2273	0.3	1.8280	-1.58322E+01
2273	0.3	1.8290	-1.58323E+01
2273	0.3	1.8300	-1.58323E+01
2273	0.3	1.8310	-1.58324E+01
2273	0.3	1.8320	-1.58324E+01
2273	0.3	1.8330	-1.58325E+01
2273	0.3	1.8340	-1.58326E+01
2273	0.3	1.8350	-1.58327E+01
2273	0.3	1.8360	-1.58328E+01
2273	0.3	1.8370	-1.58329E+01
2273	0.3	1.8380	-1.58330E+01
2273	0.3	1.8390	-1.58332E+01
2273	0.3	1.8400	-1.58334E+01
2273	0.3	1.8410	-1.58336E+01
2273	0.3	1.8420	-1.58339E+01
2273	0.3	1.8430	-1.58342E+01
2273	0.3	1.8440	-1.58345E+01
2273	0.3	1.8450	-1.58349E+01
2273	0.3	1.8460	-1.58353E+01
2273	0.3	1.8470	-1.58358E+01
2273	0.3	1.8480	-1.58363E+01
2273	0.3	1.8490	-1.58369E+01
2273	0.3	1.8500	-1.58375E+01
2273	0.3	1.8510	-1.58382E+01
2273	0.3	1.8520	-1.58390E+01
2273	0.3	1.8530	-1.58398E+01
2273	0.3	1.8540	-1.58408E+01
2273	0.3	1.8550	-1.58418E+01
2273	0.3	1.8560	-1.58429E+01
2273	0.3	1.8570	-1.58441E+01
2273	0.3	1.8580	-1.58454E+01
2273	0.3	1.8590	-1.58468E+01
2273	0.3	1.8600	-1.58483E+01
2273	0.3	1.8610	-1.58499E+01
2273	0.3	1.8620	-1.58516E+01
2273	0.3	1.8630	-1.58533E+01
2273	0.3	1.8640	-1.58552E+01
2273	0.3	1.8650	-1.58572E+01
2273	0.3	1.8660	-1.58593E+01
2273	0.3	1.8670	-1.58615E+01
2273	0.3	1.8680	-1.58639E+01
2273	0.3	1.8690	-1.58663E+01
2273	0.3	1.8700	-1.58688E+01
2273	0.3	1.8710	-1.58715E+01
2273	0.3	1.8720	-1.58742E+01
2273	0.3	1.8730	-1.58770E+01
2273	0.3	1.8740	-1.58800E+01
2273	0.3	1.8750	-1.58831E+01
2273	0.3	1.8760	-1.58862E+01
2273	0.3	1.8770	-1.58895E+01
2273	0.3	1.8780	-1.58929E+01
2273	0.3	1.8790	-1.58964E+01
2273	0.3	1.8800	-1.59000E+01
2273	0.3	1.8810	-1.59037E+01
2273	0.3	1.8820	-1.59075E+01
2273	0.3	1.8830	-1.59115E+01
2273	0.3	1.8840	-1.59155E+01
2273	0.3	1.8850	-1.59197E+01
2273	0.3	1.8860	-1.59239E+01
2273	0.3	1.8870	-1.59283E+01
2273	0.3	1.8880	-1.59328E+01
2273	0.3	1.8890	-1.59374E+01
2273	0.3	1.8900	-1.59421E+01
2273	0.3	1.8910	-1.59469E+01
2273	0.3	1.8920	-1.59518E+01
2273	0.3	1.8930	-1.59569E+01
2273	0.3	1.8940	-1.59621E+01
2273	0.3	1.8950	-1.59674E+01
2273	0.3	1.8960	-1.59728E+01
2273	0.3	1.8970	-1.59784E+01
2273	0.3	1.8980	-1.59841E+01
2273	0.3	1.8990	-1.59899E+01
2273	0.3	1.9000	-1.59958E+01
2273	0.3	1.9010	-1.60019E+01
2273	0.3	1.9020	-1.60081E+01
2273	0.3	1.9030	-1.60145E+01
2273	0.3	1.9040	-1.60209E+01
2273	0.3	1.9050	-1.60276E+01
2273	0.3	1.9060	-1.60344E+01
2273	0.3	1.9070	-1.60413E+01
2273	0.3	1.9080	-1.60483E+01
2273	0.3	1.9090	-1.60556E+01
2273	0.3	1.9100	-1.60629E+01
2273	0.3	1.9110	-1.60705E+01

2273	0.3	1.9120	-1.60781E+01
2273	0.3	1.9130	-1.60860E+01
2273	0.3	1.9140	-1.60940E+01
2273	0.3	1.9150	-1.61021E+01
2273	0.3	1.9160	-1.61105E+01
2273	0.3	1.9170	-1.61190E+01
2273	0.3	1.9180	-1.61276E+01
2273	0.3	1.9190	-1.61364E+01
2273	0.3	1.9200	-1.61454E+01
2273	0.3	1.9210	-1.61546E+01
2273	0.3	1.9220	-1.61639E+01
2273	0.3	1.9230	-1.61734E+01
2273	0.3	1.9240	-1.61831E+01
2273	0.3	1.9250	-1.61929E+01
2273	0.3	1.9260	-1.62029E+01
2273	0.3	1.9270	-1.62131E+01
2273	0.3	1.9280	-1.62234E+01
2273	0.3	1.9290	-1.62339E+01
2273	0.3	1.9300	-1.62445E+01
2273	0.3	1.9310	-1.62553E+01
2273	0.3	1.9320	-1.62663E+01
2273	0.3	1.9330	-1.62774E+01
2273	0.3	1.9340	-1.62887E+01
2273	0.3	1.9350	-1.63001E+01
2273	0.3	1.9360	-1.63116E+01
2273	0.3	1.9370	-1.63233E+01
2273	0.3	1.9380	-1.63351E+01
2273	0.3	1.9390	-1.63470E+01
2273	0.3	1.9400	-1.63591E+01
2273	0.3	1.9410	-1.63712E+01
2273	0.3	1.9420	-1.63834E+01
2273	0.3	1.9430	-1.63958E+01
2273	0.3	1.9440	-1.64082E+01
2273	0.3	1.9450	-1.64207E+01
2273	0.3	1.9460	-1.64332E+01
2273	0.3	1.9470	-1.64458E+01
2273	0.3	1.9480	-1.64584E+01
2273	0.3	1.9490	-1.64711E+01
2273	0.3	1.9500	-1.64837E+01
2273	0.3	1.9510	-1.64964E+01
2273	0.3	1.9520	-1.65091E+01
2273	0.3	1.9530	-1.65217E+01
2273	0.3	1.9540	-1.65343E+01
2273	0.3	1.9550	-1.65468E+01
2273	0.3	1.9560	-1.65593E+01
2273	0.3	1.9570	-1.65716E+01
2273	0.3	1.9580	-1.65839E+01
2273	0.3	1.9590	-1.65960E+01
2273	0.3	1.9600	-1.66080E+01
2273	0.3	1.9610	-1.66199E+01
2273	0.3	1.9620	-1.66315E+01
2273	0.3	1.9630	-1.66430E+01
2273	0.3	1.9640	-1.66542E+01
2273	0.3	1.9650	-1.66652E+01
2273	0.3	1.9660	-1.66760E+01
2273	0.3	1.9670	-1.66865E+01
2273	0.3	1.9680	-1.66967E+01
2273	0.3	1.9690	-1.67065E+01
2273	0.3	1.9700	-1.67161E+01
2273	0.3	1.9710	-1.67253E+01
2273	0.3	1.9720	-1.67342E+01
2273	0.3	1.9730	-1.67427E+01
2273	0.3	1.9740	-1.67508E+01
2273	0.3	1.9750	-1.67585E+01
2273	0.3	1.9760	-1.67658E+01
2273	0.3	1.9770	-1.67726E+01
2273	0.3		

2273	0.3	2.0040	-1.67634E+01
2273	0.3	2.0050	-1.67532E+01
2273	0.3	2.0060	-1.67426E+01
2273	0.3	2.0070	-1.67316E+01
2273	0.3	2.0080	-1.67201E+01
2273	0.3	2.0090	-1.67083E+01
2273	0.3	2.0100	-1.66961E+01
2273	0.3	2.0110	-1.66836E+01
2273	0.3	2.0120	-1.66708E+01
2273	0.3	2.0130	-1.66578E+01
2273	0.3	2.0140	-1.66444E+01
2273	0.3	2.0150	-1.66309E+01
2273	0.3	2.0160	-1.66170E+01
2273	0.3	2.0170	-1.66030E+01
2273	0.3	2.0180	-1.65888E+01
2273	0.3	2.0190	-1.65743E+01
2273	0.3	2.0200	-1.65597E+01
2273	0.3	2.0210	-1.65449E+01
2273	0.3	2.0220	-1.65299E+01
2273	0.3	2.0230	-1.65147E+01
2273	0.3	2.0240	-1.64994E+01
2273	0.3	2.0250	-1.64839E+01
2273	0.3	2.0260	-1.64682E+01
2273	0.3	2.0270	-1.64524E+01
2273	0.3	2.0280	-1.64365E+01
2273	0.3	2.0290	-1.64204E+01
2273	0.3	2.0300	-1.64042E+01
2273	0.3	2.0310	-1.63878E+01
2273	0.3	2.0320	-1.63713E+01
2273	0.3	2.0330	-1.63547E+01

2273	0.3	2.0340	-1.63380E+01
2273	0.3	2.0350	-1.63211E+01
2273	0.3	2.0360	-1.63042E+01
2273	0.3	2.0370	-1.62871E+01
2273	0.3	2.0380	-1.62698E+01
2273	0.3	2.0390	-1.62525E+01
2273	0.3	2.0400	-1.62351E+01
2273	0.3	2.0410	-1.62175E+01
2273	0.3	2.0420	-1.61999E+01
2273	0.3	2.0430	-1.61821E+01
2273	0.3	2.0440	-1.61642E+01
2273	0.3	2.0450	-1.61462E+01
2273	0.3	2.0460	-1.61281E+01
2273	0.3	2.0470	-1.61099E+01
2273	0.3	2.0480	-1.60916E+01
2273	0.3	2.0490	-1.60732E+01
2273	0.3	2.0500	-1.60547E+01
2273	0.3	2.0510	-1.60360E+01
2273	0.3	2.0520	-1.60173E+01
2273	0.3	2.0530	-1.59985E+01
2273	0.3	2.0540	-1.59796E+01
2273	0.3	2.0550	-1.59605E+01
2273	0.3	2.0560	-1.59414E+01
2273	0.3	2.0570	-1.59222E+01
2273	0.3	2.0580	-1.59028E+01
2273	0.3	2.0590	-1.58834E+01
2273	0.3	2.0600	-1.58639E+01
2273	0.3	2.0610	-1.58443E+01
2273	0.3	2.0620	-1.58246E+01
2273	0.3	2.0630	-1.58048E+01

2273	0.3	2.0640	-1.57848E+01
2273	0.3	2.0650	-1.57648E+01
2273	0.3	2.0660	-1.57447E+01
2273	0.3	2.0670	-1.57246E+01
2273	0.3	2.0680	-1.57043E+01
2273	0.3	2.0690	-1.56839E+01
2273	0.3	2.0700	-1.56634E+01
2273	0.3	2.0710	-1.56429E+01
2273	0.3	2.0720	-1.56222E+01
2273	0.3	2.0730	-1.56014E+01
2273	0.3	2.0740	-1.55806E+01
2273	0.3	2.0750	-1.55597E+01
2273	0.3	2.0760	-1.55387E+01
2273	0.3	2.0770	-1.55176E+01
2273	0.3	2.0780	-1.54964E+01
2273	0.3	2.0790	-1.54751E+01
2273	0.3	2.0800	-1.54537E+01
2273	0.3	2.0810	-1.54323E+01
2273	0.3	2.0820	-1.54107E+01
2273	0.3	2.0830	-1.53891E+01
2273	0.3	2.0840	-1.53674E+01
2273	0.3	2.0850	-1.53456E+01
2273	0.3	2.0860	-1.53237E+01
2273	0.3	2.0870	-1.53018E+01
2273	0.3	2.0880	-1.52797E+01
2273	0.3	2.0890	-1.52576E+01
2273	0.3	2.0900	-1.52354E+01

A.2.4. $(U_{0.6}Pu_{0.4})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D _{Pu} (m ² /s)
1273	0.4	1.8000	-2.48375E+01
1273	0.4	1.8010	-2.48328E+01
1273	0.4	1.8020	-2.48274E+01
1273	0.4	1.8030	-2.48224E+01
1273	0.4	1.8040	-2.48180E+01
1273	0.4	1.8050	-2.48143E+01
1273	0.4	1.8060	-2.48111E+01
1273	0.4	1.8070	-2.48085E+01
1273	0.4	1.8080	-2.48063E+01
1273	0.4	1.8090	-2.48047E+01
1273	0.4	1.8100	-2.48035E+01
1273	0.4	1.8110	-2.48027E+01
1273	0.4	1.8120	-2.48022E+01
1273	0.4	1.8130	-2.48021E+01
1273	0.4	1.8140	-2.48024E+01
1273	0.4	1.8150	-2.48029E+01
1273	0.4	1.8160	-2.48037E+01
1273	0.4	1.8170	-2.48047E+01
1273	0.4	1.8180	-2.48060E+01
1273	0.4	1.8190	-2.48075E+01
1273	0.4	1.8200	-2.48092E+01
1273	0.4	1.8210	-2.48111E+01
1273	0.4	1.8220	-2.48132E+01
1273	0.4	1.8230	-2.48154E+01
1273	0.4	1.8240	-2.48178E+01
1273	0.4	1.8250	-2.48203E+01
1273	0.4	1.8260	-2.48229E+01
1273	0.4	1.8270	-2.48257E+01
1273	0.4	1.8280	-2.48286E+01
1273	0.4	1.8290	-2.48316E+01
1273	0.4	1.8300	-2.48347E+01
1273	0.4	1.8310	-2.48379E+01
1273	0.4	1.8320	-2.48411E+01
1273	0.4	1.8330	-2.48445E+01
1273	0.4	1.8340	-2.48479E+01
1273	0.4	1.8350	-2.48514E+01
1273	0.4	1.8360	-2.48549E+01
1273	0.4	1.8370	-2.48585E+01
1273	0.4	1.8380	-2.48622E+01
1273	0.4	1.8390	-2.48659E+01
1273	0.4	1.8400	-2.48697E+01
1273	0.4	1.8410	-2.48735E+01
1273	0.4	1.8420	-2.48773E+01
1273	0.4	1.8430	-2.48812E+01
1273	0.4	1.8440	-2.48851E+01
1273	0.4	1.8450	-2.48890E+01
1273	0.4	1.8460	-2.48930E+01
1273	0.4	1.8470	-2.48970E+01
1273	0.4	1.8480	-2.49010E+01
1273	0.4	1.8490	-2.49050E+01
1273	0.4	1.8500	-2.49091E+01
1273	0.4	1.8510	-2.49132E+01
1273	0.4	1.8520	-2.49173E+01
1273	0.4	1.8530	-2.49214E+01
1273	0.4	1.8540	-2.49255E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D _{Pu} (m ² /s)
1273	0.4	1.8550	-2.49296E+01
1273	0.4	1.8560	-2.49338E+01
1273	0.4	1.8570	-2.49379E+01
1273	0.4	1.8580	-2.49421E+01
1273	0.4	1.8590	-2.49463E+01
1273	0.4	1.8600	-2.49505E+01
1273	0.4	1.8610	-2.49547E+01
1273	0.4	1.8620	-2.49589E+01
1273	0.4	1.8630	-2.49632E+01
1273	0.4	1.8640	-2.49674E+01
1273	0.4	1.8650	-2.49716E+01
1273	0.4	1.8660	-2.49759E+01
1273	0.4	1.8670	-2.49802E+01
1273	0.4	1.8680	-2.49844E+01
1273	0.4	1.8690	-2.49887E+01
1273	0.4	1.8700	-2.49930E+01
1273	0.4	1.8710	-2.49973E+01
1273	0.4	1.8720	-2.50016E+01
1273	0.4	1.8730	-2.50060E+01
1273	0.4	1.8740	-2.50103E+01
1273	0.4	1.8750	-2.50146E+01
1273	0.4	1.8760	-2.50190E+01
1273	0.4	1.8770	-2.50234E+01
1273	0.4	1.8780	-2.50277E+01
1273	0.4	1.8790	-2.50321E+01
1273	0.4	1.8800	-2.50366E+01
1273	0.4	1.8810	-2.50410E+01
1273	0.4	1.8820	-2.50454E+01
1273	0.4	1.8830	-2.50499E+01
1273	0.4	1.8840	-2.50544E+01
1273	0.4	1.8850	-2.50589E+01
1273	0.4	1.8860	-2.50634E+01
1273	0.4	1.8870	-2.50679E+01
1273	0.4	1.8880	-2.50725E+01
1273	0.4	1.8890	-2.50771E+01
1273	0.4	1.8900	-2.50817E+01
1273	0.4	1.8910	-2.50863E+01
1273	0.4	1.8920	-2.50910E+01
1273	0.4	1.8930	-2.50957E+01
1273	0.4	1.8940	-2.51004E+01
1273	0.4	1.8950	-2.51052E+01
1273	0.4	1.8960	-2.51100E+01
1273	0.4	1.8970	-2.51148E+01
1273	0.4	1.8980	-2.51197E+01
1273	0.4	1.8990	-2.51246E+01
1273	0.4	1.9000	-2.51296E+01
1273	0.4	1.9010	-2.51346E+01
1273	0.4	1.9020	-2.51396E+01
1273	0.4	1.9030	-2.51447E+01
1273	0.4	1.9040	-2.51499E+01
1273	0.4	1.9050	-2.51551E+01
1273	0.4	1.9060	-2.51604E+01
1273	0.4	1.9070	-2.51657E+01
1273	0.4	1.9080	-2.51711E+01
1273	0.4	1.9090	-2.51765E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D _{Pu} (m ² /s)
1273	0.4	1.9100	-2.51821E+01
1273	0.4	1.9110	-2.51877E+01
1273	0.4	1.9120	-2.51934E+01
1273	0.4	1.9130	-2.51991E+01
1273	0.4	1.9140	-2.52050E+01
1273	0.4	1.9150	-2.52109E+01
1273	0.4	1.9160	-2.52170E+01
1273	0.4	1.9170	-2.52231E+01
1273	0.4	1.9180	-2.52293E+01
1273	0.4	1.9190	-2.52357E+01
1273	0.4	1.9200	-2.52422E+01
1273	0.4	1.9210	-2.52488E+01
1273	0.4	1.9220	-2.52555E+01
1273	0.4	1.9230	-2.52624E+01
1273	0.4	1.9240	-2.52694E+01
1273	0.4	1.9250	-2.52766E+01
1273	0.4	1.9260	-2.52840E+01
1273	0.4	1.9270	-2.52915E+01
1273	0.4	1.9280	-2.52992E+01
1273	0.4	1.9290	-2.53071E+01
1273	0.4	1.9300	-2.53152E+01
1273	0.4	1.9310	-2.53235E+01
1273	0.4	1.9320	-2.53320E+01
1273	0.4	1.9330	-2.53407E+01
1273	0.4	1.9340	-2.53497E+01
1273	0.4	1.9350	-2.53590E+01
1273	0.4	1.9360	-2.53685E+01
1273	0.4	1.9370	-2.53783E+01
1273	0.4	1.9380	-2.53885E+01
1273	0.4	1.9390	-2.53989E+01
1273	0.4	1.9400	-2.54096E+01
1273	0.4	1.9410	-2.54207E+01
1273	0.4	1.9420	-2.54321E+01
1273	0.4	1.9430	-2.54439E+01
1273	0.4	1.9440	-2.54561E+01
1273	0.4	1.9450	-2.54686E+01
1273	0.4	1.9460	-2.54816E+01
1273	0.4	1.9470	-2.54950E+01
1273	0.4	1.9480	-2.55088E+01
1273	0.4	1.9490	-2.55231E+01
1273	0.4	1.9500	-2.55378E+01
1273	0.4	1.9510	-2.55530E+01
1273	0.4	1.9520	-2.55687E+01
1273	0.4	1.9530	-2.55849E+01
1273	0.4	1.9540	

1273	0.4	1.9650	-2.58197E+01
1273	0.4	1.9660	-2.58428E+01
1273	0.4	1.9670	-2.58664E+01
1273	0.4	1.9680	-2.58906E+01
1273	0.4	1.9690	-2.59153E+01
1273	0.4	1.9700	-2.59405E+01
1273	0.4	1.9710	-2.59662E+01
1273	0.4	1.9720	-2.59925E+01
1273	0.4	1.9730	-2.60193E+01
1273	0.4	1.9740	-2.60465E+01
1273	0.4	1.9750	-2.60743E+01
1273	0.4	1.9760	-2.61025E+01
1273	0.4	1.9770	-2.61313E+01
1273	0.4	1.9780	-2.61604E+01
1273	0.4	1.9790	-2.61901E+01
1273	0.4	1.9800	-2.62202E+01
1273	0.4	1.9810	-2.62507E+01
1273	0.4	1.9820	-2.62816E+01
1273	0.4	1.9830	-2.63129E+01
1273	0.4	1.9840	-2.63445E+01
1273	0.4	1.9850	-2.63765E+01
1273	0.4	1.9860	-2.64089E+01
1273	0.4	1.9870	-2.64415E+01
1273	0.4	1.9880	-2.64744E+01
1273	0.4	1.9890	-2.65076E+01
1273	0.4	1.9900	-2.65409E+01
1273	0.4	1.9910	-2.65744E+01
1273	0.4	1.9920	-2.66081E+01
1273	0.4	1.9930	-2.66418E+01
1273	0.4	1.9940	-2.66754E+01
1273	0.4	1.9950	-2.67091E+01
1273	0.4	1.9960	-2.67426E+01
1273	0.4	1.9970	-2.67759E+01
1273	0.4	1.9980	-2.68098E+01
1273	0.4	1.9990	-2.68441E+01
1273	0.4	2.0000	-2.68735E+01
1273	0.4	2.0010	-2.69050E+01
1273	0.4	2.0020	-2.69348E+01
1273	0.4	2.0030	-2.69629E+01
1273	0.4	2.0040	-2.69890E+01
1273	0.4	2.0050	-2.70128E+01
1273	0.4	2.0060	-2.70342E+01
1273	0.4	2.0070	-2.70530E+01
1273	0.4	2.0080	-2.70689E+01
1273	0.4	2.0090	-2.70820E+01
1273	0.4	2.0100	-2.70920E+01
1273	0.4	2.0110	-2.70989E+01
1273	0.4	2.0120	-2.71028E+01
1273	0.4	2.0130	-2.71037E+01
1273	0.4	2.0140	-2.71016E+01
1273	0.4	2.0150	-2.70967E+01
1273	0.4	2.0160	-2.70891E+01
1273	0.4	2.0170	-2.70790E+01
1273	0.4	2.0180	-2.70666E+01
1273	0.4	2.0190	-2.70521E+01
1273	0.4	2.0200	-2.70356E+01
1273	0.4	2.0210	-2.70174E+01
1273	0.4	2.0220	-2.69977E+01
1273	0.4	2.0230	-2.69765E+01
1273	0.4	2.0240	-2.69540E+01
1273	0.4	2.0250	-2.69305E+01
1273	0.4	2.0260	-2.69059E+01
1273	0.4	2.0270	-2.68805E+01
1273	0.4	2.0280	-2.68542E+01
1273	0.4	2.0290	-2.68272E+01
1273	0.4	2.0300	-2.67996E+01
1273	0.4	2.0310	-2.67714E+01
1273	0.4	2.0320	-2.67426E+01
1273	0.4	2.0330	-2.67134E+01
1273	0.4	2.0340	-2.66837E+01
1273	0.4	2.0350	-2.66536E+01
1273	0.4	2.0360	-2.66231E+01
1273	0.4	2.0370	-2.65922E+01
1273	0.4	2.0380	-2.65609E+01
1273	0.4	2.0390	-2.65293E+01
1273	0.4	2.0400	-2.64974E+01
1273	0.4	2.0410	-2.64652E+01
1273	0.4	2.0420	-2.64326E+01
1273	0.4	2.0430	-2.63998E+01
1273	0.4	2.0440	-2.63666E+01
1273	0.4	2.0450	-2.63332E+01
1273	0.4	2.0460	-2.62995E+01
1273	0.4	2.0470	-2.62655E+01
1273	0.4	2.0480	-2.62313E+01
1273	0.4	2.0490	-2.61968E+01
1273	0.4	2.0500	-2.61620E+01
1273	0.4	2.0510	-2.61270E+01
1273	0.4	2.0520	-2.60917E+01
1273	0.4	2.0530	-2.60562E+01
1273	0.4	2.0540	-2.60204E+01
1273	0.4	2.0550	-2.59844E+01
1273	0.4	2.0560	-2.59481E+01

1273	0.4	2.0570	-2.59116E+01
1273	0.4	2.0580	-2.58749E+01
1273	0.4	2.0590	-2.58380E+01
1273	0.4	2.0600	-2.58008E+01
1273	0.4	2.0610	-2.57634E+01
1273	0.4	2.0620	-2.57258E+01
1273	0.4	2.0630	-2.56880E+01
1273	0.4	2.0640	-2.56500E+01
1273	0.4	2.0650	-2.56118E+01
1273	0.4	2.0660	-2.55734E+01
1273	0.4	2.0670	-2.55349E+01
1273	0.4	2.0680	-2.54961E+01
1273	0.4	2.0690	-2.54572E+01
1273	0.4	2.0700	-2.54181E+01
1273	0.4	2.0710	-2.53788E+01
1273	0.4	2.0720	-2.53394E+01
1273	0.4	2.0730	-2.52999E+01
1273	0.4	2.0740	-2.52602E+01
1273	0.4	2.0750	-2.52203E+01
1273	0.4	2.0760	-2.51803E+01
1273	0.4	2.0770	-2.51402E+01
1273	0.4	2.0780	-2.51000E+01
1273	0.4	2.0790	-2.50596E+01
1273	0.4	2.0800	-2.50192E+01
1273	0.4	2.0810	-2.49786E+01
1273	0.4	2.0820	-2.49380E+01
1273	0.4	2.0830	-2.48972E+01
1273	0.4	2.0840	-2.48564E+01
1273	0.4	2.0850	-2.48154E+01
1273	0.4	2.0860	-2.47744E+01
1273	0.4	2.0870	-2.47333E+01
1273	0.4	2.0880	-2.46922E+01
1273	0.4	2.0890	-2.46510E+01
1273	0.4	2.0900	-2.46097E+01
1273	0.4	2.0910	-2.45683E+01
1273	0.4	2.0920	-2.45269E+01
1273	0.4	2.0930	-2.44855E+01
1273	0.4	2.0940	-2.44440E+01
1273	0.4	2.0950	-2.44025E+01
1273	0.4	2.0960	-2.43609E+01
1273	0.4	2.0970	-2.43193E+01
1273	0.4	2.0980	-2.42777E+01
1273	0.4	2.0990	-2.42360E+01
1273	0.4	2.1000	-2.41943E+01
1273	0.4	2.1010	-2.41526E+01
1273	0.4	2.1020	-2.41108E+01
1273	0.4	2.1030	-2.40691E+01
1273	0.4	2.1040	-2.40273E+01
1273	0.4	2.1050	-2.39855E+01
1273	0.4	2.1060	-2.39438E+01
1273	0.4	2.1070	-2.39020E+01
1273	0.4	2.1080	-2.38601E+01
1273	0.4	2.1090	-2.38183E+01
1273	0.4	2.1100	-2.37765E+01
1273	0.4	2.1110	-2.37347E+01
1273	0.4	2.1120	-2.36929E+01
1273	0.4	2.1130	-2.36511E+01
1273	0.4	2.1140	-2.36093E+01
1273	0.4	2.1150	-2.35675E+01
1273	0.4	2.1160	-2.35257E+01
1273	0.4	2.1170	-2.34839E+01
1273	0.4	2.1180	-2.34421E+01
1273	0.4	2.1190	-2.34003E+01
1273	0.4	2.1200	-2.33586E+01
1273	0.4	2.1210	-2.33168E+01
1273	0.4	2.1220	-2.32751E+01
1273	0.4	2.1230	-2.32334E+01
1273	0.4	2.1240	-2.31917E+01
1273	0.4	2.1250	-2.31500E+01
1273	0.4	2.1260	-2.31083E+01
1273	0.4	2.1270	-2.30666E+01
1273	0.4	2.1280	-2.30250E+01
1273	0.4	2.1290	-2.29834E+01
1273	0.4	2.1300	-2.29418E+01
1273	0.4	2.1310	-2.29002E+01
1273	0.4	2.1320	-2.28587E+01
1273	0.4	2.1330	-2.28171E+01
1273	0.4	2.1340	-2.27756E+01
1273	0.4	2.1350	-2.27341E+01
1273	0.4	2.1360	-2.26926E+01
1273	0.4	2.1370	-2.26512E+01
1273	0.4	2.1380	-2.26098E+01
1273	0.4	2.1390	-2.25684E+01
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1273	0.4	1.7820	-1.89853E+01
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1273	0.4	1.7840	-1.89851E+01
1273	0.4	1.7850	-1.89849E+01
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1273	0.4	1.7870	-1.89846E+01

1773	0.4	1.7880	-1.89844E+01
1773	0.4	1.7890	-1.89841E+01
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1773	0.4	1.7910	-1.89835E+01
1773	0.4	1.7920	-1.89832E+01
1773	0.4	1.7930	-1.89828E+01
1773	0.4	1.7940	-1.89823E+01
1773	0.4	1.7950	-1.89818E+01
1773	0.4	1.7960	-1.89812E+01
1773	0.4	1.7970	-1.89805E+01
1773	0.4	1.7980	-1.89796E+01
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1773	0.4	1.8000	-1.89778E+01
1773	0.4	1.8010	-1.89767E+01
1773	0.4	1.8020	-1.89757E+01
1773	0.4	1.8030	-1.89746E+01
1773	0.4	1.8040	-1.89736E+01
1773	0.4	1.8050	-1.89727E+01
1773	0.4	1.8060	-1.89718E+01
1773	0.4	1.8070	-1.89712E+01
1773	0.4	1.8080	-1.89706E+01
1773	0.4	1.8090	-1.89702E+01
1773	0.4	1.8100	-1.89700E+01
1773	0.4	1.8110	-1.89699E+01
1773	0.4	1.8120	-1.89700E+01
1773	0.4	1.8130	-1.89702E+01
1773	0.4	1.8140	-1.89706E+01
1773	0.4	1.8150	-1.89711E+01
1773	0.4	1.8160	-1.89718E+01
1773	0.4	1.8170	-1.89726E+01
1773	0.4	1.8180	-1.89736E+01
1773	0.4	1.8190	-1.89747E+01
1773	0.4	1.8200	-1.89759E+01
1773	0.4	1.8210	-1.89772E+01
1773	0.4	1.8220	-1.89786E+01
1773	0.4	1.8230	-1.89802E+01
1773	0.4	1.8240	-1.89818E+01
1773	0.4	1.8250	-1.89836E+01
1773	0.4	1.8260	-1.89855E+01
1773	0.4	1.8270	-1.89874E+01
1773	0.4	1.8280	-1.89895E+01
1773	0.4	1.8290	-1.89916E+01
1773	0.4	1.8300	-1.89938E+01
1773	0.4	1.8310	-1.89961E+01
1773	0.4	1.8320	-1.89985E+01
1773	0.4	1.8330	-1.90009E+01
1773	0.4	1.8340	-1.90035E+01
1773	0.4	1.8350	-1.90060E+01
1773	0.4	1.8360	-1.90087E+01
1773	0.4	1.8370	-1.90114E+01
1773	0.4	1.8380	-1.90142E+01
1773	0.4	1.8390	-1.90170E+01
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1773	0.4	1.8410	-1.90229E+01
1773	0.4	1.8420	-1.90259E+01
1773	0.4	1.8430	-1.90290E+01
1773	0.4	1.8440	-1.90321E+01
1773	0.4	1.8450	-1.90353E+01
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1773	0.4	1.8470	-1.90417E+01
1773	0.4	1.8480	-1.90450E+01
1773	0.4	1.8490	-1.90484E+01
1773	0.4	1.8500	-1.90518E+01
1773	0.4	1.8510	-1.90552E+01
1773	0.4	1.8520	-1.90587E+01
1773	0.4	1.8530	-1.90622E+01
1773	0.4		

1773	0.4	1.8800	-1.91713E+01
1773	0.4	1.8810	-1.91760E+01
1773	0.4	1.8820	-1.91806E+01
1773	0.4	1.8830	-1.91853E+01
1773	0.4	1.8840	-1.91901E+01
1773	0.4	1.8850	-1.91949E+01
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1773	0.4	1.8870	-1.92047E+01
1773	0.4	1.8880	-1.92097E+01
1773	0.4	1.8890	-1.92148E+01
1773	0.4	1.8900	-1.92199E+01
1773	0.4	1.8910	-1.92251E+01
1773	0.4	1.8920	-1.92304E+01
1773	0.4	1.8930	-1.92357E+01
1773	0.4	1.8940	-1.92411E+01
1773	0.4	1.8950	-1.92466E+01
1773	0.4	1.8960	-1.92522E+01
1773	0.4	1.8970	-1.92579E+01
1773	0.4	1.8980	-1.92636E+01
1773	0.4	1.8990	-1.92695E+01
1773	0.4	1.9000	-1.92754E+01
1773	0.4	1.9010	-1.92815E+01
1773	0.4	1.9020	-1.92876E+01
1773	0.4	1.9030	-1.92939E+01
1773	0.4	1.9040	-1.93002E+01
1773	0.4	1.9050	-1.93067E+01
1773	0.4	1.9060	-1.93133E+01
1773	0.4	1.9070	-1.93200E+01
1773	0.4	1.9080	-1.93269E+01
1773	0.4	1.9090	-1.93339E+01
1773	0.4	1.9100	-1.93410E+01
1773	0.4	1.9110	-1.93483E+01
1773	0.4	1.9120	-1.93558E+01
1773	0.4	1.9130	-1.93634E+01
1773	0.4	1.9140	-1.93711E+01
1773	0.4	1.9150	-1.93790E+01
1773	0.4	1.9160	-1.93871E+01
1773	0.4	1.9170	-1.93954E+01
1773	0.4	1.9180	-1.94039E+01
1773	0.4	1.9190	-1.94125E+01
1773	0.4	1.9200	-1.94214E+01
1773	0.4	1.9210	-1.94304E+01
1773	0.4	1.9220	-1.94397E+01
1773	0.4	1.9230	-1.94492E+01
1773	0.4	1.9240	-1.94588E+01
1773	0.4	1.9250	-1.94688E+01
1773	0.4	1.9260	-1.94789E+01
1773	0.4	1.9270	-1.94893E+01
1773	0.4	1.9280	-1.94999E+01
1773	0.4	1.9290	-1.95107E+01
1773	0.4	1.9300	-1.95218E+01
1773	0.4	1.9310	-1.95332E+01
1773	0.4	1.9320	-1.95448E+01
1773	0.4	1.9330	-1.95566E+01
1773	0.4	1.9340	-1.95687E+01
1773	0.4	1.9350	-1.95811E+01
1773	0.4	1.9360	-1.95938E+01
1773	0.4	1.9370	-1.96067E+01
1773	0.4	1.9380	-1.96199E+01
1773	0.4	1.9390	-1.96333E+01
1773	0.4	1.9400	-1.96470E+01
1773	0.4	1.9410	-1.96610E+01
1773	0.4	1.9420	-1.96752E+01
1773	0.4	1.9430	-1.96898E+01
1773	0.4	1.9440	-1.97045E+01
1773	0.4	1.9450	-1.97196E+01
1773	0.4	1.9460	-1.97349E+01
1773	0.4	1.9470	-1.97504E+01
1773	0.4	1.9480	-1.97662E+01
1773	0.4	1.9490	-1.97823E+01
1773	0.4	1.9500	-1.97986E+01
1773	0.4	1.9510	-1.98151E+01
1773	0.4	1.9520	-1.98319E+01
1773	0.4	1.9530	-1.98488E+01
1773	0.4	1.9540	-1.98660E+01
1773	0.4	1.9550	-1.98834E+01
1773	0.4	1.9560	-1.99010E+01
1773	0.4	1.9570	-1.99187E+01
1773	0.4	1.9580	-1.99366E+01
1773	0.4	1.9590	-1.99547E+01
1773	0.4	1.9600	-1.99729E+01
1773	0.4	1.9610	-1.99913E+01
1773	0.4	1.9620	-2.00097E+01
1773	0.4	1.9630	-2.00283E+01
1773	0.4	1.9640	-2.00469E+01
1773	0.4	1.9650	-2.00656E+01
1773	0.4	1.9660	-2.00843E+01
1773	0.4	1.9670	-2.01031E+01
1773	0.4	1.9680	-2.01218E+01
1773	0.4	1.9690	-2.01405E+01
1773	0.4	1.9700	-2.01592E+01
1773	0.4	1.9710	-2.01778E+01

1773	0.4	1.9720	-2.01962E+01
1773	0.4	1.9730	-2.02145E+01
1773	0.4	1.9740	-2.02327E+01
1773	0.4	1.9750	-2.02506E+01
1773	0.4	1.9760	-2.02684E+01
1773	0.4	1.9770	-2.02858E+01
1773	0.4	1.9780	-2.03030E+01
1773	0.4	1.9790	-2.03198E+01
1773	0.4	1.9800	-2.03362E+01
1773	0.4	1.9810	-2.03522E+01
1773	0.4	1.9820	-2.03678E+01
1773	0.4	1.9830	-2.03829E+01
1773	0.4	1.9840	-2.03974E+01
1773	0.4	1.9850	-2.04114E+01
1773	0.4	1.9860	-2.04248E+01
1773	0.4	1.9870	-2.04375E+01
1773	0.4	1.9880	-2.04496E+01
1773	0.4	1.9890	-2.04610E+01
1773	0.4	1.9900	-2.04717E+01
1773	0.4	1.9910	-2.04816E+01
1773	0.4	1.9920	-2.04907E+01
1773	0.4	1.9930	-2.04990E+01
1773	0.4	1.9940	-2.05065E+01
1773	0.4	1.9950	-2.05132E+01
1773	0.4	1.9960	-2.05190E+01
1773	0.4	1.9970	-2.05240E+01
1773	0.4	1.9980	-2.05281E+01
1773	0.4	1.9990	-2.05312E+01
1773	0.4	2.0000	-2.05328E+01
1773	0.4	2.0010	-2.05298E+01
1773	0.4	2.0020	-2.05249E+01
1773	0.4	2.0030	-2.05187E+01
1773	0.4	2.0040	-2.05113E+01
1773	0.4	2.0050	-2.05028E+01
1773	0.4	2.0060	-2.04934E+01
1773	0.4	2.0070	-2.04829E+01
1773	0.4	2.0080	-2.04716E+01
1773	0.4	2.0090	-2.04594E+01
1773	0.4	2.0100	-2.04464E+01
1773	0.4	2.0110	-2.04327E+01
1773	0.4	2.0120	-2.04183E+01
1773	0.4	2.0130	-2.04033E+01
1773	0.4	2.0140	-2.03877E+01
1773	0.4	2.0150	-2.03716E+01
1773	0.4	2.0160	-2.03550E+01
1773	0.4	2.0170	-2.03379E+01
1773	0.4	2.0180	-2.03203E+01
1773	0.4	2.0190	-2.03024E+01
1773	0.4	2.0200	-2.02841E+01
1773	0.4	2.0210	-2.02654E+01
1773	0.4	2.0220	-2.02464E+01
1773	0.4	2.0230	-2.02271E+01
1773	0.4	2.0240	-2.02075E+01
1773	0.4	2.0250	-2.01876E+01
1773	0.4	2.0260	-2.01675E+01
1773	0.4	2.0270	-2.01471E+01
1773	0.4	2.0280	-2.01264E+01
1773	0.4	2.0290	-2.01056E+01
1773	0.4	2.0300	-2.00845E+01
1773	0.4	2.0310	-2.00633E+01
1773	0.4	2.0320	-2.00418E+01
1773	0.4	2.0330	-2.00201E+01
1773	0.4	2.0340	-1.99983E+01
1773	0.4	2.0350	-1.99762E+01
1773	0.4	2.0360	-1.99540E+01
1773	0.4	2.0370	-1.99316E+01
1773	0.4	2.0380	-1.99090E+01
1773	0.4	2.0390	-1.98863E+01
1773	0.4	2.0400	-1.98634E+01
1773	0.4	2.0410	-1.98403E+01
1773	0.4	2.0420	-1.98171E+01
1773	0.4	2.0430	-1.97937E+01
1773	0.4	2.0440	-1.97701E+01
1773	0.4	2.0450	-1.97464E+01
1773	0.4	2.0460	-1.97225E+01
1773	0.4	2.0470	-1.96985E+01
1773	0.4	2.0480	-1.96743E+01
1773	0.4	2.0490	-1.96500E+01
1773	0.4	2.0500	-1.96255E+01
1773	0.4	2.0510	-1.96008E+01
1773	0.4	2.0520	-1.95760E+01
1773	0.4	2.0530	-1.95510E+01
1773	0.4	2.0540	-1.95259E+01
1773	0.4	2.0550	-1.95007E+01
1773	0.4	2.0560	-1.94753E+01
1773	0.4	2.0570	-1.94497E+01
1773	0.4	2.0580	-1.94240E+01
1773	0.4	2.0590	-1.93982E+01
1773	0.4	2.0600	-1.93722E+01
1773	0.4	2.0610	-1.93460E+01
1773	0.4	2.0620	-1.93197E+01
1773	0.4	2.0630	-1.92933E+01

1773	0.4	2.0640	-1.92667E+01
1773	0.4	2.0650	-1.92400E+01
1773	0.4	2.0660	-1.92131E+01
1773	0.4	2.0670	-1.91861E+01
1773	0.4	2.0680	-1.91589E+01
1773	0.4	2.0690	-1.91316E+01
1773	0.4	2.0700	-1.91042E+01
1773	0.4	2.0710	-1.90766E+01
1773	0.4	2.0720	-1.90489E+01
1773	0.4	2.0730	-1.90211E+01
1773	0.4	2.0740	-1.89931E+01
1773	0.4	2.0750	-1.89650E+01
1773	0.4	2.0760	-1.89368E+01
1773	0.4	2.0770	-1.89084E+01
1773	0.4	2.0780	-1.88799E+01
1773	0.4	2.0790	-1.88513E+01
1773	0.4	2.0800	-1.88225E+01
1773	0.4	2.0810	-1.87936E+01
1773	0.4	2.0820	-1.87646E+01
1773	0.4	2.0830	-1.87355E+01
1773	0.4	2.0840	-1.87063E+01
1773	0.4	2.0850	-1.86769E+01
1773	0.4	2.0860	-1.86475E+01
1773	0.4	2.0870	-1.86179E+01
1773	0.4	2.0880	-1.85882E+01
1773	0.4	2.0890	-1.85584E+01
1773	0.4	2.0900	-1.85286E+01
1773	0.4	2.0910	-1.84986E+01
1773	0.4	2.0920	-1.84685E+01
1773	0.4	2.0930	-1.84383E+01
1773	0.4	2.0940	-1.84080E+01
1773	0.4	2.0950	-1.83776E+01
1773	0.4	2.0960	-1.83472E+01
1773	0.4	2.0970	-1.83166E+01
1773	0.4	2.0980	-1.82860E+01
1773	0.4	2.0990	-1.82552E+01
1773	0.4	2.1000	-1.82244E+01
1773	0.4	2.1010	-1.81936E+01
1773	0.4	2.1020	-1.81626E+01
1773	0.4	2.1030	-1.81316E+01
1773	0.4	2.1040	-1.81005E+01
1773	0.4	2.1050	-1.80693E+01
1773	0.4	2.1060	-1.80381E+01
1773	0.4	2.1070	-1.80068E+01
1773	0.4	2.1080	-1.79755E+01
1773	0.4	2.1090	-1.79441E+01
1773	0.4	2.1100	-1.79126E+01
1773	0.4	2.1110	-1.78811E+01
1773	0.4	2.1120	-1.78495E+01
1773	0.4	2.1130	-1.78179E+01
1773	0.4	2.1140	-1.77862E+01
1773	0.4	2.1150	-1.77545E+01
1773	0.4	2.1160	-1.77228E+01
1773	0.4	2.1170	-1.76910E+01
1773	0.4	2.1180	-1.76592E+01
1773	0.4	2.1190	-1.76273E+01
1773	0.4	2.1200	-1.75954E+01
2273	0.4	1.7300	-1.56789E+01
2273	0.4	1.7310	-1.56789E+01
2273	0.4	1.7320	-1.56789E+01
2273	0.4	1.7330	-1.56788E+01
2273	0.4	1.7340	-1.56788E+01
2273	0.4	1.7350	-1.56787E+01
2273	0.4	1.7360	-1.56787E+01
2273	0.4	1.7370	-1.56787E+01
2273	0.4	1.7380	-1.56786E+01
2273	0.4		

2273	0.4	1.7650	-1.56769E+01
2273	0.4	1.7660	-1.56768E+01
2273	0.4	1.7670	-1.56767E+01
2273	0.4	1.7680	-1.56766E+01
2273	0.4	1.7690	-1.56765E+01
2273	0.4	1.7700	-1.56763E+01
2273	0.4	1.7710	-1.56762E+01
2273	0.4	1.7720	-1.56761E+01
2273	0.4	1.7730	-1.56760E+01
2273	0.4	1.7740	-1.56759E+01
2273	0.4	1.7750	-1.56758E+01
2273	0.4	1.7760	-1.56756E+01
2273	0.4	1.7770	-1.56755E+01
2273	0.4	1.7780	-1.56754E+01
2273	0.4	1.7790	-1.56752E+01
2273	0.4	1.7800	-1.56751E+01
2273	0.4	1.7810	-1.56749E+01
2273	0.4	1.7820	-1.56748E+01
2273	0.4	1.7830	-1.56746E+01
2273	0.4	1.7840	-1.56745E+01
2273	0.4	1.7850	-1.56743E+01
2273	0.4	1.7860	-1.56742E+01
2273	0.4	1.7870	-1.56740E+01
2273	0.4	1.7880	-1.56739E+01
2273	0.4	1.7890	-1.56737E+01
2273	0.4	1.7900	-1.56736E+01
2273	0.4	1.7910	-1.56734E+01
2273	0.4	1.7920	-1.56733E+01
2273	0.4	1.7930	-1.56732E+01
2273	0.4	1.7940	-1.56731E+01
2273	0.4	1.7950	-1.56730E+01
2273	0.4	1.7960	-1.56729E+01
2273	0.4	1.7970	-1.56729E+01
2273	0.4	1.7980	-1.56729E+01
2273	0.4	1.7990	-1.56729E+01
2273	0.4	1.8000	-1.56729E+01
2273	0.4	1.8010	-1.56730E+01
2273	0.4	1.8020	-1.56731E+01
2273	0.4	1.8030	-1.56733E+01
2273	0.4	1.8040	-1.56735E+01
2273	0.4	1.8050	-1.56737E+01
2273	0.4	1.8060	-1.56740E+01
2273	0.4	1.8070	-1.56744E+01
2273	0.4	1.8080	-1.56748E+01
2273	0.4	1.8090	-1.56753E+01
2273	0.4	1.8100	-1.56759E+01
2273	0.4	1.8110	-1.56765E+01
2273	0.4	1.8120	-1.56771E+01
2273	0.4	1.8130	-1.56779E+01
2273	0.4	1.8140	-1.56787E+01
2273	0.4	1.8150	-1.56796E+01
2273	0.4	1.8160	-1.56806E+01
2273	0.4	1.8170	-1.56816E+01
2273	0.4	1.8180	-1.56827E+01
2273	0.4	1.8190	-1.56839E+01
2273	0.4	1.8200	-1.56851E+01
2273	0.4	1.8210	-1.56865E+01
2273	0.4	1.8220	-1.56879E+01
2273	0.4	1.8230	-1.56893E+01
2273	0.4	1.8240	-1.56908E+01
2273	0.4	1.8250	-1.56924E+01
2273	0.4	1.8260	-1.56941E+01
2273	0.4	1.8270	-1.56958E+01
2273	0.4	1.8280	-1.56976E+01
2273	0.4	1.8290	-1.56995E+01
2273	0.4	1.8300	-1.57015E+01
2273	0.4	1.8310	-1.57034E+01
2273	0.4	1.8320	-1.57055E+01
2273	0.4	1.8330	-1.57076E+01
2273	0.4	1.8340	-1.57098E+01
2273	0.4	1.8350	-1.57121E+01
2273	0.4	1.8360	-1.57144E+01
2273	0.4	1.8370	-1.57167E+01
2273	0.4	1.8380	-1.57192E+01
2273	0.4	1.8390	-1.57216E+01
2273	0.4	1.8400	-1.57242E+01
2273	0.4	1.8410	-1.57268E+01
2273	0.4	1.8420	-1.57294E+01
2273	0.4	1.8430	-1.57321E+01
2273	0.4	1.8440	-1.57349E+01
2273	0.4	1.8450	-1.57377E+01
2273	0.4	1.8460	-1.57406E+01
2273	0.4	1.8470	-1.57435E+01
2273	0.4	1.8480	-1.57465E+01
2273	0.4	1.8490	-1.57496E+01
2273	0.4	1.8500	-1.57526E+01
2273	0.4	1.8510	-1.57558E+01
2273	0.4	1.8520	-1.57590E+01
2273	0.4	1.8530	-1.57622E+01
2273	0.4	1.8540	-1.57655E+01
2273	0.4	1.8550	-1.57689E+01
2273	0.4	1.8560	-1.57723E+01

2273	0.4	1.8570	-1.57758E+01
2273	0.4	1.8580	-1.57793E+01
2273	0.4	1.8590	-1.57829E+01
2273	0.4	1.8600	-1.57865E+01
2273	0.4	1.8610	-1.57902E+01
2273	0.4	1.8620	-1.57940E+01
2273	0.4	1.8630	-1.57978E+01
2273	0.4	1.8640	-1.58017E+01
2273	0.4	1.8650	-1.58056E+01
2273	0.4	1.8660	-1.58096E+01
2273	0.4	1.8670	-1.58136E+01
2273	0.4	1.8680	-1.58177E+01
2273	0.4	1.8690	-1.58219E+01
2273	0.4	1.8700	-1.58261E+01
2273	0.4	1.8710	-1.58304E+01
2273	0.4	1.8720	-1.58348E+01
2273	0.4	1.8730	-1.58392E+01
2273	0.4	1.8740	-1.58437E+01
2273	0.4	1.8750	-1.58483E+01
2273	0.4	1.8760	-1.58529E+01
2273	0.4	1.8770	-1.58576E+01
2273	0.4	1.8780	-1.58624E+01
2273	0.4	1.8790	-1.58673E+01
2273	0.4	1.8800	-1.58722E+01
2273	0.4	1.8810	-1.58773E+01
2273	0.4	1.8820	-1.58824E+01
2273	0.4	1.8830	-1.58876E+01
2273	0.4	1.8840	-1.58929E+01
2273	0.4	1.8850	-1.58982E+01
2273	0.4	1.8860	-1.59037E+01
2273	0.4	1.8870	-1.59092E+01
2273	0.4	1.8880	-1.59149E+01
2273	0.4	1.8890	-1.59206E+01
2273	0.4	1.8900	-1.59265E+01
2273	0.4	1.8910	-1.59324E+01
2273	0.4	1.8920	-1.59385E+01
2273	0.4	1.8930	-1.59446E+01
2273	0.4	1.8940	-1.59509E+01
2273	0.4	1.8950	-1.59573E+01
2273	0.4	1.8960	-1.59638E+01
2273	0.4	1.8970	-1.59704E+01
2273	0.4	1.8980	-1.59771E+01
2273	0.4	1.8990	-1.59840E+01
2273	0.4	1.9000	-1.59909E+01
2273	0.4	1.9010	-1.59980E+01
2273	0.4	1.9020	-1.60053E+01
2273	0.4	1.9030	-1.60126E+01
2273	0.4	1.9040	-1.60201E+01
2273	0.4	1.9050	-1.60278E+01
2273	0.4	1.9060	-1.60355E+01
2273	0.4	1.9070	-1.60434E+01
2273	0.4	1.9080	-1.60515E+01
2273	0.4	1.9090	-1.60597E+01
2273	0.4	1.9100	-1.60680E+01
2273	0.4	1.9110	-1.60765E+01
2273	0.4	1.9120	-1.60851E+01
2273	0.4	1.9130	-1.60939E+01
2273	0.4	1.9140	-1.61028E+01
2273	0.4	1.9150	-1.61119E+01
2273	0.4	1.9160	-1.61211E+01
2273	0.4	1.9170	-1.61305E+01
2273	0.4	1.9180	-1.61401E+01
2273	0.4	1.9190	-1.61497E+01
2273	0.4	1.9200	-1.61596E+01
2273	0.4	1.9210	-1.61696E+01
2273	0.4	1.9220	-1.61797E+01
2273	0.4	1.9230	-1.61900E+01
2273	0.4	1.9240	-1.62004E+01
2273	0.4	1.9250	-1.62110E+01
2273	0.4	1.9260	-1.62217E+01
2273	0.4	1.9270	-1.62325E+01
2273	0.4	1.9280	-1.62435E+01
2273	0.4	1.9290	-1.62546E+01
2273	0.4	1.9300	-1.62659E+01
2273	0.4	1.9310	-1.62772E+01
2273	0.4	1.9320	-1.62887E+01
2273	0.4	1.9330	-1.63003E+01
2273	0.4	1.9340	-1.63120E+01
2273	0.4	1.9350	-1.63238E+01
2273	0.4	1.9360	-1.63357E+01
2273	0.4	1.9370	-1.63477E+01
2273	0.4	1.9380	-1.63598E+01
2273	0.4	1.9390	-1.63720E+01
2273	0.4	1.9400	-1.63842E+01
2273	0.4	1.9410	-1.63964E+01
2273	0.4	1.9420	-1.64088E+01
2273	0.4	1.9430	-1.64211E+01
2273	0.4	1.9440	-1.64335E+01
2273	0.4	1.9450	-1.64459E+01
2273	0.4	1.9460	-1.64582E+01
2273	0.4	1.9470	-1.64706E+01
2273	0.4	1.9480	-1.64830E+01

2273	0.4	1.9490	-1.64953E+01
2273	0.4	1.9500	-1.65075E+01
2273	0.4	1.9510	-1.65197E+01
2273	0.4	1.9520	-1.65318E+01
2273	0.4	1.9530	-1.65438E+01
2273	0.4	1.9540	-1.65557E+01
2273	0.4	1.9550	-1.65675E+01
2273	0.4	1.9560	-1.65791E+01
2273	0.4	1.9570	-1.65906E+01
2273	0.4	1.9580	-1.66019E+01
2273	0.4	1.9590	-1.66130E+01
2273	0.4	1.9600	-1.66238E+01
2273	0.4	1.9610	-1.66345E+01
2273	0.4	1.9620	-1.66449E+01
2273	0.4	1.9630	-1.66550E+01
2273	0.4	1.9640	-1.66648E+01
2273	0.4	1.9650	-1.66744E+01
2273	0.4	1.9660	-1.66836E+01
2273	0.4	1.9670	-1.66925E+01
2273	0.4	1.9680	-1.67010E+01
2273	0.4	1.9690	-1.67092E+01
2273	0.4	1.9700	-1.67169E+01
2273	0.4	1.9710	-1.67243E+01
2273	0.4	1.9720	-1.67313E+01
2273	0.4	1.9730	-1.67379E+01
2273	0.4	1.9740	-1.67440E+01
2273	0.4	1.9750	-1.67497E+01
2273	0.4	1.9760	-1.67549E+01
2273	0.4	1.9770	-1.67597E+01
2273	0.4	1.9780	-1.67640E+01
2273	0.4	1.9790	-1.67679E+01
2273	0.4	1.9800	-1.67712E+01
2273	0.4	1.9810	-1.67741E+01
2273	0.4	1.9820	-1.67765E+01
2273	0.4	1.9830	-1.67785E+01
2273	0.4	1.9840	-1.67799E+01
2273	0.4	1.9850	-1.67809E+01
2273	0.4	1.9860	-1.67814E+01
2273	0.4	1.9870	-1.67814E+01
2273	0.4	1.9880	-1.67809E+01
2273	0.4	1.9890	-1.67800E+01
2273	0.4	1.9900	-1.67786E+01
2273	0.4	1.9910	-1.67767E+01
2273	0.4	1.9920	-1.67744E+01
2273	0.4	1.9930	-1.67716E+01
2273	0.4	1.9940	-1.67684E+01
2273	0.4	1.9950	-1.67646E+01
2273	0.4	1.9960	-1.67603E+01
2273	0.4	1.9970	-1.67554E+01
2273	0.4	1.9980	-1.67498E+01
2273	0.4	1.9990	-1.67434E+01
2273	0.4	2.0000	-1.67359E+01
2273	0.4	2.0010	-1.67271E+01
2273	0.4	2.0020	-1.67173E+01
2273	0.4	2.0030	-1.67065E+01
2273	0.4	2.0040	-1.66951E+01
2273	0.4	2.0050	-1.66830E+01
2273	0.4	2.0060	-1.66705E+01
2273	0.4	2.0070	-1.66576E+01
2273	0.4	2.0080	-1.66443E+01
2273	0.4	2.0090	-1.66307E+01
2273	0.4	2.0100	-1.66168E+01
2273	0.4	2.0110	-1.66026E+01
2273	0.4	2.0120	-1.65881E+01
2273	0.4	2.0130	-1.65734E+01
2273	0.4	2.0140	-1.65585E+01
2273	0.4		

2273	0.4	2.0410	-1.60940E+01
2273	0.4	2.0420	-1.60751E+01
2273	0.4	2.0430	-1.60560E+01
2273	0.4	2.0440	-1.60369E+01
2273	0.4	2.0450	-1.60176E+01
2273	0.4	2.0460	-1.59983E+01
2273	0.4	2.0470	-1.59788E+01

2273	0.4	2.0480	-1.59593E+01
2273	0.4	2.0490	-1.59396E+01
2273	0.4	2.0500	-1.59199E+01
2273	0.4	2.0510	-1.59000E+01
2273	0.4	2.0520	-1.58801E+01
2273	0.4	2.0530	-1.58600E+01
2273	0.4	2.0540	-1.58398E+01

2273	0.4	2.0550	-1.58196E+01
2273	0.4	2.0560	-1.57992E+01
2273	0.4	2.0570	-1.57788E+01
2273	0.4	2.0580	-1.57582E+01
2273	0.4	2.0590	-1.57376E+01
2273	0.4	2.0600	-1.57168E+01

A.2.5. ($U_{0.5}Pu_{0.5}$) O_{2+x} :

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{Pu} (m ² /s)
1273	0.5	1.7500	-2.43846E+01
1273	0.5	1.7510	-2.43788E+01
1273	0.5	1.7520	-2.43721E+01
1273	0.5	1.7530	-2.43657E+01
1273	0.5	1.7540	-2.43599E+01
1273	0.5	1.7550	-2.43547E+01
1273	0.5	1.7560	-2.43501E+01
1273	0.5	1.7570	-2.43460E+01
1273	0.5	1.7580	-2.43424E+01
1273	0.5	1.7590	-2.43393E+01
1273	0.5	1.7600	-2.43367E+01
1273	0.5	1.7610	-2.43344E+01
1273	0.5	1.7620	-2.43325E+01
1273	0.5	1.7630	-2.43310E+01
1273	0.5	1.7640	-2.43298E+01
1273	0.5	1.7650	-2.43289E+01
1273	0.5	1.7660	-2.43283E+01
1273	0.5	1.7670	-2.43280E+01
1273	0.5	1.7680	-2.43279E+01
1273	0.5	1.7690	-2.43280E+01
1273	0.5	1.7700	-2.43284E+01
1273	0.5	1.7710	-2.43290E+01
1273	0.5	1.7720	-2.43298E+01
1273	0.5	1.7730	-2.43307E+01
1273	0.5	1.7740	-2.43319E+01
1273	0.5	1.7750	-2.43332E+01
1273	0.5	1.7760	-2.43346E+01
1273	0.5	1.7770	-2.43362E+01
1273	0.5	1.7780	-2.43379E+01
1273	0.5	1.7790	-2.43398E+01
1273	0.5	1.7800	-2.43417E+01
1273	0.5	1.7810	-2.43438E+01
1273	0.5	1.7820	-2.43460E+01
1273	0.5	1.7830	-2.43483E+01
1273	0.5	1.7840	-2.43507E+01
1273	0.5	1.7850	-2.43532E+01
1273	0.5	1.7860	-2.43557E+01
1273	0.5	1.7870	-2.43583E+01
1273	0.5	1.7880	-2.43610E+01
1273	0.5	1.7890	-2.43638E+01
1273	0.5	1.7900	-2.43667E+01
1273	0.5	1.7910	-2.43696E+01
1273	0.5	1.7920	-2.43725E+01
1273	0.5	1.7930	-2.43755E+01
1273	0.5	1.7940	-2.43786E+01
1273	0.5	1.7950	-2.43817E+01
1273	0.5	1.7960	-2.43848E+01
1273	0.5	1.7970	-2.43880E+01
1273	0.5	1.7980	-2.43912E+01
1273	0.5	1.7990	-2.43945E+01
1273	0.5	1.8000	-2.43978E+01
1273	0.5	1.8010	-2.44011E+01
1273	0.5	1.8020	-2.44045E+01
1273	0.5	1.8030	-2.44079E+01
1273	0.5	1.8040	-2.44113E+01
1273	0.5	1.8050	-2.44147E+01
1273	0.5	1.8060	-2.44181E+01
1273	0.5	1.8070	-2.44216E+01
1273	0.5	1.8080	-2.44251E+01
1273	0.5	1.8090	-2.44286E+01
1273	0.5	1.8100	-2.44321E+01
1273	0.5	1.8110	-2.44357E+01
1273	0.5	1.8120	-2.44392E+01
1273	0.5	1.8130	-2.44428E+01
1273	0.5	1.8140	-2.44463E+01
1273	0.5	1.8150	-2.44499E+01
1273	0.5	1.8160	-2.44535E+01
1273	0.5	1.8170	-2.44571E+01
1273	0.5	1.8180	-2.44607E+01
1273	0.5	1.8190	-2.44643E+01
1273	0.5	1.8200	-2.44679E+01
1273	0.5	1.8210	-2.44715E+01
1273	0.5	1.8220	-2.44751E+01
1273	0.5	1.8230	-2.44788E+01
1273	0.5	1.8240	-2.44824E+01
1273	0.5	1.8250	-2.44860E+01
1273	0.5	1.8260	-2.44897E+01
1273	0.5	1.8270	-2.44933E+01
1273	0.5	1.8280	-2.44969E+01
1273	0.5	1.8290	-2.45006E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{Pu} (m ² /s)
1273	0.5	1.8300	-2.45042E+01
1273	0.5	1.8310	-2.45079E+01
1273	0.5	1.8320	-2.45115E+01
1273	0.5	1.8330	-2.45152E+01
1273	0.5	1.8340	-2.45188E+01
1273	0.5	1.8350	-2.45225E+01
1273	0.5	1.8360	-2.45261E+01
1273	0.5	1.8370	-2.45298E+01
1273	0.5	1.8380	-2.45334E+01
1273	0.5	1.8390	-2.45371E+01
1273	0.5	1.8400	-2.45407E+01
1273	0.5	1.8410	-2.45444E+01
1273	0.5	1.8420	-2.45481E+01
1273	0.5	1.8430	-2.45517E+01
1273	0.5	1.8440	-2.45554E+01
1273	0.5	1.8450	-2.45591E+01
1273	0.5	1.8460	-2.45628E+01
1273	0.5	1.8470	-2.45664E+01
1273	0.5	1.8480	-2.45701E+01
1273	0.5	1.8490	-2.45738E+01
1273	0.5	1.8500	-2.45775E+01
1273	0.5	1.8510	-2.45812E+01
1273	0.5	1.8520	-2.45849E+01
1273	0.5	1.8530	-2.45886E+01
1273	0.5	1.8540	-2.45923E+01
1273	0.5	1.8550	-2.45960E+01
1273	0.5	1.8560	-2.45997E+01
1273	0.5	1.8570	-2.46035E+01
1273	0.5	1.8580	-2.46072E+01
1273	0.5	1.8590	-2.46110E+01
1273	0.5	1.8600	-2.46147E+01
1273	0.5	1.8610	-2.46185E+01
1273	0.5	1.8620	-2.46223E+01
1273	0.5	1.8630	-2.46260E+01
1273	0.5	1.8640	-2.46298E+01
1273	0.5	1.8650	-2.46336E+01
1273	0.5	1.8660	-2.46375E+01
1273	0.5	1.8670	-2.46413E+01
1273	0.5	1.8680	-2.46452E+01
1273	0.5	1.8690	-2.46490E+01
1273	0.5	1.8700	-2.46529E+01
1273	0.5	1.8710	-2.46568E+01
1273	0.5	1.8720	-2.46607E+01
1273	0.5	1.8730	-2.46646E+01
1273	0.5	1.8740	-2.46686E+01
1273	0.5	1.8750	-2.46725E+01
1273	0.5	1.8760	-2.46765E+01
1273	0.5	1.8770	-2.46805E+01
1273	0.5	1.8780	-2.46846E+01
1273	0.5	1.8790	-2.46886E+01
1273	0.5	1.8800	-2.46927E+01
1273	0.5	1.8810	-2.46968E+01
1273	0.5	1.8820	-2.47009E+01
1273	0.5	1.8830	-2.47051E+01
1273	0.5	1.8840	-2.47092E+01
1273	0.5	1.8850	-2.47135E+01
1273	0.5	1.8860	-2.47177E+01
1273	0.5	1.8870	-2.47220E+01
1273	0.5	1.8880	-2.47263E+01
1273	0.5	1.8890	-2.47306E+01
1273	0.5	1.8900	-2.47350E+01
1273	0.5	1.8910	-2.47394E+01
1273	0.5	1.8920	-2.47439E+01
1273	0.5	1.8930	-2.47484E+01
1273	0.5	1.8940	-2.47529E+01
1273	0.5	1.8950	-2.47575E+01
1273	0.5	1.8960	-2.47621E+01
1273	0.5	1.8970	-2.47668E+01
1273	0.5	1.8980	-2.47715E+01
1273	0.5	1.8990	-2.47763E+01
1273	0.5	1.9000	-2.47812E+01
1273	0.5	1.9010	-2.47861E+01
1273	0.5	1.9020	-2.47910E+01
1273	0.5	1.9030	-2.47961E+01
1273	0.5	1.9040	-2.48012E+01
1273	0.5	1.9050	-2.48063E+01
1273	0.5	1.9060	-2.48116E+01
1273	0.5	1.9070	-2.48169E+01
1273	0.5	1.9080	-2.48223E+01
1273	0.5	1.9090	-2.48278E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{Pu} (m ² /s)
1273	0.5	1.9100	-2.48333E+01
1273	0.5	1.9110	-2.48390E+01
1273	0.5	1.9120	-2.48448E+01
1273	0.5	1.9130	-2.48506E+01
1273	0.5	1.9140	-2.48566E+01
1273	0.5	1.9150	-2.48627E+01
1273	0.5	1.9160	-2.48689E+01
1273	0.5	1.9170	-2.48752E+01
1273	0.5	1.9180	-2.48817E+01
1273	0.5	1.9190	-2.48883E+01
1273	0.5	1.9200	-2.48951E+01
1273	0.5	1.9210	-2.49020E+01
1273	0.5	1.9220	-2.49091E+01
1273	0.5	1.9230	-2.49163E+01
1273	0.5	1.9240	-2.49237E+01
1273	0.5	1.9250	-2.49314E+01
1273	0.5	1.9260	-2.49392E+01
1273	0.5	1.9270	-2.49472E+01
1273	0.5	1.9280	-2.49554E+01
1273	0.5	1.9290	-2.49639E+01
1273	0.5	1.9300	-2.49726E+01
1273	0.5	1.9310	-2.49816E+01
1273	0.5	1.9320	-2.49908E+01
1273	0.5	1.9330	-2.50003E+01
1273	0.5	1.9340	-2.50101E+01
1273	0.5	1.9350	-2.50201E+01
1273	0.5	1.9360	-2.50305E+01
1273	0.5	1.9370	-2.50412E+01
1273	0.5	1.9380	-2.50523E+01
1273	0.5	1.9390	-2.50637E+01
1273	0.5	1.9400	-2.50755E+01
1273	0.5	1.9410	-2.50876E+01
1273	0.5	1.9420	-2.51001E+01
1273	0.5	1.9430	-2.51130E+01
1273	0.5	1.9440	-2.51264E+01
1273	0.5	1.9450	-2.51401E+01
1273	0.5	1.9460	-2.51543E+01
1273	0.5	1.9470	-2.51689E+01
1273	0.5	1.9480	-2.51840E+01
1273	0.5	1.9490	-2.51996E+01
1273	0.5	1.9500	-2.52156E+01
1273	0.5	1.9510	-2.52321E+01
1273	0.5	1.9520	-2.52490E+01
1273	0.5	1.9530	-2.52665E+01
1273	0.5	1.9540	-2.52844E+01
1273	0.5	1.9550	-2.53029E+01
1273	0.5	1.9560	-2.53218E+01
1273	0.5	1.9570	-2.53413E+01
1273	0.5	1.9580	-2.53612E+01
1273	0.5	1.9590	-2.53817E+01
1273	0.5	1.9600	-2.54026E+01
1273	0.5	1.9610	-2.54241E+01
1273	0.5	1.9620	-2.54461E+01
1273	0.5	1.9630	-2.54685E+01
1273	0.5	1.9640	-2.54915E+01
1273	0.5	1.9650	-2.55150E+01
1273	0.5	1.9660	-2.55389E+01
1273	0.5	1.9670	-2.55633E+01
1273	0.5	1.9680	-2.55882E+01
1273	0.5	1.9690	-2.56135E+01
1273	0.5	1.9700	-2.56394E+01
1273	0.5	1.9710	-2.56656E+01

1273	0.5	1.9900	-2.62293E+01
1273	0.5	1.9910	-2.62606E+01
1273	0.5	1.9920	-2.62916E+01
1273	0.5	1.9930	-2.63225E+01
1273	0.5	1.9940	-2.63530E+01
1273	0.5	1.9950	-2.63831E+01
1273	0.5	1.9960	-2.64128E+01
1273	0.5	1.9970	-2.64418E+01
1273	0.5	1.9980	-2.64701E+01
1273	0.5	1.9990	-2.64976E+01
1273	0.5	2.0000	-2.65241E+01
1273	0.5	2.0010	-2.65482E+01
1273	0.5	2.0020	-2.65701E+01
1273	0.5	2.0030	-2.65896E+01
1273	0.5	2.0040	-2.66065E+01
1273	0.5	2.0050	-2.66206E+01
1273	0.5	2.0060	-2.66318E+01
1273	0.5	2.0070	-2.66400E+01
1273	0.5	2.0080	-2.66452E+01
1273	0.5	2.0090	-2.66473E+01
1273	0.5	2.0100	-2.66464E+01
1273	0.5	2.0110	-2.66426E+01
1273	0.5	2.0120	-2.66360E+01
1273	0.5	2.0130	-2.66267E+01
1273	0.5	2.0140	-2.66150E+01
1273	0.5	2.0150	-2.66009E+01
1273	0.5	2.0160	-2.65848E+01
1273	0.5	2.0170	-2.65666E+01
1273	0.5	2.0180	-2.65468E+01
1273	0.5	2.0190	-2.65254E+01
1273	0.5	2.0200	-2.65026E+01
1273	0.5	2.0210	-2.64785E+01
1273	0.5	2.0220	-2.64533E+01
1273	0.5	2.0230	-2.64271E+01
1273	0.5	2.0240	-2.64000E+01
1273	0.5	2.0250	-2.63722E+01
1273	0.5	2.0260	-2.63436E+01
1273	0.5	2.0270	-2.63144E+01
1273	0.5	2.0280	-2.62846E+01
1273	0.5	2.0290	-2.62542E+01
1273	0.5	2.0300	-2.62234E+01
1273	0.5	2.0310	-2.61921E+01
1273	0.5	2.0320	-2.61605E+01
1273	0.5	2.0330	-2.61284E+01
1273	0.5	2.0340	-2.60960E+01
1273	0.5	2.0350	-2.60632E+01
1273	0.5	2.0360	-2.60301E+01
1273	0.5	2.0370	-2.59966E+01
1273	0.5	2.0380	-2.59629E+01
1273	0.5	2.0390	-2.59288E+01
1273	0.5	2.0400	-2.58945E+01
1273	0.5	2.0410	-2.58599E+01
1273	0.5	2.0420	-2.58250E+01
1273	0.5	2.0430	-2.57898E+01
1273	0.5	2.0440	-2.57544E+01
1273	0.5	2.0450	-2.57186E+01
1273	0.5	2.0460	-2.56826E+01
1273	0.5	2.0470	-2.56464E+01
1273	0.5	2.0480	-2.56099E+01
1273	0.5	2.0490	-2.55731E+01
1273	0.5	2.0500	-2.55361E+01
1273	0.5	2.0510	-2.54988E+01
1273	0.5	2.0520	-2.54612E+01
1273	0.5	2.0530	-2.54234E+01
1273	0.5	2.0540	-2.53854E+01
1273	0.5	2.0550	-2.53471E+01
1273	0.5	2.0560	-2.53086E+01
1273	0.5	2.0570	-2.52698E+01
1273	0.5	2.0580	-2.52308E+01
1273	0.5	2.0590	-2.51915E+01
1273	0.5	2.0600	-2.51521E+01
1273	0.5	2.0610	-2.51124E+01
1273	0.5	2.0620	-2.50724E+01
1273	0.5	2.0630	-2.50323E+01
1273	0.5	2.0640	-2.49919E+01
1273	0.5	2.0650	-2.49513E+01
1273	0.5	2.0660	-2.49106E+01
1273	0.5	2.0670	-2.48696E+01
1273	0.5	2.0680	-2.48284E+01
1273	0.5	2.0690	-2.47870E+01
1273	0.5	2.0700	-2.47455E+01
1273	0.5	2.0710	-2.47037E+01
1273	0.5	2.0720	-2.46618E+01
1273	0.5	2.0730	-2.46197E+01
1273	0.5	2.0740	-2.45775E+01
1273	0.5	2.0750	-2.45351E+01
1273	0.5	2.0760	-2.44925E+01
1273	0.5	2.0770	-2.44498E+01
1273	0.5	2.0780	-2.44069E+01
1273	0.5	2.0790	-2.43640E+01
1273	0.5	2.0800	-2.43208E+01
1273	0.5	2.0810	-2.42776E+01

1273	0.5	2.0820	-2.42342E+01
1273	0.5	2.0830	-2.41908E+01
1273	0.5	2.0840	-2.41472E+01
1273	0.5	2.0850	-2.41035E+01
1273	0.5	2.0860	-2.40597E+01
1273	0.5	2.0870	-2.40159E+01
1273	0.5	2.0880	-2.39719E+01
1273	0.5	2.0890	-2.39279E+01
1273	0.5	2.0900	-2.38838E+01
1273	0.5	2.0910	-2.38396E+01
1273	0.5	2.0920	-2.37954E+01
1273	0.5	2.0930	-2.37511E+01
1273	0.5	2.0940	-2.37067E+01
1273	0.5	2.0950	-2.36623E+01
1273	0.5	2.0960	-2.36179E+01
1273	0.5	2.0970	-2.35734E+01
1273	0.5	2.0980	-2.35288E+01
1273	0.5	2.0990	-2.34843E+01
1273	0.5	2.1000	-2.34397E+01
1273	0.5	2.1010	-2.33950E+01
1273	0.5	2.1020	-2.33504E+01
1273	0.5	2.1030	-2.33057E+01
1273	0.5	2.1040	-2.32610E+01
1273	0.5	2.1050	-2.32163E+01
1273	0.5	2.1060	-2.31715E+01
1273	0.5	2.1070	-2.31268E+01
1273	0.5	2.1080	-2.30820E+01
1273	0.5	2.1090	-2.30373E+01
1273	0.5	2.1100	-2.29925E+01
1273	0.5	2.1110	-2.29478E+01
1273	0.5	2.1120	-2.29030E+01
1273	0.5	2.1130	-2.28583E+01
1273	0.5	2.1140	-2.28135E+01
1273	0.5	2.1150	-2.27688E+01
1273	0.5	2.1160	-2.27240E+01
1273	0.5	2.1170	-2.26793E+01
1273	0.5	2.1180	-2.26346E+01
1273	0.5	2.1190	-2.25899E+01
1273	0.5	2.1200	-2.25452E+01
1273	0.5	2.1210	-2.25005E+01
1273	0.5	2.1220	-2.24559E+01
1273	0.5	2.1230	-2.24112E+01
1273	0.5	2.1240	-2.23666E+01
1273	0.5	2.1250	-2.23220E+01
1273	0.5	2.1260	-2.22774E+01
1273	0.5	2.1270	-2.22329E+01
1273	0.5	2.1280	-2.21883E+01
1273	0.5	2.1290	-2.21438E+01
1273	0.5	2.1300	-2.20993E+01
1273	0.5	2.17400	-1.87233E+01
1273	0.5	2.17410	-1.87230E+01
1273	0.5	2.17420	-1.87225E+01
1273	0.5	2.17430	-1.87221E+01
1273	0.5	2.17440	-1.87215E+01
1273	0.5	2.17450	-1.87208E+01
1273	0.5	2.17460	-1.87200E+01
1273	0.5	2.17470	-1.87190E+01
1273	0.5	2.17480	-1.87179E+01
1273	0.5	2.17490	-1.87166E+01
1273	0.5	2.17500	-1.87152E+01
1273	0.5	2.17510	-1.87136E+01
1273	0.5	2.17520	-1.87119E+01
1273	0.5	2.17530	-1.87101E+01
1273	0.5	2.17540	-1.87083E+01
1273	0.5	2.17550	-1.87065E+01
1273	0.5	2.17560	-1.87048E+01
1273	0.5	2.17570	-1.87032E+01
1273	0.5	2.17580	-1.87017E+01
1273	0.5	2.17590	-1.87004E+01
1273	0.5	2.17600	-1.86992E+01
1273	0.5	2.17610	-1.86981E+01
1273	0.5	2.17620	-1.86972E+01
1273	0.5	2.17630	-1.86964E+01
1273	0.5	2.17640	-1.86958E+01
1273	0.5	2.17650	-1.86953E+01
1273	0.5	2.17660	-1.86950E+01
1273	0.5	2.17670	-1.86948E+01
1273	0.5	2.17680	-1.86947E+01
1273	0.5	2.17690	-1.86947E+01
1273	0.5	2.17700	-1.86949E+01
1273	0.5	2.17710	-1.86952E+01
1273	0.5	2.17720	-1.86956E+01
1273	0.5	2.17730	-1.86961E+01
1273	0.5	2.17740	-1.86968E+01
1273	0.5	2.17750	-1.86975E+01
1273	0.5	2.17760	-1.86983E+01
1273	0.5	2.17770	-1.86993E+01
1273	0.5	2.17780	-1.87003E+01
1273	0.5	2.17790	-1.87014E+01
1273	0.5	2.17800	-1.87026E+01
1273	0.5	2.17810	-1.87038E+01
1273	0.5	2.17820	-1.87052E+01

1773	0.5	1.7830	-1.87066E+01
1773	0.5	1.7840	-1.87082E+01
1773	0.5	1.7850	-1.87097E+01
1773	0.5	1.7860	-1.87114E+01
1773	0.5	1.7870	-1.87131E+01
1773	0.5	1.7880	-1.87149E+01
1773	0.5	1.7890	-1.87167E+01
1773	0.5	1.7900	-1.87186E+01
1773	0.5	1.7910	-1.87206E+01
1773	0.5	1.7920	-1.87226E+01
1773	0.5	1.7930	-1.87247E+01
1773	0.5	1.7940	-1.87268E+01
1773	0.5	1.7950	-1.87290E+01
1773	0.5	1.7960	-1.87312E+01
1773	0.5	1.7970	-1.87335E+01
1773	0.5	1.7980	-1.87358E+01
1773	0.5	1.7990	-1.87381E+01
1773	0.5	1.8000	-1.87405E+01
1773	0.5	1.8010	-1.87430E+01
1773	0.5	1.8020	-1.87455E+01
1773	0.5	1.8030	-1.87480E+01
1773	0.5	1.8040	-1.87506E+01
1773	0.5	1.8050	-1.87532E+01
1773	0.5	1.8060	-1.87558E+01
1773	0.5	1.8070	-1.87584E+01
1773	0.5	1.8080	-1.87611E+01
1773	0.5	1.8090	-1.87639E+01
1773	0.5	1.8100	-1.87666E+01
1773	0.5	1.8110	-1.87694E+01
1773	0.5	1.8120	-1.87723E+01
1773	0.5	1.8130	-1.87751E+01
1773	0.5	1.8140	-1.87780E+01
1773	0.5	1.8150	-1.87809E+01
1773	0.5	1.8160	-1.87838E+01
1773	0.5	1.8170	-1.87868E+01
1773	0.5	1.8180	-1.87898E+01
1773	0.5	1.8190	-1.87928E+01
1773	0.5	1.8200	-1.87958E+01
1773	0.5	1.8210	-1.87989E+01
1773	0.5	1.8220	-1.88019E+01
1773	0.5	1.8230	-1.88050E+01
1773	0.5	1.8240	-1.88082E+01
1773	0.5	1.8250	-1.88113E+01
1773	0.5	1.8260	-1.88145E+01
1773	0.5	1.8270	-1.88177E+01
1773	0.5	1.8280	-1.88209E+01
1773	0.5	1.8290	-1.88241E+01
1773	0.5	1.8300	-1.88274E+01
1773	0.5	1.8310	-1.88306E+01
1773	0.5	1.8320	-1.88339E+01
1773	0.5	1.8330	-1.88372E+01
1773	0.5	1.8340	-1.88406E+01
1773	0.5	1.8350	-1.88439E+01
1773	0.5	1.8360	-1.88473E+01
1773	0.5	1.8370	-1.88507E+01
1773	0.5	1.8380	-1.88541E+01
1773	0.5	1.8390	-1.88575E+01
1773	0.5	1.8400	-1.88609E+01
1773	0.5	1.8410	-1.88644E+01
1773	0.5	1.8420	-1.88679E+01
1773	0.5	1.8430	-1.88714E+01
1773	0.5	1.8440	-1.88749E+01
1773	0.5	1.8450	-1.88784E+01
1773	0.5	1.8460	-1.88820E+01
1773	0.5	1.8470	-1.88856E+01
1773	0.5	1.8	

1773	0.5	1.8750	-1.89960E+01
1773	0.5	1.8760	-1.90004E+01
1773	0.5	1.8770	-1.90049E+01
1773	0.5	1.8780	-1.90094E+01
1773	0.5	1.8790	-1.90139E+01
1773	0.5	1.8800	-1.90186E+01
1773	0.5	1.8810	-1.90232E+01
1773	0.5	1.8820	-1.90279E+01
1773	0.5	1.8830	-1.90327E+01
1773	0.5	1.8840	-1.90376E+01
1773	0.5	1.8850	-1.90425E+01
1773	0.5	1.8860	-1.90474E+01
1773	0.5	1.8870	-1.90525E+01
1773	0.5	1.8880	-1.90576E+01
1773	0.5	1.8890	-1.90628E+01
1773	0.5	1.8900	-1.90680E+01
1773	0.5	1.8910	-1.90734E+01
1773	0.5	1.8920	-1.90788E+01
1773	0.5	1.8930	-1.90843E+01
1773	0.5	1.8940	-1.90899E+01
1773	0.5	1.8950	-1.90955E+01
1773	0.5	1.8960	-1.91013E+01
1773	0.5	1.8970	-1.91072E+01
1773	0.5	1.8980	-1.91132E+01
1773	0.5	1.8990	-1.91192E+01
1773	0.5	1.9000	-1.91254E+01
1773	0.5	1.9010	-1.91318E+01
1773	0.5	1.9020	-1.91382E+01
1773	0.5	1.9030	-1.91447E+01
1773	0.5	1.9040	-1.91514E+01
1773	0.5	1.9050	-1.91582E+01
1773	0.5	1.9060	-1.91652E+01
1773	0.5	1.9070	-1.91723E+01
1773	0.5	1.9080	-1.91795E+01
1773	0.5	1.9090	-1.91869E+01
1773	0.5	1.9100	-1.91945E+01
1773	0.5	1.9110	-1.92022E+01
1773	0.5	1.9120	-1.92101E+01
1773	0.5	1.9130	-1.92182E+01
1773	0.5	1.9140	-1.92264E+01
1773	0.5	1.9150	-1.92348E+01
1773	0.5	1.9160	-1.92434E+01
1773	0.5	1.9170	-1.92522E+01
1773	0.5	1.9180	-1.92612E+01
1773	0.5	1.9190	-1.92704E+01
1773	0.5	1.9200	-1.92799E+01
1773	0.5	1.9210	-1.92895E+01
1773	0.5	1.9220	-1.92993E+01
1773	0.5	1.9230	-1.93094E+01
1773	0.5	1.9240	-1.93196E+01
1773	0.5	1.9250	-1.93301E+01
1773	0.5	1.9260	-1.93409E+01
1773	0.5	1.9270	-1.93519E+01
1773	0.5	1.9280	-1.93631E+01
1773	0.5	1.9290	-1.93745E+01
1773	0.5	1.9300	-1.93862E+01
1773	0.5	1.9310	-1.93981E+01
1773	0.5	1.9320	-1.94103E+01
1773	0.5	1.9330	-1.94227E+01
1773	0.5	1.9340	-1.94354E+01
1773	0.5	1.9350	-1.94483E+01
1773	0.5	1.9360	-1.94614E+01
1773	0.5	1.9370	-1.94748E+01
1773	0.5	1.9380	-1.94885E+01
1773	0.5	1.9390	-1.95024E+01
1773	0.5	1.9400	-1.95165E+01
1773	0.5	1.9410	-1.95309E+01
1773	0.5	1.9420	-1.95454E+01
1773	0.5	1.9430	-1.95603E+01
1773	0.5	1.9440	-1.95753E+01
1773	0.5	1.9450	-1.95906E+01
1773	0.5	1.9460	-1.96060E+01
1773	0.5	1.9470	-1.96217E+01
1773	0.5	1.9480	-1.96376E+01
1773	0.5	1.9490	-1.96536E+01
1773	0.5	1.9500	-1.96699E+01
1773	0.5	1.9510	-1.96863E+01
1773	0.5	1.9520	-1.97028E+01
1773	0.5	1.9530	-1.97196E+01
1773	0.5	1.9540	-1.97364E+01
1773	0.5	1.9550	-1.97534E+01
1773	0.5	1.9560	-1.97704E+01
1773	0.5	1.9570	-1.97876E+01
1773	0.5	1.9580	-1.98048E+01
1773	0.5	1.9590	-1.98221E+01
1773	0.5	1.9600	-1.98395E+01
1773	0.5	1.9610	-1.98568E+01
1773	0.5	1.9620	-1.98741E+01
1773	0.5	1.9630	-1.98915E+01
1773	0.5	1.9640	-1.99087E+01
1773	0.5	1.9650	-1.99259E+01
1773	0.5	1.9660	-1.99430E+01

1773	0.5	1.9670	-1.99600E+01
1773	0.5	1.9680	-1.99768E+01
1773	0.5	1.9690	-1.99934E+01
1773	0.5	1.9700	-2.00098E+01
1773	0.5	1.9710	-2.00260E+01
1773	0.5	1.9720	-2.00419E+01
1773	0.5	1.9730	-2.00574E+01
1773	0.5	1.9740	-2.00727E+01
1773	0.5	1.9750	-2.00875E+01
1773	0.5	1.9760	-2.01019E+01
1773	0.5	1.9770	-2.01159E+01
1773	0.5	1.9780	-2.01293E+01
1773	0.5	1.9790	-2.01423E+01
1773	0.5	1.9800	-2.01547E+01
1773	0.5	1.9810	-2.01665E+01
1773	0.5	1.9820	-2.01776E+01
1773	0.5	1.9830	-2.01882E+01
1773	0.5	1.9840	-2.01980E+01
1773	0.5	1.9850	-2.02071E+01
1773	0.5	1.9860	-2.02155E+01
1773	0.5	1.9870	-2.02231E+01
1773	0.5	1.9880	-2.02299E+01
1773	0.5	1.9890	-2.02360E+01
1773	0.5	1.9900	-2.02412E+01
1773	0.5	1.9910	-2.02456E+01
1773	0.5	1.9920	-2.02492E+01
1773	0.5	1.9930	-2.02520E+01
1773	0.5	1.9940	-2.02540E+01
1773	0.5	1.9950	-2.02551E+01
1773	0.5	1.9960	-2.02554E+01
1773	0.5	1.9970	-2.02549E+01
1773	0.5	1.9980	-2.02536E+01
1773	0.5	1.9990	-2.02515E+01
1773	0.5	2.0000	-2.02476E+01
1773	0.5	2.0010	-2.02389E+01
1773	0.5	2.0020	-2.02283E+01
1773	0.5	2.0030	-2.02166E+01
1773	0.5	2.0040	-2.02040E+01
1773	0.5	2.0050	-2.01906E+01
1773	0.5	2.0060	-2.01763E+01
1773	0.5	2.0070	-2.01614E+01
1773	0.5	2.0080	-2.01457E+01
1773	0.5	2.0090	-2.01294E+01
1773	0.5	2.0100	-2.01126E+01
1773	0.5	2.0110	-2.00952E+01
1773	0.5	2.0120	-2.00773E+01
1773	0.5	2.0130	-2.00589E+01
1773	0.5	2.0140	-2.00401E+01
1773	0.5	2.0150	-2.00209E+01
1773	0.5	2.0160	-2.00013E+01
1773	0.5	2.0170	-1.99813E+01
1773	0.5	2.0180	-1.99611E+01
1773	0.5	2.0190	-1.99405E+01
1773	0.5	2.0200	-1.99197E+01
1773	0.5	2.0210	-1.98985E+01
1773	0.5	2.0220	-1.98772E+01
1773	0.5	2.0230	-1.98555E+01
1773	0.5	2.0240	-1.98337E+01
1773	0.5	2.0250	-1.98116E+01
1773	0.5	2.0260	-1.97893E+01
1773	0.5	2.0270	-1.97668E+01
1773	0.5	2.0280	-1.97441E+01
1773	0.5	2.0290	-1.97213E+01
1773	0.5	2.0300	-1.96982E+01
1773	0.5	2.0310	-1.96749E+01
1773	0.5	2.0320	-1.96515E+01
1773	0.5	2.0330	-1.96279E+01
1773	0.5	2.0340	-1.96042E+01
1773	0.5	2.0350	-1.95802E+01
1773	0.5	2.0360	-1.95561E+01
1773	0.5	2.0370	-1.95319E+01
1773	0.5	2.0380	-1.95075E+01
1773	0.5	2.0390	-1.94829E+01
1773	0.5	2.0400	-1.94582E+01
1773	0.5	2.0410	-1.94333E+01
1773	0.5	2.0420	-1.94083E+01
1773	0.5	2.0430	-1.93831E+01
1773	0.5	2.0440	-1.93577E+01
1773	0.5	2.0450	-1.93322E+01
1773	0.5	2.0460	-1.93066E+01
1773	0.5	2.0470	-1.92808E+01
1773	0.5	2.0480	-1.92549E+01
1773	0.5	2.0490	-1.92288E+01
1773	0.5	2.0500	-1.92025E+01
1773	0.5	2.0510	-1.91761E+01
1773	0.5	2.0520	-1.91496E+01
1773	0.5	2.0530	-1.91229E+01
1773	0.5	2.0540	-1.90961E+01
1773	0.5	2.0550	-1.90691E+01
1773	0.5	2.0560	-1.90420E+01
1773	0.5	2.0570	-1.90147E+01
1773	0.5	2.0580	-1.89872E+01

1773	0.5	2.0590	-1.89597E+01
1773	0.5	2.0600	-1.89319E+01
1773	0.5	2.0610	-1.89041E+01
1773	0.5	2.0620	-1.88760E+01
1773	0.5	2.0630	-1.88479E+01
1773	0.5	2.0640	-1.88196E+01
1773	0.5	2.0650	-1.87911E+01
1773	0.5	2.0660	-1.87625E+01
1773	0.5	2.0670	-1.87338E+01
1773	0.5	2.0680	-1.87049E+01
1773	0.5	2.0690	-1.86758E+01
1773	0.5	2.0700	-1.86467E+01
1773	0.5	2.0710	-1.86173E+01
1773	0.5	2.0720	-1.85879E+01
1773	0.5	2.0730	-1.85583E+01
1773	0.5	2.0740	-1.85285E+01
1773	0.5	2.0750	-1.84987E+01
1773	0.5	2.0760	-1.84687E+01
1773	0.5	2.0770	-1.84385E+01
1773	0.5	2.0780	-1.84082E+01
1773	0.5	2.0790	-1.83778E+01
1773	0.5	2.0800	-1.83473E+01
1773	0.5	2.0810	-1.83166E+01
1773	0.5	2.0820	-1.82858E+01
1773	0.5	2.0830	-1.82549E+01
1773	0.5	2.0840	-1.82238E+01
1773	0.5	2.0850	-1.81926E+01
1773	0.5	2.0860	-1.81613E+01
1773	0.5	2.0870	-1.81299E+01
1773	0.5	2.0880	-1.80984E+01
1773	0.5	2.0890	-1.80667E+01
1773	0.5	2.0900	-1.80350E+01
1773	0.5	2.0910	-1.80031E+01
1773	0.5	2.0920	-1.79711E+01
1773	0.5	2.0930	-1.79391E+01
1773	0.5	2.0940	-1.79069E+01
1773	0.5	2.0950	-1.78746E+01
1773	0.5	2.0960	-1.78422E+01
1773	0.5	2.0970	-1.78098E+01
1773	0.5	2.0980	-1.77772E+01
1773	0.5	2.0990	-1.77445E+01
1773	0.5	2.1000	-1.77118E+01
2273	0.5	1.7000	-1.55247E+01
2273	0.5	1.7010	-1.55246E+01
2273	0.5	1.7020	-1.55245E+01
2273	0.5	1.7030	-1.55244E+01
2273	0.5	1.7040	-1.55243E+01
2273	0.5	1.7050	-1.55242E+01
2273	0.5	1.7060	-1.55241E+01
2273	0.5	1.7070	-1.55240E+01
2273	0.5	1.7080	-1.55239E+01
2273	0.5	1.7090	-1.55237E+01
2273	0.5	1.7100	-1.55236E+01
2273	0.5	1.7110	-1.55235E+01
2273	0.5	1.7120	-1.55234E+01
2273	0.5	1.7130	-1.55232E+01
2273	0.5	1.7140	-1.55231E+01
2273	0.5	1.7150	-1.55229E+01
2273	0.5	1.7160	-1.55228E+01
2273	0.5	1.7170	-1.55226E+01
2273	0.5	1.7180	-1.55225E+01
2273	0.5	1.7190	-1.55223E+01
2273	0.5	1.7200	-1.55221E+01
2273	0.5	1.7210	-1.55219E+01
2273	0.5	1.7220	-1.55217E+01
2273	0.5	1.7230	-1.55215E+01
2273	0.5		

2273	0.5	1.7500	-1.55119E+01
2273	0.5	1.7510	-1.55114E+01
2273	0.5	1.7520	-1.55110E+01
2273	0.5	1.7530	-1.55106E+01
2273	0.5	1.7540	-1.55102E+01
2273	0.5	1.7550	-1.55099E+01
2273	0.5	1.7560	-1.55096E+01
2273	0.5	1.7570	-1.55093E+01
2273	0.5	1.7580	-1.55090E+01
2273	0.5	1.7590	-1.55088E+01
2273	0.5	1.7600	-1.55087E+01
2273	0.5	1.7610	-1.55086E+01
2273	0.5	1.7620	-1.55085E+01
2273	0.5	1.7630	-1.55085E+01
2273	0.5	1.7640	-1.55086E+01
2273	0.5	1.7650	-1.55087E+01
2273	0.5	1.7660	-1.55089E+01
2273	0.5	1.7670	-1.55091E+01
2273	0.5	1.7680	-1.55094E+01
2273	0.5	1.7690	-1.55098E+01
2273	0.5	1.7700	-1.55102E+01
2273	0.5	1.7710	-1.55107E+01
2273	0.5	1.7720	-1.55112E+01
2273	0.5	1.7730	-1.55118E+01
2273	0.5	1.7740	-1.55124E+01
2273	0.5	1.7750	-1.55132E+01
2273	0.5	1.7760	-1.55139E+01
2273	0.5	1.7770	-1.55148E+01
2273	0.5	1.7780	-1.55157E+01
2273	0.5	1.7790	-1.55166E+01
2273	0.5	1.7800	-1.55176E+01
2273	0.5	1.7810	-1.55187E+01
2273	0.5	1.7820	-1.55198E+01
2273	0.5	1.7830	-1.55210E+01
2273	0.5	1.7840	-1.55222E+01
2273	0.5	1.7850	-1.55235E+01
2273	0.5	1.7860	-1.55248E+01
2273	0.5	1.7870	-1.55262E+01
2273	0.5	1.7880	-1.55276E+01
2273	0.5	1.7890	-1.55291E+01
2273	0.5	1.7900	-1.55306E+01
2273	0.5	1.7910	-1.55322E+01
2273	0.5	1.7920	-1.55338E+01
2273	0.5	1.7930	-1.55355E+01
2273	0.5	1.7940	-1.55372E+01
2273	0.5	1.7950	-1.55389E+01
2273	0.5	1.7960	-1.55407E+01
2273	0.5	1.7970	-1.55426E+01
2273	0.5	1.7980	-1.55445E+01
2273	0.5	1.7990	-1.55464E+01
2273	0.5	1.8000	-1.55483E+01
2273	0.5	1.8010	-1.55503E+01
2273	0.5	1.8020	-1.55524E+01
2273	0.5	1.8030	-1.55545E+01
2273	0.5	1.8040	-1.55566E+01
2273	0.5	1.8050	-1.55587E+01
2273	0.5	1.8060	-1.55609E+01
2273	0.5	1.8070	-1.55631E+01
2273	0.5	1.8080	-1.55654E+01
2273	0.5	1.8090	-1.55677E+01
2273	0.5	1.8100	-1.55700E+01
2273	0.5	1.8110	-1.55724E+01
2273	0.5	1.8120	-1.55748E+01
2273	0.5	1.8130	-1.55772E+01
2273	0.5	1.8140	-1.55797E+01
2273	0.5	1.8150	-1.55822E+01
2273	0.5	1.8160	-1.55847E+01
2273	0.5	1.8170	-1.55873E+01
2273	0.5	1.8180	-1.55899E+01
2273	0.5	1.8190	-1.55925E+01
2273	0.5	1.8200	-1.55952E+01
2273	0.5	1.8210	-1.55978E+01
2273	0.5	1.8220	-1.56006E+01
2273	0.5	1.8230	-1.56033E+01
2273	0.5	1.8240	-1.56061E+01
2273	0.5	1.8250	-1.56089E+01
2273	0.5	1.8260	-1.56118E+01
2273	0.5	1.8270	-1.56146E+01
2273	0.5	1.8280	-1.56175E+01
2273	0.5	1.8290	-1.56205E+01
2273	0.5	1.8300	-1.56234E+01
2273	0.5	1.8310	-1.56264E+01
2273	0.5	1.8320	-1.56295E+01
2273	0.5	1.8330	-1.56325E+01
2273	0.5	1.8340	-1.56356E+01
2273	0.5	1.8350	-1.56387E+01
2273	0.5	1.8360	-1.56419E+01
2273	0.5	1.8370	-1.56451E+01
2273	0.5	1.8380	-1.56483E+01
2273	0.5	1.8390	-1.56515E+01
2273	0.5	1.8400	-1.56548E+01
2273	0.5	1.8410	-1.56581E+01

2273	0.5	1.8420	-1.56614E+01
2273	0.5	1.8430	-1.56648E+01
2273	0.5	1.8440	-1.56682E+01
2273	0.5	1.8450	-1.56717E+01
2273	0.5	1.8460	-1.56752E+01
2273	0.5	1.8470	-1.56787E+01
2273	0.5	1.8480	-1.56822E+01
2273	0.5	1.8490	-1.56858E+01
2273	0.5	1.8500	-1.56895E+01
2273	0.5	1.8510	-1.56931E+01
2273	0.5	1.8520	-1.56968E+01
2273	0.5	1.8530	-1.57006E+01
2273	0.5	1.8540	-1.57044E+01
2273	0.5	1.8550	-1.57082E+01
2273	0.5	1.8560	-1.57121E+01
2273	0.5	1.8570	-1.57160E+01
2273	0.5	1.8580	-1.57199E+01
2273	0.5	1.8590	-1.57239E+01
2273	0.5	1.8600	-1.57280E+01
2273	0.5	1.8610	-1.57321E+01
2273	0.5	1.8620	-1.57362E+01
2273	0.5	1.8630	-1.57404E+01
2273	0.5	1.8640	-1.57447E+01
2273	0.5	1.8650	-1.57490E+01
2273	0.5	1.8660	-1.57533E+01
2273	0.5	1.8670	-1.57578E+01
2273	0.5	1.8680	-1.57622E+01
2273	0.5	1.8690	-1.57667E+01
2273	0.5	1.8700	-1.57713E+01
2273	0.5	1.8710	-1.57760E+01
2273	0.5	1.8720	-1.57807E+01
2273	0.5	1.8730	-1.57855E+01
2273	0.5	1.8740	-1.57903E+01
2273	0.5	1.8750	-1.57952E+01
2273	0.5	1.8760	-1.58002E+01
2273	0.5	1.8770	-1.58052E+01
2273	0.5	1.8780	-1.58104E+01
2273	0.5	1.8790	-1.58156E+01
2273	0.5	1.8800	-1.58209E+01
2273	0.5	1.8810	-1.58262E+01
2273	0.5	1.8820	-1.58317E+01
2273	0.5	1.8830	-1.58372E+01
2273	0.5	1.8840	-1.58428E+01
2273	0.5	1.8850	-1.58485E+01
2273	0.5	1.8860	-1.58543E+01
2273	0.5	1.8870	-1.58602E+01
2273	0.5	1.8880	-1.58662E+01
2273	0.5	1.8890	-1.58723E+01
2273	0.5	1.8900	-1.58784E+01
2273	0.5	1.8910	-1.58847E+01
2273	0.5	1.8920	-1.58911E+01
2273	0.5	1.8930	-1.58976E+01
2273	0.5	1.8940	-1.59042E+01
2273	0.5	1.8950	-1.59109E+01
2273	0.5	1.8960	-1.59177E+01
2273	0.5	1.8970	-1.59247E+01
2273	0.5	1.8980	-1.59317E+01
2273	0.5	1.8990	-1.59389E+01
2273	0.5	1.9000	-1.59462E+01
2273	0.5	1.9010	-1.59536E+01
2273	0.5	1.9020	-1.59611E+01
2273	0.5	1.9030	-1.59688E+01
2273	0.5	1.9040	-1.59766E+01
2273	0.5	1.9050	-1.59845E+01
2273	0.5	1.9060	-1.59926E+01
2273	0.5	1.9070	-1.60007E+01
2273	0.5	1.9080	-1.60090E+01
2273	0.5	1.9090	-1.60175E+01
2273	0.5	1.9100	-1.60260E+01
2273	0.5	1.9110	-1.60347E+01
2273	0.5	1.9120	-1.60436E+01
2273	0.5	1.9130	-1.60525E+01
2273	0.5	1.9140	-1.60616E+01
2273	0.5	1.9150	-1.60708E+01
2273	0.5	1.9160	-1.60802E+01
2273	0.5	1.9170	-1.60897E+01
2273	0.5	1.9180	-1.60993E+01
2273	0.5	1.9190	-1.61090E+01
2273	0.5	1.9200	-1.61188E+01
2273	0.5	1.9210	-1.61288E+01
2273	0.5	1.9220	-1.61389E+01
2273	0.5	1.9230	-1.61491E+01
2273	0.5	1.9240	-1.61594E+01
2273	0.5	1.9250	-1.61698E+01
2273	0.5	1.9260	-1.61803E+01
2273	0.5	1.9270	-1.61909E+01
2273	0.5	1.9280	-1.62016E+01
2273	0.5	1.9290	-1.62124E+01
2273	0.5	1.9300	-1.62232E+01
2273	0.5	1.9310	-1.62342E+01
2273	0.5	1.9320	-1.62452E+01
2273	0.5	1.9330	-1.62562E+01

2273	0.5	1.9340	-1.62673E+01
2273	0.5	1.9350	-1.62784E+01
2273	0.5	1.9360	-1.62896E+01
2273	0.5	1.9370	-1.63008E+01
2273	0.5	1.9380	-1.63120E+01
2273	0.5	1.9390	-1.63232E+01
2273	0.5	1.9400	-1.63344E+01
2273	0.5	1.9410	-1.63455E+01
2273	0.5	1.9420	-1.63567E+01
2273	0.5	1.9430	-1.63677E+01
2273	0.5	1.9440	-1.63788E+01
2273	0.5	1.9450	-1.63897E+01
2273	0.5	1.9460	-1.64006E+01
2273	0.5	1.9470	-1.64113E+01
2273	0.5	1.9480	-1.64220E+01
2273	0.5	1.9490	-1.64325E+01
2273	0.5	1.9500	-1.64428E+01
2273	0.5	1.9510	-1.64530E+01
2273	0.5	1.9520	-1.64630E+01
2273	0.5	1.9530	-1.64729E+01
2273	0.5	1.9540	-1.64825E+01
2273	0.5	1.9550	-1.64919E+01
2273	0.5	1.9560	-1.65010E+01
2273	0.5	1.9570	-1.65099E+01
2273	0.5	1.9580	-1.65185E+01
2273	0.5	1.9590	-1.65268E+01
2273	0.5	1.9600	-1.65348E+01
2273	0.5	1.9610	-1.65425E+01
2273	0.5	1.9620	-1.65498E+01
2273	0.5	1.9630	-1.65568E+01
2273	0.5	1.9640	-1.65634E+01
2273	0.5	1.9650	-1.65697E+01
2273	0.5	1.9660	-1.65755E+01
2273	0.5	1.9670	-1.65810E+01
2273	0.5	1.9680	-1.65860E+01
2273	0.5	1.9690	-1.65906E+01
2273	0.5	1.9700	-1.65948E+01
2273	0.5	1.9710	-1.65986E+01
2273	0.5	1.9720	-1.66019E+01
2273	0.5	1.9730	-1.66048E+01
2273	0.5	1.9740	-1.66072E+01
2273	0.5	1.9750	-1.66092E+01
2273	0.5	1.9760	-1.66107E+01
2273	0.5	1.9770	-1.66117E+01
2273	0.5	1.9780	-1.66123E+01
2273	0.5	1.9790	-1.66125E+01
2273	0.5	1.9800	-1.66121E+01
2273	0.5	1.9810	-1.66114E+01
2273	0.5	1.9820	-1.66102E+01
2273	0.5	1.9830	-1.66085E+01
2273	0.5	1.9840	-1.66065E+01
2273	0.5	1.9850	-1.66039E+01
2273	0.5	1.9860	-1.66010E+01
2273	0.5	1.9870	-1.65977E+01
2273	0.5	1.9880	-1.65939E+01
2273	0.5	1.9890	-1.65897E+01
2273	0.5	1.9900	-1.65851E+01
2273	0.5	1.9910	-1.65802E+01
2273	0.5	1.9920	-1.65748E+01
2273	0.5	1.9930	-1.65690E+01
2273	0.5	1.9940	-1.65628E+01
2273	0.5	1.9950	-1.65562E+01
2273	0.5	1.9960	-1.65491E+01
2273	0.5	1.9970	-1.65414E+01
2273	0.5	1.9980	-1.65332E+01
2273	0.5	1.9990	-1.65241E+01
2273	0.5		

2273	0.5	2.0260	-1.60947E+01
2273	0.5	2.0270	-1.60761E+01
2273	0.5	2.0280	-1.60574E+01
2273	0.5	2.0290	-1.60385E+01
2273	0.5	2.0300	-1.60196E+01

2273	0.5	2.0310	-1.60005E+01
2273	0.5	2.0320	-1.59813E+01
2273	0.5	2.0330	-1.59621E+01
2273	0.5	2.0340	-1.59427E+01
2273	0.5	2.0350	-1.59231E+01

2273	0.5	2.0360	-1.59035E+01
2273	0.5	2.0370	-1.58838E+01
2273	0.5	2.0380	-1.58640E+01
2273	0.5	2.0390	-1.58441E+01
2273	0.5	2.0400	-1.58240E+01

A.2.6. $(U_{0.4}Pu_{0.6})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)
1273	0.6	1.7000	-2.39317E+01
1273	0.6	1.7010	-2.39246E+01
1273	0.6	1.7020	-2.39161E+01
1273	0.6	1.7030	-2.39080E+01
1273	0.6	1.7040	-2.39005E+01
1273	0.6	1.7050	-2.38936E+01
1273	0.6	1.7060	-2.38872E+01
1273	0.6	1.7070	-2.38815E+01
1273	0.6	1.7080	-2.38762E+01
1273	0.6	1.7090	-2.38714E+01
1273	0.6	1.7100	-2.38670E+01
1273	0.6	1.7110	-2.38631E+01
1273	0.6	1.7120	-2.38596E+01
1273	0.6	1.7130	-2.38564E+01
1273	0.6	1.7140	-2.38536E+01
1273	0.6	1.7150	-2.38511E+01
1273	0.6	1.7160	-2.38489E+01
1273	0.6	1.7170	-2.38470E+01
1273	0.6	1.7180	-2.38454E+01
1273	0.6	1.7190	-2.38440E+01
1273	0.6	1.7200	-2.38428E+01
1273	0.6	1.7210	-2.38419E+01
1273	0.6	1.7220	-2.38412E+01
1273	0.6	1.7230	-2.38408E+01
1273	0.6	1.7240	-2.38405E+01
1273	0.6	1.7250	-2.38404E+01
1273	0.6	1.7260	-2.38404E+01
1273	0.6	1.7270	-2.38407E+01
1273	0.6	1.7280	-2.38411E+01
1273	0.6	1.7290	-2.38416E+01
1273	0.6	1.7300	-2.38423E+01
1273	0.6	1.7310	-2.38432E+01
1273	0.6	1.7320	-2.38441E+01
1273	0.6	1.7330	-2.38452E+01
1273	0.6	1.7340	-2.38464E+01
1273	0.6	1.7350	-2.38477E+01
1273	0.6	1.7360	-2.38491E+01
1273	0.6	1.7370	-2.38506E+01
1273	0.6	1.7380	-2.38523E+01
1273	0.6	1.7390	-2.38540E+01
1273	0.6	1.7400	-2.38558E+01
1273	0.6	1.7410	-2.38577E+01
1273	0.6	1.7420	-2.38596E+01
1273	0.6	1.7430	-2.38617E+01
1273	0.6	1.7440	-2.38638E+01
1273	0.6	1.7450	-2.38660E+01
1273	0.6	1.7460	-2.38682E+01
1273	0.6	1.7470	-2.38705E+01
1273	0.6	1.7480	-2.38729E+01
1273	0.6	1.7490	-2.38754E+01
1273	0.6	1.7500	-2.38778E+01
1273	0.6	1.7510	-2.38804E+01
1273	0.6	1.7520	-2.38830E+01
1273	0.6	1.7530	-2.38856E+01
1273	0.6	1.7540	-2.38883E+01
1273	0.6	1.7550	-2.38910E+01
1273	0.6	1.7560	-2.38938E+01
1273	0.6	1.7570	-2.38966E+01
1273	0.6	1.7580	-2.38994E+01
1273	0.6	1.7590	-2.39023E+01
1273	0.6	1.7600	-2.39052E+01
1273	0.6	1.7610	-2.39082E+01
1273	0.6	1.7620	-2.39112E+01
1273	0.6	1.7630	-2.39142E+01
1273	0.6	1.7640	-2.39172E+01
1273	0.6	1.7650	-2.39203E+01
1273	0.6	1.7660	-2.39233E+01
1273	0.6	1.7670	-2.39264E+01
1273	0.6	1.7680	-2.39296E+01
1273	0.6	1.7690	-2.39327E+01
1273	0.6	1.7700	-2.39359E+01
1273	0.6	1.7710	-2.39390E+01
1273	0.6	1.7720	-2.39422E+01
1273	0.6	1.7730	-2.39455E+01
1273	0.6	1.7740	-2.39487E+01
1273	0.6	1.7750	-2.39519E+01
1273	0.6	1.7760	-2.39552E+01
1273	0.6	1.7770	-2.39585E+01
1273	0.6	1.7780	-2.39617E+01
T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)
1273	0.6	1.7790	-2.39650E+01
1273	0.6	1.7800	-2.39683E+01
1273	0.6	1.7810	-2.39716E+01
1273	0.6	1.7820	-2.39750E+01
1273	0.6	1.7830	-2.39783E+01
1273	0.6	1.7840	-2.39816E+01
1273	0.6	1.7850	-2.39850E+01
1273	0.6	1.7860	-2.39883E+01
1273	0.6	1.7870	-2.39917E+01
1273	0.6	1.7880	-2.39950E+01
1273	0.6	1.7890	-2.39984E+01
1273	0.6	1.7900	-2.40017E+01
1273	0.6	1.7910	-2.40051E+01
1273	0.6	1.7920	-2.40085E+01
1273	0.6	1.7930	-2.40118E+01
1273	0.6	1.7940	-2.40152E+01
1273	0.6	1.7950	-2.40186E+01
1273	0.6	1.7960	-2.40220E+01
1273	0.6	1.7970	-2.40254E+01
1273	0.6	1.7980	-2.40288E+01
1273	0.6	1.7990	-2.40321E+01
1273	0.6	1.8000	-2.40355E+01
1273	0.6	1.8010	-2.40389E+01
1273	0.6	1.8020	-2.40423E+01
1273	0.6	1.8030	-2.40457E+01
1273	0.6	1.8040	-2.40491E+01
1273	0.6	1.8050	-2.40525E+01
1273	0.6	1.8060	-2.40559E+01
1273	0.6	1.8070	-2.40593E+01
1273	0.6	1.8080	-2.40626E+01
1273	0.6	1.8090	-2.40660E+01
1273	0.6	1.8100	-2.40694E+01
1273	0.6	1.8110	-2.40728E+01
1273	0.6	1.8120	-2.40762E+01
1273	0.6	1.8130	-2.40796E+01
1273	0.6	1.8140	-2.40830E+01
1273	0.6	1.8150	-2.40864E+01
1273	0.6	1.8160	-2.40898E+01
1273	0.6	1.8170	-2.40932E+01
1273	0.6	1.8180	-2.40966E+01
1273	0.6	1.8190	-2.41000E+01
1273	0.6	1.8200	-2.41033E+01
1273	0.6	1.8210	-2.41067E+01
1273	0.6	1.8220	-2.41101E+01
1273	0.6	1.8230	-2.41135E+01
1273	0.6	1.8240	-2.41169E+01
1273	0.6	1.8250	-2.41203E+01
1273	0.6	1.8260	-2.41237E+01
1273	0.6	1.8270	-2.41271E+01
1273	0.6	1.8280	-2.41305E+01
1273	0.6	1.8290	-2.41339E+01
1273	0.6	1.8300	-2.41373E+01
1273	0.6	1.8310	-2.41407E+01
1273	0.6	1.8320	-2.41442E+01
1273	0.6	1.8330	-2.41476E+01
1273	0.6	1.8340	-2.41510E+01
1273	0.6	1.8350	-2.41544E+01
1273	0.6	1.8360	-2.41578E+01
1273	0.6	1.8370	-2.41613E+01
1273	0.6	1.8380	-2.41647E+01
1273	0.6	1.8390	-2.41681E+01
1273	0.6	1.8400	-2.41716E+01
1273	0.6	1.8410	-2.41750E+01
1273	0.6	1.8420	-2.41785E+01
1273	0.6	1.8430	-2.41820E+01
1273	0.6	1.8440	-2.41854E+01
1273	0.6	1.8450	-2.41889E+01
1273	0.6	1.8460	-2.41924E+01
1273	0.6	1.8470	-2.41959E+01
1273	0.6	1.8480	-2.41994E+01
1273	0.6	1.8490	-2.42029E+01
1273	0.6	1.8500	-2.42064E+01
1273	0.6	1.8510	-2.42099E+01
1273	0.6	1.8520	-2.42134E+01
1273	0.6	1.8530	-2.42170E+01
1273	0.6	1.8540	-2.42205E+01
1273	0.6	1.8550	-2.42241E+01
1273	0.6	1.8560	-2.42277E+01
1273	0.6	1.8570	-2.42313E+01
T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)
1273	0.6	1.8580	-2.42349E+01
1273	0.6	1.8590	-2.42385E+01
1273	0.6	1.8600	-2.42421E+01
1273	0.6	1.8610	-2.42457E+01
1273	0.6	1.8620	-2.42494E+01
1273	0.6	1.8630	-2.42531E+01
1273	0.6	1.8640	-2.42567E+01
1273	0.6	1.8650	-2.42604E+01
1273	0.6	1.8660	-2.42642E+01
1273	0.6	1.8670	-2.42679E+01
1273	0.6	1.8680	-2.42717E+01
1273	0.6	1.8690	-2.42754E+01
1273	0.6	1.8700	-2.42792E+01
1273	0.6	1.8710	-2.42830E+01
1273	0.6	1.8720	-2.42869E+01
1273	0.6	1.8730	-2.42907E+01
1273	0.6	1.8740	-2.42946E+01
1273	0.6	1.8750	-2.42985E+01
1273	0.6	1.8760	-2.43024E+01
1273	0.6	1.8770	-2.43064E+01
1273	0.6	1.8780	-2.43104E+01
1273	0.6	1.8790	-2.43144E+01
1273	0.6	1.8800	-2.43184E+01
1273	0.6	1.8810	-2.43225E+01
1273	0.6	1.8820	-2.43266E+01
1273	0.6	1.8830	-2.43307E+01
1273	0.6	1.8840	-2.43348E+01
1273	0.6	1.8850	-2.43390E+01
1273	0.6	1.8860	-2.43433E+01
1273	0.6	1.8870	-2.43475E+01
1273	0.6	1.8880	-2.43518E+01
1273	0.6	1.8890	-2.43562E+01
1273	0.6	1.8900	-2.43605E+01
1273	0.6	1.8910	-2.43650E+01
1273	0.6	1.8920	-2.43694E+01
1273	0.6	1.8930	-2.43740E+01
1273	0.6	1.8940	-2.43785E+01
1273	0.6	1.8950	-2.43832E+01
1273	0.6	1.8960	-2.43878E+01
1273	0.6	1.8970	-2.43926E+01
1273	0.6	1.8980	-2.43973E+01
1273	0.6	1.8990	-2.44022E+01
1273	0.6	1.9000	-2.44071E+01
1273	0.6	1.9010	-2.44121E+01
1273	0.6	1.9020	-2.44171E+01
1273	0.6	1.9030	-2.44223E+01
1273	0.6	1.9040	-2.44275E+01
1273	0.6	1.9050	-2.44327E+01
1273	0.6	1.9060	-2.44381E+01
1273	0.6	1.9070	-2.44435E+01
1273	0.6	1.9080	-2.44491E+01
1273	0.6	1.9090	-2.44547E+01
1273	0.6	1.9100	-2.44605E+01
1273	0.6	1.9110	-2.44663E+01
1273	0.6	1.9120	-2.44723E+01
1273	0.6	1.9130	-2.44783E+01
1273	0.6	1.9140	-2.44845E+01
1273	0.6	1.9150	-2.44908E+01
1273	0.6	1.9160	-2.44973E+01
1273	0.6	1.9170	-2.45039E+01
1273	0.6	1.9180	-2.45107E+01
1273	0.6	1.9190	-2.45176E+01
1273	0.6	1.9200	-2.45247E+01
1273	0.6	1.9210	-2.45319E+01
1273	0.6	1.9220	-2.45394E+01
1273	0.6	1.9230	

1273	0.6	1.9400	-2.47160E+01
1273	0.6	1.9410	-2.47289E+01
1273	0.6	1.9420	-2.47421E+01
1273	0.6	1.9430	-2.47558E+01
1273	0.6	1.9440	-2.47699E+01
1273	0.6	1.9450	-2.47845E+01
1273	0.6	1.9460	-2.47994E+01
1273	0.6	1.9470	-2.48148E+01
1273	0.6	1.9480	-2.48307E+01
1273	0.6	1.9490	-2.48470E+01
1273	0.6	1.9500	-2.48637E+01
1273	0.6	1.9510	-2.48809E+01
1273	0.6	1.9520	-2.48986E+01
1273	0.6	1.9530	-2.49167E+01
1273	0.6	1.9540	-2.49353E+01
1273	0.6	1.9550	-2.49543E+01
1273	0.6	1.9560	-2.49738E+01
1273	0.6	1.9570	-2.49938E+01
1273	0.6	1.9580	-2.50142E+01
1273	0.6	1.9590	-2.50350E+01
1273	0.6	1.9600	-2.50563E+01
1273	0.6	1.9610	-2.50781E+01
1273	0.6	1.9620	-2.51002E+01
1273	0.6	1.9630	-2.51228E+01
1273	0.6	1.9640	-2.51458E+01
1273	0.6	1.9650	-2.51692E+01
1273	0.6	1.9660	-2.51930E+01
1273	0.6	1.9670	-2.52171E+01
1273	0.6	1.9680	-2.52416E+01
1273	0.6	1.9690	-2.52665E+01
1273	0.6	1.9700	-2.52916E+01
1273	0.6	1.9710	-2.53171E+01
1273	0.6	1.9720	-2.53428E+01
1273	0.6	1.9730	-2.53688E+01
1273	0.6	1.9740	-2.53950E+01
1273	0.6	1.9750	-2.54215E+01
1273	0.6	1.9760	-2.54480E+01
1273	0.6	1.9770	-2.54748E+01
1273	0.6	1.9780	-2.55016E+01
1273	0.6	1.9790	-2.55284E+01
1273	0.6	1.9800	-2.55553E+01
1273	0.6	1.9810	-2.55821E+01
1273	0.6	1.9820	-2.56088E+01
1273	0.6	1.9830	-2.56353E+01
1273	0.6	1.9840	-2.56617E+01
1273	0.6	1.9850	-2.56877E+01
1273	0.6	1.9860	-2.57133E+01
1273	0.6	1.9870	-2.57385E+01
1273	0.6	1.9880	-2.57631E+01
1273	0.6	1.9890	-2.57871E+01
1273	0.6	1.9900	-2.58103E+01
1273	0.6	1.9910	-2.58327E+01
1273	0.6	1.9920	-2.58541E+01
1273	0.6	1.9930	-2.58745E+01
1273	0.6	1.9940	-2.58937E+01
1273	0.6	1.9950	-2.59116E+01
1273	0.6	1.9960	-2.59281E+01
1273	0.6	1.9970	-2.59431E+01
1273	0.6	1.9980	-2.59566E+01
1273	0.6	1.9990	-2.59684E+01
1273	0.6	2.0000	-2.59785E+01
1273	0.6	2.0010	-2.59871E+01
1273	0.6	2.0020	-2.59822E+01
1273	0.6	2.0030	-2.59799E+01
1273	0.6	2.0040	-2.59748E+01
1273	0.6	2.0050	-2.59671E+01
1273	0.6	2.0060	-2.59569E+01
1273	0.6	2.0070	-2.59443E+01
1273	0.6	2.0080	-2.59295E+01
1273	0.6	2.0090	-2.59127E+01
1273	0.6	2.0100	-2.58940E+01
1273	0.6	2.0110	-2.58736E+01
1273	0.6	2.0120	-2.58516E+01
1273	0.6	2.0130	-2.58283E+01
1273	0.6	2.0140	-2.58038E+01
1273	0.6	2.0150	-2.57781E+01
1273	0.6	2.0160	-2.57515E+01
1273	0.6	2.0170	-2.57239E+01
1273	0.6	2.0180	-2.56956E+01
1273	0.6	2.0190	-2.56665E+01
1273	0.6	2.0200	-2.56368E+01
1273	0.6	2.0210	-2.56064E+01
1273	0.6	2.0220	-2.55756E+01
1273	0.6	2.0230	-2.55443E+01
1273	0.6	2.0240	-2.55125E+01
1273	0.6	2.0250	-2.54803E+01
1273	0.6	2.0260	-2.54477E+01
1273	0.6	2.0270	-2.54147E+01
1273	0.6	2.0280	-2.53814E+01
1273	0.6	2.0290	-2.53478E+01
1273	0.6	2.0300	-2.53138E+01
1273	0.6	2.0310	-2.52796E+01

1273	0.6	2.0320	-2.52450E+01
1273	0.6	2.0330	-2.52102E+01
1273	0.6	2.0340	-2.51751E+01
1273	0.6	2.0350	-2.51397E+01
1273	0.6	2.0360	-2.51040E+01
1273	0.6	2.0370	-2.50681E+01
1273	0.6	2.0380	-2.50318E+01
1273	0.6	2.0390	-2.49954E+01
1273	0.6	2.0400	-2.49586E+01
1273	0.6	1.7000	-1.84532E+01
1273	0.6	1.7010	-1.84509E+01
1273	0.6	1.7020	-1.84485E+01
1273	0.6	1.7030	-1.84458E+01
1273	0.6	1.7040	-1.84431E+01
1273	0.6	1.7050	-1.84404E+01
1273	0.6	1.7060	-1.84377E+01
1273	0.6	1.7070	-1.84350E+01
1273	0.6	1.7080	-1.84325E+01
1273	0.6	1.7090	-1.84301E+01
1273	0.6	1.7100	-1.84278E+01
1273	0.6	1.7110	-1.84256E+01
1273	0.6	1.7120	-1.84236E+01
1273	0.6	1.7130	-1.84218E+01
1273	0.6	1.7140	-1.84201E+01
1273	0.6	1.7150	-1.84185E+01
1273	0.6	1.7160	-1.84171E+01
1273	0.6	1.7170	-1.84158E+01
1273	0.6	1.7180	-1.84146E+01
1273	0.6	1.7190	-1.84136E+01
1273	0.6	1.7200	-1.84127E+01
1273	0.6	1.7210	-1.84119E+01
1273	0.6	1.7220	-1.84112E+01
1273	0.6	1.7230	-1.84107E+01
1273	0.6	1.7240	-1.84102E+01
1273	0.6	1.7250	-1.84099E+01
1273	0.6	1.7260	-1.84097E+01
1273	0.6	1.7270	-1.84095E+01
1273	0.6	1.7280	-1.84095E+01
1273	0.6	1.7290	-1.84096E+01
1273	0.6	1.7300	-1.84097E+01
1273	0.6	1.7310	-1.84100E+01
1273	0.6	1.7320	-1.84103E+01
1273	0.6	1.7330	-1.84107E+01
1273	0.6	1.7340	-1.84112E+01
1273	0.6	1.7350	-1.84118E+01
1273	0.6	1.7360	-1.84125E+01
1273	0.6	1.7370	-1.84132E+01
1273	0.6	1.7380	-1.84140E+01
1273	0.6	1.7390	-1.84149E+01
1273	0.6	1.7400	-1.84158E+01
1273	0.6	1.7410	-1.84168E+01
1273	0.6	1.7420	-1.84179E+01
1273	0.6	1.7430	-1.84190E+01
1273	0.6	1.7440	-1.84202E+01
1273	0.6	1.7450	-1.84214E+01
1273	0.6	1.7460	-1.84227E+01
1273	0.6	1.7470	-1.84241E+01
1273	0.6	1.7480	-1.84255E+01
1273	0.6	1.7490	-1.84269E+01
1273	0.6	1.7500	-1.84284E+01
1273	0.6	1.7510	-1.84300E+01
1273	0.6	1.7520	-1.84316E+01
1273	0.6	1.7530	-1.84332E+01
1273	0.6	1.7540	-1.84349E+01
1273	0.6	1.7550	-1.84367E+01
1273	0.6	1.7560	-1.84385E+01
1273	0.6	1.7570	-1.84403E+01
1273	0.6	1.7580	-1.84421E+01
1273	0.6	1.7590	-1.84440E+01
1273	0.6	1.7600	-1.84460E+01
1273	0.6	1.7610	-1.84479E+01
1273	0.6	1.7620	-1.84500E+01
1273	0.6	1.7630	-1.84520E+01
1273	0.6	1.7640	-1.84541E+01
1273	0.6	1.7650	-1.84562E+01
1273	0.6	1.7660	-1.84583E+01
1273	0.6	1.7670	-1.84605E+01
1273	0.6	1.7680	-1.84627E+01
1273	0.6	1.7690	-1.84650E+01
1273	0.6	1.7700	-1.84672E+01
1273	0.6	1.7710	-1.84695E+01
1273	0.6	1.7720	-1.84718E+01
1273	0.6	1.7730	-1.84742E+01
1273	0.6	1.7740	-1.84766E+01
1273	0.6	1.7750	-1.84790E+01
1273	0.6	1.7760	-1.84814E+01
1273	0.6	1.7770	-1.84838E+01
1273	0.6	1.7780	-1.84863E+01
1273	0.6	1.7790	-1.84888E+01
1273	0.6	1.7800	-1.84913E+01
1273	0.6	1.7810	-1.84939E+01
1273	0.6	1.7820	-1.84964E+01

1773	0.6	1.7830	-1.84990E+01
1773	0.6	1.7840	-1.85016E+01
1773	0.6	1.7850	-1.85042E+01
1773	0.6	1.7860	-1.85069E+01
1773	0.6	1.7870	-1.85096E+01
1773	0.6	1.7880	-1.85122E+01
1773	0.6	1.7890	-1.85149E+01
1773	0.6	1.7900	-1.85177E+01
1773	0.6	1.7910	-1.85204E+01
1773	0.6	1.7920	-1.85232E+01
1773	0.6	1.7930	-1.85259E+01
1773	0.6	1.7940	-1.85287E+01
1773	0.6	1.7950	-1.85315E+01
1773	0.6	1.7960	-1.85344E+01
1773	0.6	1.7970	-1.85372E+01
1773	0.6	1.7980	-1.85401E+01
1773	0.6	1.7990	-1.85429E+01
1773	0.6	1.8000	-1.85458E+01
1773	0.6	1.8010	-1.85487E+01
1773	0.6	1.8020	-1.85517E+01
1773	0.6	1.8030	-1.85546E+01
1773	0.6	1.8040	-1.85575E+01
1773	0.6	1.8050	-1.85605E+01
1773	0.6	1.8060	-1.85635E+01
1773	0.6	1.8070	-1.85665E+01
1773	0.6	1.8080	-1.85695E+01
1773	0.6	1.8090	-1.85725E+01
1773	0.6	1.8100	-1.85755E+01
1773	0.6	1.8110	-1.85786E+01
1773	0.6	1.8120	-1.85816E+01
1773	0.6	1.8130	-1.85847E+01
1773	0.6	1.8140	-1.85878E+01
1773	0.6	1.8150	-1.85909E+01
1773	0.6	1.8160	-1.85940E+01
1773	0.6	1.8170	-1.85971E+01
1773	0.6	1.8180	-1.86003E+01
1773	0.6	1.8190	-1.86034E+01
1773	0.6	1.8200	-1.86066E+01
1773	0.6	1.8210	-1.86098E+01
1773	0.6	1.8220	-1.86130E+01
1773	0.6	1.8230	-1.86162E+01
1773	0.6	1.8240	-1.86194E+01
1773	0.6	1.8250	-1.86226E+01
1773	0.6	1.8260	-1.86259E+01
1773	0.6	1.8270	-1.86291E+01
1773	0.6	1.8280	-1.86324E+01
1773	0.6	1.8290	-1.86357E+01
1773	0.6	1.8300	-1.86390E+01
1773	0.6	1.8310	-1.86423E+01
1773	0.6	1.8320	-1.86456E+01
1773	0.6	1.8330	-1.86490E+01
1773	0.6	1.8340	-1.86523E+01
1773	0.6	1.8350	-1.86557E+01
1773	0.6	1.8360	-1.86591E+01
1773	0.6	1.8370	-1.86625E+01
1773	0.6	1.8380	-1.86659E+01
1773	0.6	1.8390	-1.86694E+01
1773	0.6	1.8400	-1.86728E+01
1773	0.6	1.8410	-1.86763E+01
1773	0.6	1.8420	-1.86798E+01
1773	0.6	1.8430	-1.86833E+01
1773	0.6	1.8440	-1.86868E+01
1773	0.6	1.8450	-1.86903E+01
1773	0.6	1.8460	-1.86939E+01
1773	0.6	1.8470	-1.86975E+01
1773	0.6	1.8480	-1.87011E+01
1773	0.6		

1773	0.6	1.8750	-1.88080E+01
1773	0.6	1.8760	-1.88124E+01
1773	0.6	1.8770	-1.88170E+01
1773	0.6	1.8780	-1.88215E+01
1773	0.6	1.8790	-1.88261E+01
1773	0.6	1.8800	-1.88308E+01
1773	0.6	1.8810	-1.88355E+01
1773	0.6	1.8820	-1.88403E+01
1773	0.6	1.8830	-1.88452E+01
1773	0.6	1.8840	-1.88501E+01
1773	0.6	1.8850	-1.88550E+01
1773	0.6	1.8860	-1.88601E+01
1773	0.6	1.8870	-1.88652E+01
1773	0.6	1.8880	-1.88704E+01
1773	0.6	1.8890	-1.88757E+01
1773	0.6	1.8900	-1.88810E+01
1773	0.6	1.8910	-1.88865E+01
1773	0.6	1.8920	-1.88920E+01
1773	0.6	1.8930	-1.88976E+01
1773	0.6	1.8940	-1.89033E+01
1773	0.6	1.8950	-1.89091E+01
1773	0.6	1.8960	-1.89150E+01
1773	0.6	1.8970	-1.89210E+01
1773	0.6	1.8980	-1.89271E+01
1773	0.6	1.8990	-1.89333E+01
1773	0.6	1.9000	-1.89397E+01
1773	0.6	1.9010	-1.89461E+01
1773	0.6	1.9020	-1.89527E+01
1773	0.6	1.9030	-1.89594E+01
1773	0.6	1.9040	-1.89663E+01
1773	0.6	1.9050	-1.89732E+01
1773	0.6	1.9060	-1.89803E+01
1773	0.6	1.9070	-1.89876E+01
1773	0.6	1.9080	-1.89950E+01
1773	0.6	1.9090	-1.90026E+01
1773	0.6	1.9100	-1.90103E+01
1773	0.6	1.9110	-1.90181E+01
1773	0.6	1.9120	-1.90262E+01
1773	0.6	1.9130	-1.90344E+01
1773	0.6	1.9140	-1.90428E+01
1773	0.6	1.9150	-1.90513E+01
1773	0.6	1.9160	-1.90600E+01
1773	0.6	1.9170	-1.90690E+01
1773	0.6	1.9180	-1.90781E+01
1773	0.6	1.9190	-1.90874E+01
1773	0.6	1.9200	-1.90968E+01
1773	0.6	1.9210	-1.91065E+01
1773	0.6	1.9220	-1.91164E+01
1773	0.6	1.9230	-1.91265E+01
1773	0.6	1.9240	-1.91368E+01
1773	0.6	1.9250	-1.91473E+01
1773	0.6	1.9260	-1.91579E+01
1773	0.6	1.9270	-1.91688E+01
1773	0.6	1.9280	-1.91799E+01
1773	0.6	1.9290	-1.91912E+01
1773	0.6	1.9300	-1.92027E+01
1773	0.6	1.9310	-1.92144E+01
1773	0.6	1.9320	-1.92263E+01
1773	0.6	1.9330	-1.92384E+01
1773	0.6	1.9340	-1.92507E+01
1773	0.6	1.9350	-1.92632E+01
1773	0.6	1.9360	-1.92759E+01
1773	0.6	1.9370	-1.92888E+01
1773	0.6	1.9380	-1.93018E+01
1773	0.6	1.9390	-1.93150E+01
1773	0.6	1.9400	-1.93283E+01
1773	0.6	1.9410	-1.93419E+01
1773	0.6	1.9420	-1.93555E+01
1773	0.6	1.9430	-1.93693E+01
1773	0.6	1.9440	-1.93832E+01
1773	0.6	1.9450	-1.93973E+01
1773	0.6	1.9460	-1.94114E+01
1773	0.6	1.9470	-1.94256E+01
1773	0.6	1.9480	-1.94399E+01
1773	0.6	1.9490	-1.94543E+01
1773	0.6	1.9500	-1.94687E+01
1773	0.6	1.9510	-1.94831E+01
1773	0.6	1.9520	-1.94975E+01
1773	0.6	1.9530	-1.95119E+01
1773	0.6	1.9540	-1.95263E+01
1773	0.6	1.9550	-1.95406E+01
1773	0.6	1.9560	-1.95548E+01
1773	0.6	1.9570	-1.95690E+01
1773	0.6	1.9580	-1.95830E+01
1773	0.6	1.9590	-1.95968E+01
1773	0.6	1.9600	-1.96105E+01
1773	0.6	1.9610	-1.96240E+01
1773	0.6	1.9620	-1.96372E+01
1773	0.6	1.9630	-1.96501E+01
1773	0.6	1.9640	-1.96628E+01
1773	0.6	1.9650	-1.96751E+01
1773	0.6	1.9660	-1.96871E+01

1773	0.6	1.9670	-1.96987E+01
1773	0.6	1.9680	-1.97099E+01
1773	0.6	1.9690	-1.97206E+01
1773	0.6	1.9700	-1.97308E+01
1773	0.6	1.9710	-1.97405E+01
1773	0.6	1.9720	-1.97497E+01
1773	0.6	1.9730	-1.97583E+01
1773	0.6	1.9740	-1.97664E+01
1773	0.6	1.9750	-1.97738E+01
1773	0.6	1.9760	-1.97806E+01
1773	0.6	1.9770	-1.97876E+01
1773	0.6	1.9780	-1.97921E+01
1773	0.6	1.9790	-1.97969E+01
1773	0.6	1.9800	-1.98009E+01
1773	0.6	1.9810	-1.98042E+01
1773	0.6	1.9820	-1.98068E+01
1773	0.6	1.9830	-1.98087E+01
1773	0.6	1.9840	-1.98098E+01
1773	0.6	1.9850	-1.98103E+01
1773	0.6	1.9860	-1.98099E+01
1773	0.6	1.9870	-1.98089E+01
1773	0.6	1.9880	-1.98071E+01
1773	0.6	1.9890	-1.98047E+01
1773	0.6	1.9900	-1.98015E+01
1773	0.6	1.9910	-1.97977E+01
1773	0.6	1.9920	-1.97932E+01
1773	0.6	1.9930	-1.97881E+01
1773	0.6	1.9940	-1.97823E+01
1773	0.6	1.9950	-1.97759E+01
1773	0.6	1.9960	-1.97689E+01
1773	0.6	1.9970	-1.97613E+01
1773	0.6	1.9980	-1.97531E+01
1773	0.6	1.9990	-1.97443E+01
1773	0.6	2.0000	-1.97339E+01
1773	0.6	2.0010	-1.97187E+01
1773	0.6	2.0020	-1.97018E+01
1773	0.6	2.0030	-1.96843E+01
1773	0.6	2.0040	-1.96662E+01
1773	0.6	2.0050	-1.96476E+01
1773	0.6	2.0060	-1.96285E+01
1773	0.6	2.0070	-1.96090E+01
1773	0.6	2.0080	-1.95891E+01
1773	0.6	2.0090	-1.95688E+01
1773	0.6	2.0100	-1.95482E+01
1773	0.6	2.0110	-1.95272E+01
1773	0.6	2.0120	-1.95060E+01
1773	0.6	2.0130	-1.94845E+01
1773	0.6	2.0140	-1.94626E+01
1773	0.6	2.0150	-1.94406E+01
1773	0.6	2.0160	-1.94183E+01
1773	0.6	2.0170	-1.93957E+01
1773	0.6	2.0180	-1.93730E+01
1773	0.6	2.0190	-1.93500E+01
1773	0.6	2.0200	-1.93268E+01
1773	0.6	2.0210	-1.93034E+01
1773	0.6	2.0220	-1.92799E+01
1773	0.6	2.0230	-1.92561E+01
1773	0.6	2.0240	-1.92322E+01
1773	0.6	2.0250	-1.92081E+01
1773	0.6	2.0260	-1.91838E+01
1773	0.6	2.0270	-1.91594E+01
1773	0.6	2.0280	-1.91347E+01
1773	0.6	2.0290	-1.91100E+01
1773	0.6	2.0300	-1.90850E+01
1773	0.6	2.0310	-1.90599E+01
1773	0.6	2.0320	-1.90347E+01
1773	0.6	2.0330	-1.90093E+01
1773	0.6	2.0340	-1.89837E+01
1773	0.6	2.0350	-1.89580E+01
1773	0.6	2.0360	-1.89321E+01
1773	0.6	2.0370	-1.89061E+01
1773	0.6	2.0380	-1.88800E+01
1773	0.6	2.0390	-1.88537E+01
1773	0.6	2.0400	-1.88272E+01
1773	0.6	2.0410	-1.88006E+01
1773	0.6	2.0420	-1.87738E+01
1773	0.6	2.0430	-1.87469E+01
1773	0.6	2.0440	-1.87198E+01
1773	0.6	2.0450	-1.86926E+01
1773	0.6	2.0460	-1.86653E+01
1773	0.6	2.0470	-1.86378E+01
1773	0.6	2.0480	-1.86101E+01
1773	0.6	2.0490	-1.85823E+01
1773	0.6	2.0500	-1.85543E+01
1773	0.6	2.0510	-1.85262E+01
1773	0.6	2.0520	-1.84980E+01
1773	0.6	2.0530	-1.84695E+01
1773	0.6	2.0540	-1.84410E+01
1773	0.6	2.0550	-1.84123E+01
1773	0.6	2.0560	-1.83834E+01
1773	0.6	2.0570	-1.83544E+01
1773	0.6	2.0580	-1.83252E+01

1773	0.6	2.0590	-1.82959E+01
1773	0.6	2.0600	-1.82664E+01
1773	0.6	2.0610	-1.82368E+01
1773	0.6	2.0620	-1.82071E+01
1773	0.6	2.0630	-1.81771E+01
1773	0.6	2.0640	-1.81471E+01
1773	0.6	2.0650	-1.81168E+01
1773	0.6	2.0660	-1.80865E+01
1773	0.6	2.0670	-1.80559E+01
1773	0.6	2.0680	-1.80253E+01
1773	0.6	2.0690	-1.79944E+01
1773	0.6	2.0700	-1.79635E+01
1773	0.6	2.0710	-1.79323E+01
1773	0.6	2.0720	-1.79011E+01
1773	0.6	2.0730	-1.78697E+01
1773	0.6	2.0740	-1.78381E+01
1773	0.6	2.0750	-1.78064E+01
1773	0.6	2.0760	-1.77745E+01
1773	0.6	2.0770	-1.77425E+01
1773	0.6	2.0780	-1.77104E+01
1773	0.6	2.0790	-1.76781E+01
1773	0.6	2.0800	-1.76457E+01
2273	0.6	1.6700	-1.53691E+01
2273	0.6	1.6710	-1.53689E+01
2273	0.6	1.6720	-1.53686E+01
2273	0.6	1.6730	-1.53684E+01
2273	0.6	1.6740	-1.53681E+01
2273	0.6	1.6750	-1.53678E+01
2273	0.6	1.6760	-1.53675E+01
2273	0.6	1.6770	-1.53672E+01
2273	0.6	1.6780	-1.53669E+01
2273	0.6	1.6790	-1.53666E+01
2273	0.6	1.6800	-1.53662E+01
2273	0.6	1.6810	-1.53658E+01
2273	0.6	1.6820	-1.53654E+01
2273	0.6	1.6830	-1.53649E+01
2273	0.6	1.6840	-1.53645E+01
2273	0.6	1.6850	-1.53640E+01
2273	0.6	1.6860	-1.53634E+01
2273	0.6	1.6870	-1.53629E+01
2273	0.6	1.6880	-1.53623E+01
2273	0.6	1.6890	-1.53617E+01
2273	0.6	1.6900	-1.53611E+01
2273	0.6	1.6910	-1.53604E+01
2273	0.6	1.6920	-1.53597E+01
2273	0.6	1.6930	-1.53589E+01
2273	0.6	1.6940	-1.53581E+01
2273	0.6	1.6950	-1.53573E+01
2273	0.6	1.6960	-1.53565E+01
2273	0.6	1.6970	-1.53556E+01
2273	0.6	1.6980	-1.53547E+01
2273	0.6	1.6990	-1.53538E+01
2273	0.6	1.7000	-1.53528E+01
2273	0.6	1.7010	-1.53518E+01
2273	0.6	1.7020	-1.53509E+01
2273	0.6	1.7030	-1.53499E+01
2273	0.6	1.7040	-1.53489E+01
2273	0.6	1.7050	-1.53479E+01
2273	0.6	1.7060	-1.53469E+01
2273	0.6	1.7070	-1.53459E+01
2273	0.6	1.7080	-1.53450E+01
2273	0.6	1.7090	-1.53441E+01
2273	0.6	1.7100	-1.53432E+01
2273	0.6	1.7110	-1.53423E+01
2273	0.6	1.7120	-1.53415E+01
2273	0.6	1.7130	-1.53408E+01
2273	0.6		

2273	0.6	1.7400	-1.53401E+01
2273	0.6	1.7410	-1.53408E+01
2273	0.6	1.7420	-1.53416E+01
2273	0.6	1.7430	-1.53424E+01
2273	0.6	1.7440	-1.53432E+01
2273	0.6	1.7450	-1.53441E+01
2273	0.6	1.7460	-1.53451E+01
2273	0.6	1.7470	-1.53460E+01
2273	0.6	1.7480	-1.53470E+01
2273	0.6	1.7490	-1.53481E+01
2273	0.6	1.7500	-1.53492E+01
2273	0.6	1.7510	-1.53503E+01
2273	0.6	1.7520	-1.53515E+01
2273	0.6	1.7530	-1.53527E+01
2273	0.6	1.7540	-1.53540E+01
2273	0.6	1.7550	-1.53553E+01
2273	0.6	1.7560	-1.53566E+01
2273	0.6	1.7570	-1.53580E+01
2273	0.6	1.7580	-1.53594E+01
2273	0.6	1.7590	-1.53608E+01
2273	0.6	1.7600	-1.53622E+01
2273	0.6	1.7610	-1.53637E+01
2273	0.6	1.7620	-1.53653E+01
2273	0.6	1.7630	-1.53668E+01
2273	0.6	1.7640	-1.53684E+01
2273	0.6	1.7650	-1.53701E+01
2273	0.6	1.7660	-1.53717E+01
2273	0.6	1.7670	-1.53734E+01
2273	0.6	1.7680	-1.53751E+01
2273	0.6	1.7690	-1.53769E+01
2273	0.6	1.7700	-1.53786E+01
2273	0.6	1.7710	-1.53804E+01
2273	0.6	1.7720	-1.53823E+01
2273	0.6	1.7730	-1.53841E+01
2273	0.6	1.7740	-1.53860E+01
2273	0.6	1.7750	-1.53879E+01
2273	0.6	1.7760	-1.53899E+01
2273	0.6	1.7770	-1.53918E+01
2273	0.6	1.7780	-1.53938E+01
2273	0.6	1.7790	-1.53958E+01
2273	0.6	1.7800	-1.53979E+01
2273	0.6	1.7810	-1.53999E+01
2273	0.6	1.7820	-1.54020E+01
2273	0.6	1.7830	-1.54041E+01
2273	0.6	1.7840	-1.54063E+01
2273	0.6	1.7850	-1.54085E+01
2273	0.6	1.7860	-1.54106E+01
2273	0.6	1.7870	-1.54128E+01
2273	0.6	1.7880	-1.54151E+01
2273	0.6	1.7890	-1.54173E+01
2273	0.6	1.7900	-1.54196E+01
2273	0.6	1.7910	-1.54219E+01
2273	0.6	1.7920	-1.54242E+01
2273	0.6	1.7930	-1.54266E+01
2273	0.6	1.7940	-1.54290E+01
2273	0.6	1.7950	-1.54313E+01
2273	0.6	1.7960	-1.54338E+01
2273	0.6	1.7970	-1.54362E+01
2273	0.6	1.7980	-1.54386E+01
2273	0.6	1.7990	-1.54411E+01
2273	0.6	1.8000	-1.54436E+01
2273	0.6	1.8010	-1.54461E+01
2273	0.6	1.8020	-1.54487E+01
2273	0.6	1.8030	-1.54512E+01
2273	0.6	1.8040	-1.54538E+01
2273	0.6	1.8050	-1.54564E+01
2273	0.6	1.8060	-1.54590E+01
2273	0.6	1.8070	-1.54617E+01
2273	0.6	1.8080	-1.54643E+01
2273	0.6	1.8090	-1.54670E+01
2273	0.6	1.8100	-1.54697E+01
2273	0.6	1.8110	-1.54724E+01
2273	0.6	1.8120	-1.54752E+01
2273	0.6	1.8130	-1.54779E+01
2273	0.6	1.8140	-1.54807E+01
2273	0.6	1.8150	-1.54835E+01
2273	0.6	1.8160	-1.54864E+01
2273	0.6	1.8170	-1.54892E+01
2273	0.6	1.8180	-1.54921E+01
2273	0.6	1.8190	-1.54950E+01
2273	0.6	1.8200	-1.54979E+01
2273	0.6	1.8210	-1.55008E+01
2273	0.6	1.8220	-1.55038E+01
2273	0.6	1.8230	-1.55067E+01
2273	0.6	1.8240	-1.55097E+01
2273	0.6	1.8250	-1.55128E+01
2273	0.6	1.8260	-1.55158E+01
2273	0.6	1.8270	-1.55189E+01
2273	0.6	1.8280	-1.55220E+01
2273	0.6	1.8290	-1.55251E+01
2273	0.6	1.8300	-1.55282E+01
2273	0.6	1.8310	-1.55314E+01

2273	0.6	1.8320	-1.55345E+01
2273	0.6	1.8330	-1.55378E+01
2273	0.6	1.8340	-1.55410E+01
2273	0.6	1.8350	-1.55443E+01
2273	0.6	1.8360	-1.55475E+01
2273	0.6	1.8370	-1.55509E+01
2273	0.6	1.8380	-1.55542E+01
2273	0.6	1.8390	-1.55576E+01
2273	0.6	1.8400	-1.55609E+01
2273	0.6	1.8410	-1.55644E+01
2273	0.6	1.8420	-1.55678E+01
2273	0.6	1.8430	-1.55713E+01
2273	0.6	1.8440	-1.55748E+01
2273	0.6	1.8450	-1.55784E+01
2273	0.6	1.8460	-1.55819E+01
2273	0.6	1.8470	-1.55855E+01
2273	0.6	1.8480	-1.55892E+01
2273	0.6	1.8490	-1.55928E+01
2273	0.6	1.8500	-1.55965E+01
2273	0.6	1.8510	-1.56003E+01
2273	0.6	1.8520	-1.56041E+01
2273	0.6	1.8530	-1.56079E+01
2273	0.6	1.8540	-1.56117E+01
2273	0.6	1.8550	-1.56156E+01
2273	0.6	1.8560	-1.56195E+01
2273	0.6	1.8570	-1.56235E+01
2273	0.6	1.8580	-1.56275E+01
2273	0.6	1.8590	-1.56316E+01
2273	0.6	1.8600	-1.56357E+01
2273	0.6	1.8610	-1.56398E+01
2273	0.6	1.8620	-1.56440E+01
2273	0.6	1.8630	-1.56482E+01
2273	0.6	1.8640	-1.56525E+01
2273	0.6	1.8650	-1.56568E+01
2273	0.6	1.8660	-1.56612E+01
2273	0.6	1.8670	-1.56657E+01
2273	0.6	1.8680	-1.56702E+01
2273	0.6	1.8690	-1.56747E+01
2273	0.6	1.8700	-1.56793E+01
2273	0.6	1.8710	-1.56840E+01
2273	0.6	1.8720	-1.56887E+01
2273	0.6	1.8730	-1.56935E+01
2273	0.6	1.8740	-1.56983E+01
2273	0.6	1.8750	-1.57032E+01
2273	0.6	1.8760	-1.57082E+01
2273	0.6	1.8770	-1.57132E+01
2273	0.6	1.8780	-1.57184E+01
2273	0.6	1.8790	-1.57235E+01
2273	0.6	1.8800	-1.57288E+01
2273	0.6	1.8810	-1.57341E+01
2273	0.6	1.8820	-1.57395E+01
2273	0.6	1.8830	-1.57450E+01
2273	0.6	1.8840	-1.57506E+01
2273	0.6	1.8850	-1.57562E+01
2273	0.6	1.8860	-1.57619E+01
2273	0.6	1.8870	-1.57677E+01
2273	0.6	1.8880	-1.57736E+01
2273	0.6	1.8890	-1.57796E+01
2273	0.6	1.8900	-1.57857E+01
2273	0.6	1.8910	-1.57918E+01
2273	0.6	1.8920	-1.57981E+01
2273	0.6	1.8930	-1.58044E+01
2273	0.6	1.8940	-1.58108E+01
2273	0.6	1.8950	-1.58174E+01
2273	0.6	1.8960	-1.58240E+01
2273	0.6	1.8970	-1.58307E+01
2273	0.6	1.8980	-1.58375E+01
2273	0.6	1.8990	-1.58445E+01
2273	0.6	1.9000	-1.58515E+01
2273	0.6	1.9010	-1.58586E+01
2273	0.6	1.9020	-1.58658E+01
2273	0.6	1.9030	-1.58731E+01
2273	0.6	1.9040	-1.58805E+01
2273	0.6	1.9050	-1.58880E+01
2273	0.6	1.9060	-1.58956E+01
2273	0.6	1.9070	-1.59033E+01
2273	0.6	1.9080	-1.59111E+01
2273	0.6	1.9090	-1.59190E+01
2273	0.6	1.9100	-1.59270E+01
2273	0.6	1.9110	-1.59351E+01
2273	0.6	1.9120	-1.59433E+01
2273	0.6	1.9130	-1.59515E+01
2273	0.6	1.9140	-1.59599E+01
2273	0.6	1.9150	-1.59683E+01
2273	0.6	1.9160	-1.59768E+01
2273	0.6	1.9170	-1.59854E+01
2273	0.6	1.9180	-1.59940E+01
2273	0.6	1.9190	-1.60028E+01
2273	0.6	1.9200	-1.60115E+01
2273	0.6	1.9210	-1.60204E+01
2273	0.6	1.9220	-1.60292E+01
2273	0.6	1.9230	-1.60382E+01

2273	0.6	1.9240	-1.60471E+01
2273	0.6	1.9250	-1.60556E+01
2273	0.6	1.9260	-1.60652E+01
2273	0.6	1.9270	-1.60742E+01
2273	0.6	1.9280	-1.60832E+01
2273	0.6	1.9290	-1.60923E+01
2273	0.6	1.9300	-1.61013E+01
2273	0.6	1.9310	-1.61103E+01
2273	0.6	1.9320	-1.61193E+01
2273	0.6	1.9330	-1.61282E+01
2273	0.6	1.9340	-1.61371E+01
2273	0.6	1.9350	-1.61460E+01
2273	0.6	1.9360	-1.61547E+01
2273	0.6	1.9370	-1.61634E+01
2273	0.6	1.9380	-1.61719E+01
2273	0.6	1.9390	-1.61804E+01
2273	0.6	1.9400	-1.61887E+01
2273	0.6	1.9410	-1.61969E+01
2273	0.6	1.9420	-1.62050E+01
2273	0.6	1.9430	-1.62128E+01
2273	0.6	1.9440	-1.62205E+01
2273	0.6	1.9450	-1.62281E+01
2273	0.6	1.9460	-1.62354E+01
2273	0.6	1.9470	-1.62424E+01
2273	0.6	1.9480	-1.62493E+01
2273	0.6	1.9490	-1.62559E+01
2273	0.6	1.9500	-1.62622E+01
2273	0.6	1.9510	-1.62683E+01
2273	0.6	1.9520	-1.62741E+01
2273	0.6	1.9530	-1.62796E+01
2273	0.6	1.9540	-1.62848E+01
2273	0.6	1.9550	-1.62896E+01
2273	0.6	1.9560	-1.62941E+01
2273	0.6	1.9570	-1.62983E+01
2273	0.6	1.9580	-1.63021E+01
2273	0.6	1.9590	-1.63056E+01
2273	0.6	1.9600	-1.63087E+01
2273	0.6	1.9610	-1.63114E+01
2273	0.6	1.9620	-1.63137E+01
2273	0.6	1.9630	-1.63156E+01
2273	0.6	1.9640	-1.63172E+01
2273	0.6	1.9650	-1.63183E+01
2273	0.6	1.9660	-1.63191E+01
2273	0.6	1.9670	-1.63194E+01
2273	0.6	1.9680	-1.63194E+01
2273	0.6	1.9690	-1.63189E+01
2273	0.6	1.9700	-1.63180E+01
2273	0.6	1.9710	-1.63167E+01
2273	0.6	1.9720	-1.63151E+01
2273	0.6	1.9730	-1.63130E+01
2273	0.6	1.9740	-1.63105E+01
2273	0.6	1.9750	-1.63077E+01
2273	0.6	1.9760	-1.63044E+01
2273	0.6	1.9770	-1.63008E+01
2273	0.6	1.9780	-1.62968E+01
2273	0.6	1.9790	-1.62924E+01
2273	0.6	1.9800	-1.62877E+01
2273	0.6	1.9810	-1.62826E+01
2273	0.6	1.9820	-1.62772E+01
2273	0.6	1.9830	-1.62714E+01
2273	0.6	1.9840	-1.62653E+01
2273	0.6	1.9850	-1.62589E+01
2273	0.6	1.9860	-1.62521E+01
2273	0.6	1.9870	-1.62450E+01
2273	0.6	1.9880	-1.62376E+01
2273	0.6	1.9890	-1.62299E+01
2273	0.6		

2273	0.6	2.0160	-1.58511E+01
2273	0.6	2.0170	-1.58324E+01
2273	0.6	2.0180	-1.58136E+01
2273	0.6	2.0190	-1.57946E+01
2273	0.6	2.0200	-1.57756E+01

2273	0.6	2.0210	-1.57564E+01
2273	0.6	2.0220	-1.57371E+01
2273	0.6	2.0230	-1.57176E+01
2273	0.6	2.0240	-1.56981E+01
2273	0.6	2.0250	-1.56784E+01

2273	0.6	2.0260	-1.56586E+01
2273	0.6	2.0270	-1.56387E+01
2273	0.6	2.0280	-1.56187E+01
2273	0.6	2.0290	-1.55986E+01
2273	0.6	2.0300	-1.55784E+01

A.2.7. $(U_{0.3}Pu_{0.7})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{pu} _{pu} (m ² /s)
1273	0.7	1.6600	-2.33935E+01
1273	0.7	1.6610	-2.33875E+01
1273	0.7	1.6620	-2.33820E+01
1273	0.7	1.6630	-2.33768E+01
1273	0.7	1.6640	-2.33720E+01
1273	0.7	1.6650	-2.33676E+01
1273	0.7	1.6660	-2.33635E+01
1273	0.7	1.6670	-2.33596E+01
1273	0.7	1.6680	-2.33561E+01
1273	0.7	1.6690	-2.33528E+01
1273	0.7	1.6700	-2.33498E+01
1273	0.7	1.6710	-2.33471E+01
1273	0.7	1.6720	-2.33446E+01
1273	0.7	1.6730	-2.33423E+01
1273	0.7	1.6740	-2.33402E+01
1273	0.7	1.6750	-2.33383E+01
1273	0.7	1.6760	-2.33366E+01
1273	0.7	1.6770	-2.33351E+01
1273	0.7	1.6780	-2.33338E+01
1273	0.7	1.6790	-2.33327E+01
1273	0.7	1.6800	-2.33317E+01
1273	0.7	1.6810	-2.33309E+01
1273	0.7	1.6820	-2.33302E+01
1273	0.7	1.6830	-2.33297E+01
1273	0.7	1.6840	-2.33293E+01
1273	0.7	1.6850	-2.33290E+01
1273	0.7	1.6860	-2.33289E+01
1273	0.7	1.6870	-2.33289E+01
1273	0.7	1.6880	-2.33290E+01
1273	0.7	1.6890	-2.33292E+01
1273	0.7	1.6900	-2.33296E+01
1273	0.7	1.6910	-2.33300E+01
1273	0.7	1.6920	-2.33305E+01
1273	0.7	1.6930	-2.33312E+01
1273	0.7	1.6940	-2.33319E+01
1273	0.7	1.6950	-2.33327E+01
1273	0.7	1.6960	-2.33337E+01
1273	0.7	1.6970	-2.33347E+01
1273	0.7	1.6980	-2.33358E+01
1273	0.7	1.6990	-2.33369E+01
1273	0.7	1.7000	-2.33382E+01
1273	0.7	1.7010	-2.33395E+01
1273	0.7	1.7020	-2.33409E+01
1273	0.7	1.7030	-2.33423E+01
1273	0.7	1.7040	-2.33438E+01
1273	0.7	1.7050	-2.33454E+01
1273	0.7	1.7060	-2.33471E+01
1273	0.7	1.7070	-2.33488E+01
1273	0.7	1.7080	-2.33506E+01
1273	0.7	1.7090	-2.33524E+01
1273	0.7	1.7100	-2.33543E+01
1273	0.7	1.7110	-2.33562E+01
1273	0.7	1.7120	-2.33582E+01
1273	0.7	1.7130	-2.33602E+01
1273	0.7	1.7140	-2.33623E+01
1273	0.7	1.7150	-2.33644E+01
1273	0.7	1.7160	-2.33666E+01
1273	0.7	1.7170	-2.33688E+01
1273	0.7	1.7180	-2.33711E+01
1273	0.7	1.7190	-2.33734E+01
1273	0.7	1.7200	-2.33757E+01
1273	0.7	1.7210	-2.33781E+01
1273	0.7	1.7220	-2.33805E+01
1273	0.7	1.7230	-2.33830E+01
1273	0.7	1.7240	-2.33855E+01
1273	0.7	1.7250	-2.33880E+01
1273	0.7	1.7260	-2.33906E+01
1273	0.7	1.7270	-2.33932E+01
1273	0.7	1.7280	-2.33958E+01
1273	0.7	1.7290	-2.33984E+01
1273	0.7	1.7300	-2.34011E+01
1273	0.7	1.7310	-2.34038E+01
1273	0.7	1.7320	-2.34065E+01
1273	0.7	1.7330	-2.34093E+01
1273	0.7	1.7340	-2.34121E+01
1273	0.7	1.7350	-2.34149E+01
1273	0.7	1.7360	-2.34177E+01
1273	0.7	1.7370	-2.34205E+01
1273	0.7	1.7380	-2.34234E+01
1273	0.7	1.7400	-2.34292E+01

1273	0.7	1.7410	-2.34322E+01
1273	0.7	1.7420	-2.34351E+01
1273	0.7	1.7430	-2.34381E+01
1273	0.7	1.7440	-2.34411E+01
1273	0.7	1.7450	-2.34441E+01
1273	0.7	1.7460	-2.34471E+01
1273	0.7	1.7470	-2.34501E+01
1273	0.7	1.7480	-2.34532E+01
1273	0.7	1.7490	-2.34563E+01
1273	0.7	1.7500	-2.34593E+01
1273	0.7	1.7510	-2.34624E+01
1273	0.7	1.7520	-2.34655E+01
1273	0.7	1.7530	-2.34687E+01
1273	0.7	1.7540	-2.34718E+01
1273	0.7	1.7550	-2.34749E+01
1273	0.7	1.7560	-2.34781E+01
1273	0.7	1.7570	-2.34813E+01
1273	0.7	1.7580	-2.34844E+01
1273	0.7	1.7590	-2.34876E+01
1273	0.7	1.7600	-2.34908E+01
1273	0.7	1.7610	-2.34940E+01
1273	0.7	1.7620	-2.34972E+01
1273	0.7	1.7630	-2.35005E+01
1273	0.7	1.7640	-2.35037E+01
1273	0.7	1.7650	-2.35069E+01
1273	0.7	1.7660	-2.35102E+01
1273	0.7	1.7670	-2.35134E+01
1273	0.7	1.7680	-2.35167E+01
1273	0.7	1.7690	-2.35200E+01
1273	0.7	1.7700	-2.35232E+01
1273	0.7	1.7710	-2.35265E+01
1273	0.7	1.7720	-2.35298E+01
1273	0.7	1.7730	-2.35331E+01
1273	0.7	1.7740	-2.35364E+01
1273	0.7	1.7750	-2.35397E+01
1273	0.7	1.7760	-2.35430E+01
1273	0.7	1.7770	-2.35463E+01
1273	0.7	1.7780	-2.35496E+01
1273	0.7	1.7790	-2.35529E+01
1273	0.7	1.7800	-2.35563E+01
1273	0.7	1.7810	-2.35596E+01
1273	0.7	1.7820	-2.35629E+01
1273	0.7	1.7830	-2.35663E+01
1273	0.7	1.7840	-2.35696E+01
1273	0.7	1.7850	-2.35729E+01
1273	0.7	1.7860	-2.35763E+01
1273	0.7	1.7870	-2.35796E+01
1273	0.7	1.7880	-2.35830E+01
1273	0.7	1.7890	-2.35863E+01
1273	0.7	1.7900	-2.35897E+01
1273	0.7	1.7910	-2.35930E+01
1273	0.7	1.7920	-2.35964E+01
1273	0.7	1.7930	-2.35998E+01
1273	0.7	1.7940	-2.36031E+01
1273	0.7	1.7950	-2.36065E+01
1273	0.7	1.7960	-2.36099E+01
1273	0.7	1.7970	-2.36133E+01
1273	0.7	1.7980	-2.36166E+01
1273	0.7	1.7990	-2.36200E+01
1273	0.7	1.8000	-2.36234E+01
1273	0.7	1.8010	-2.36268E+01
1273	0.7	1.8020	-2.36302E+01
1273	0.7	1.8030	-2.36336E+01
1273	0.7	1.8040	-2.36369E+01
1273	0.7	1.8050	-2.36403E+01
1273	0.7	1.8060	-2.36437E+01
1273	0.7	1.8070	-2.36471E+01
1273	0.7	1.8080	-2.36505E+01
1273	0.7	1.8090	-2.36539E+01
1273	0.7	1.8100	-2.36573E+01
1273	0.7	1.8110	-2.36608E+01
1273	0.7	1.8120	-2.36642E+01
1273	0.7	1.8130	-2.36676E+01
1273	0.7	1.8140	-2.36710E+01
1273	0.7	1.8150	-2.36744E+01
1273	0.7	1.8160	-2.36778E+01
1273	0.7	1.8170	-2.36813E+01
1273	0.7	1.8180	-2.36847E+01
1273	0.7	1.8190	-2.36881E+01
1273	0.7	1.8200	-2.36916E+01
1273	0.7	1.8210	-2.36950E+01
1273	0.7	1.8220	-2.36985E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ^{pu} _{pu} (m ² /s)
1273	0.7	1.8230	-2.37019E+01
1273	0.7	1.8240	-2.37054E+01
1273	0.7	1.8250	-2.37088E+01
1273	0.7	1.8260	-2.37123E+01
1273	0.7	1.8270	-2.37158E+01
1273	0.7	1.8280	-2.37192E+01
1273	0.7	1.8290	-2.37227E+01
1273	0.7	1.8300	-2.37262E+01
1273	0.7	1.8310	-2.37297E+01
1273	0.7	1.8320	-2.37332E+01
1273	0.7	1.8330	-2.37367E+01
1273	0.7	1.8340	-2.37402E+01
1273	0.7	1.8350	-2.37437E+01
1273	0.7	1.8360	-2.37472E+01
1273	0.7	1.8370	-2.37507E+01
1273	0.7	1.8380	-2.37543E+01
1273	0.7	1.8390	-2.37578E+01
1273	0.7	1.8400	-2.37613E+01
1273	0.7	1.8410	-2.37649E+01
1273	0.7	1.8420	-2.37685E+01
1273	0.7	1.8430	-2.37720E+01
1273	0.7	1.8440	-2.37756E+01
1273	0.7	1.8450	-2.37792E+01
1273	0.7	1.8460	-2.37828E+01
1273	0.7	1.8470	-2.37864E+01
1273	0.7	1.8480	-2.37900E+01
1273	0.7	1.8490	-2.37936E+01
1273	0.7	1.8500	-2.37973E+01
1273	0.7	1.8510	-2.38009E+01
1273	0.7	1.8520	-2.38046E+01
1273	0.7	1.8530	-2.38083E+01
1273	0.7	1.8540	-2.38119E+01
1273	0.7	1.8550	-2.38156E+01
1273	0.7	1.8560	-2.38193E+01
1273	0.7	1.8570	-2.38231E+01
1273	0.7	1.8580	-2.38268E+01
1273	0.7	1.8590	-2.38305E+01
1273	0.7	1.8600	-2.38343E+01
1273	0.7	1.8610	-2.38381E+01
1273	0.7	1.8620	-2.38419E+01
1273	0.7	1.8630	-2.38457E+01
1273	0.7	1.8640	-2.38495E+01
1273	0.7	1.8650	-2.38534E+01
1273	0.7	1.8660	-2.38572E+01
1273	0.7	1.8670	-2.38611E+01
1273	0.7	1.8680	-2.38650E+01
1273	0.7	1.8690	-2.38689E+01
1273	0.7	1.8700	-2.38729E+01
1273	0.7	1.8710	-2.38768E+01
1273	0.7	1.8720	-2.38808E+01
1273	0.7	1.8730	-2.38848E+01
1273	0.7	1.8740	-2.38888E+01
1273	0.7	1.8750	-2.38929E+01
1273	0.7	1.8760	-2.38970E+01
1273	0.7	1.8770	-2.39011E+01
1273	0.7	1.8780	-2.39052E+01
1273	0.7	1.8790	-2.39094E+01
1273	0.7	1.8800	-2.39135E+01
1273	0.7	1.8810	-2.39178E+01
1273	0.7	1.8820	-2.39220E+01
1273	0.7	1.8830	-2.39263E+01
1273	0.7	1.8840	-2.39306E+01
1273	0.7	1.8850	-2.39349E+01
1273	0.7	1.8860	-2.39393E+01
1273	0.7	1.8870	-2.39437E+01
1273	0.7	1.8880	-2.39482E+01

1273	0.7	1.9070	-2.40430E+01
1273	0.7	1.9080	-2.40487E+01
1273	0.7	1.9090	-2.40545E+01
1273	0.7	1.9100	-2.40604E+01
1273	0.7	1.9110	-2.40664E+01
1273	0.7	1.9120	-2.40726E+01
1273	0.7	1.9130	-2.40788E+01
1273	0.7	1.9140	-2.40852E+01
1273	0.7	1.9150	-2.40917E+01
1273	0.7	1.9160	-2.40983E+01
1273	0.7	1.9170	-2.41051E+01
1273	0.7	1.9180	-2.41121E+01
1273	0.7	1.9190	-2.41192E+01
1273	0.7	1.9200	-2.41264E+01
1273	0.7	1.9210	-2.41339E+01
1273	0.7	1.9220	-2.41415E+01
1273	0.7	1.9230	-2.41493E+01
1273	0.7	1.9240	-2.41573E+01
1273	0.7	1.9250	-2.41655E+01
1273	0.7	1.9260	-2.41740E+01
1273	0.7	1.9270	-2.41826E+01
1273	0.7	1.9280	-2.41915E+01
1273	0.7	1.9290	-2.42007E+01
1273	0.7	1.9300	-2.42101E+01
1273	0.7	1.9310	-2.42198E+01
1273	0.7	1.9320	-2.42297E+01
1273	0.7	1.9330	-2.42399E+01
1273	0.7	1.9340	-2.42505E+01
1273	0.7	1.9350	-2.42613E+01
1273	0.7	1.9360	-2.42724E+01
1273	0.7	1.9370	-2.42839E+01
1273	0.7	1.9380	-2.42957E+01
1273	0.7	1.9390	-2.43078E+01
1273	0.7	1.9400	-2.43203E+01
1273	0.7	1.9410	-2.43331E+01
1273	0.7	1.9420	-2.43463E+01
1273	0.7	1.9430	-2.43598E+01
1273	0.7	1.9440	-2.43737E+01
1273	0.7	1.9450	-2.43880E+01
1273	0.7	1.9460	-2.44026E+01
1273	0.7	1.9470	-2.44176E+01
1273	0.7	1.9480	-2.44329E+01
1273	0.7	1.9490	-2.44487E+01
1273	0.7	1.9500	-2.44647E+01
1273	0.7	1.9510	-2.44812E+01
1273	0.7	1.9520	-2.44979E+01
1273	0.7	1.9530	-2.45151E+01
1273	0.7	1.9540	-2.45325E+01
1273	0.7	1.9550	-2.45502E+01
1273	0.7	1.9560	-2.45683E+01
1273	0.7	1.9570	-2.45866E+01
1273	0.7	1.9580	-2.46052E+01
1273	0.7	1.9590	-2.46240E+01
1273	0.7	1.9600	-2.46430E+01
1273	0.7	1.9610	-2.46623E+01
1273	0.7	1.9620	-2.46817E+01
1273	0.7	1.9630	-2.47012E+01
1273	0.7	1.9640	-2.47208E+01
1273	0.7	1.9650	-2.47404E+01
1273	0.7	1.9660	-2.47601E+01
1273	0.7	1.9670	-2.47797E+01
1273	0.7	1.9680	-2.47992E+01
1273	0.7	1.9690	-2.48186E+01
1273	0.7	1.9700	-2.48378E+01
1273	0.7	1.9710	-2.48568E+01
1273	0.7	1.9720	-2.48754E+01
1273	0.7	1.9730	-2.48937E+01
1273	0.7	1.9740	-2.49115E+01
1273	0.7	1.9750	-2.49287E+01
1273	0.7	1.9760	-2.49454E+01
1273	0.7	1.9770	-2.49614E+01
1273	0.7	1.9780	-2.49767E+01
1273	0.7	1.9790	-2.49911E+01
1273	0.7	1.9800	-2.50046E+01
1273	0.7	1.9810	-2.50171E+01
1273	0.7	1.9820	-2.50286E+01
1273	0.7	1.9830	-2.50389E+01
1273	0.7	1.9840	-2.50481E+01
1273	0.7	1.9850	-2.50560E+01
1273	0.7	1.9860	-2.50626E+01
1273	0.7	1.9870	-2.50678E+01
1273	0.7	1.9880	-2.50717E+01
1273	0.7	1.9890	-2.50742E+01
1273	0.7	1.9900	-2.50752E+01
1273	0.7	1.9910	-2.50749E+01
1273	0.7	1.9920	-2.50731E+01
1273	0.7	1.9930	-2.50700E+01
1273	0.7	1.9940	-2.50654E+01
1273	0.7	1.9950	-2.50595E+01
1273	0.7	1.9960	-2.50524E+01
1273	0.7	1.9970	-2.50439E+01
1273	0.7	1.9980	-2.50342E+01

1273	0.7	1.9990	-2.50234E+01
1273	0.7	2.0000	-2.50114E+01
1273	0.7	2.0010	-2.49901E+01
1273	0.7	2.0020	-2.49675E+01
1273	0.7	2.0030	-2.49436E+01
1273	0.7	2.0040	-2.49187E+01
1273	0.7	2.0050	-2.48929E+01
1273	0.7	2.0060	-2.48661E+01
1273	0.7	2.0070	-2.48385E+01
1273	0.7	2.0080	-2.48102E+01
1273	0.7	2.0090	-2.47812E+01
1273	0.7	2.0100	-2.47516E+01
1273	0.7	2.0110	-2.47215E+01
1273	0.7	2.0120	-2.46909E+01
1273	0.7	2.0130	-2.46597E+01
1273	0.7	2.0140	-2.46282E+01
1273	0.7	2.0150	-2.45962E+01
1273	0.7	2.0160	-2.45639E+01
1273	0.7	2.0170	-2.45312E+01
1273	0.7	2.0180	-2.44981E+01
1273	0.7	2.0190	-2.44648E+01
1273	0.7	2.0200	-2.44311E+01
1273	0.7	2.0210	-2.43971E+01
1273	0.7	2.0220	-2.43628E+01
1273	0.7	2.0230	-2.43283E+01
1273	0.7	2.0240	-2.42934E+01
1273	0.7	2.0250	-2.42583E+01
1273	0.7	2.0260	-2.42229E+01
1273	0.7	2.0270	-2.41873E+01
1273	0.7	2.0280	-2.41513E+01
1273	0.7	2.0290	-2.41152E+01
1273	0.7	2.0300	-2.40787E+01
1273	0.7	2.0310	-2.40420E+01
1273	0.7	2.0320	-2.40051E+01
1273	0.7	2.0330	-2.39679E+01
1273	0.7	2.0340	-2.39304E+01
1273	0.7	2.0350	-2.38927E+01
1273	0.7	2.0360	-2.38547E+01
1273	0.7	2.0370	-2.38165E+01
1273	0.7	2.0380	-2.37780E+01
1273	0.7	2.0390	-2.37392E+01
1273	0.7	2.0400	-2.37002E+01
1273	0.7	2.0410	-2.36609E+01
1273	0.7	2.0420	-2.36214E+01
1273	0.7	2.0430	-2.35816E+01
1273	0.7	2.0440	-2.35415E+01
1273	0.7	2.0450	-2.35012E+01
1273	0.7	2.0460	-2.34606E+01
1273	0.7	2.0470	-2.34197E+01
1273	0.7	2.0480	-2.33786E+01
1273	0.7	2.0490	-2.33372E+01
1273	0.7	2.0500	-2.32955E+01
1273	0.7	2.0510	-2.32536E+01
1273	0.7	2.0520	-2.32114E+01
1273	0.7	2.0530	-2.31689E+01
1273	0.7	2.0540	-2.31262E+01
1273	0.7	2.0550	-2.30832E+01
1273	0.7	2.0560	-2.30400E+01
1273	0.7	2.0570	-2.29964E+01
1273	0.7	2.0580	-2.29527E+01
1273	0.7	2.0590	-2.29086E+01
1273	0.7	2.0600	-2.28644E+01
1273	0.7	2.0610	-2.28198E+01
1273	0.7	2.0620	-2.27750E+01
1273	0.7	2.0630	-2.27300E+01
1273	0.7	2.0640	-2.26847E+01
1273	0.7	2.0650	-2.26392E+01
1273	0.7	2.0660	-2.25935E+01
1273	0.7	2.0670	-2.25475E+01
1273	0.7	2.0680	-2.25013E+01
1273	0.7	2.0690	-2.24549E+01
1273	0.7	2.0700	-2.24083E+01
1273	0.7	2.0710	-2.23615E+01
1273	0.7	2.0720	-2.23145E+01
1273	0.7	2.0730	-2.22673E+01
1273	0.7	2.0740	-2.22199E+01
1273	0.7	2.0750	-2.21723E+01
1273	0.7	2.0760	-2.21245E+01
1273	0.7	2.0770	-2.20766E+01
1273	0.7	2.0780	-2.20286E+01
1273	0.7	2.0790	-2.19803E+01
1273	0.7	2.0800	-2.19320E+01
1273	0.7	2.0810	-2.18835E+01
1273	0.7	2.0820	-2.18349E+01
1273	0.7	2.0830	-2.17861E+01
1273	0.7	2.0840	-2.17372E+01
1273	0.7	2.0850	-2.16883E+01
1273	0.7	2.0860	-2.16392E+01
1273	0.7	2.0870	-2.15900E+01
1273	0.7	2.0880	-2.15408E+01
1273	0.7	2.0890	-2.14914E+01
1273	0.7	2.0900	-2.14420E+01

1273	0.7	2.0910	-2.13925E+01
1273	0.7	2.0920	-2.13430E+01
1273	0.7	2.0930	-2.12934E+01
1273	0.7	2.0940	-2.12437E+01
1273	0.7	2.0950	-2.11940E+01
1273	0.7	2.0960	-2.11442E+01
1273	0.7	2.0970	-2.10945E+01
1273	0.7	2.0980	-2.10446E+01
1273	0.7	2.0990	-2.09948E+01
1273	0.7	2.1000	-2.09449E+01
1273	0.7	2.1010	-2.08950E+01
1273	0.7	2.1020	-2.08451E+01
1273	0.7	2.1030	-2.07952E+01
1273	0.7	2.1040	-2.07453E+01
1273	0.7	2.1050	-2.06954E+01
1273	0.7	2.1060	-2.06455E+01
1273	0.7	2.1070	-2.05956E+01
1273	0.7	2.1080	-2.05456E+01
1273	0.7	2.1090	-2.04957E+01
1273	0.7	2.1100	-2.04458E+01
1273	0.7	1.6500	-1.81919E+01
1273	0.7	1.6510	-1.81889E+01
1273	0.7	1.6520	-1.81854E+01
1273	0.7	1.6530	-1.81817E+01
1273	0.7	1.6540	-1.81778E+01
1273	0.7	1.6550	-1.81739E+01
1273	0.7	1.6560	-1.81699E+01
1273	0.7	1.6570	-1.81660E+01
1273	0.7	1.6580	-1.81622E+01
1273	0.7	1.6590	-1.81585E+01
1273	0.7	1.6600	-1.81549E+01
1273	0.7	1.6610	-1.81515E+01
1273	0.7	1.6620	-1.81482E+01
1273	0.7	1.6630	-1.81451E+01
1273	0.7	1.6640	-1.81421E+01
1273	0.7	1.6650	-1.81392E+01
1273	0.7	1.6660	-1.81365E+01
1273	0.7	1.6670	-1.81339E+01
1273	0.7	1.6680	-1.81315E+01
1273	0.7	1.6690	-1.81292E+01
1273	0.7	1.6700	-1.81270E+01
1273	0.7	1.6710	-1.81250E+01
1273	0.7	1.6720	-1.81231E+01
1273	0.7	1.6730	-1.81212E+01
1273	0.7	1.6740	-1.81196E+01
1273	0.7	1.6750	-1.81180E+01
1273	0.7	1.6760	-1.81165E+01
1273	0.7	1.6770	-1.81151E+01
1273	0.7	1.6780	-1.81139E+01
1273	0.7	1.6790	-1.81127E+01
1273	0.7	1.6800	-1.81117E+01
1273	0.7	1.6810	-1.81107E+01
1273	0.7	1.6820	-1.81098E+01
1273	0.7	1.6830	-1.81090E+01
1273	0.7	1.6840	-1.81083E+01
1273	0.7	1.6850	-1.81077E+01
1273	0.7	1.6860	-1.81072E+01
1273	0.7	1.6870	-1.81067E+01
1273	0.7	1.6880	-1.81063E+01
1273	0.7	1.6890	-1.81060E+01
1273	0.7	1.6900	-1.81058E+01
1273	0.7	1.6910	-1.81057E+01
1273	0.7	1.6920	-1.81056E+01
1273	0.7	1.6930	-1.81055E+01
1273	0.7	1.6940	-1.81056E+01
1273	0.7	1.6950	-1.81057E+01
1273	0.7		

1773	0.7	1.7220	-1.81284E+01
1773	0.7	1.7230	-1.81298E+01
1773	0.7	1.7240	-1.81313E+01
1773	0.7	1.7250	-1.81328E+01
1773	0.7	1.7260	-1.81343E+01
1773	0.7	1.7270	-1.81358E+01
1773	0.7	1.7280	-1.81374E+01
1773	0.7	1.7290	-1.81391E+01
1773	0.7	1.7300	-1.81407E+01
1773	0.7	1.7310	-1.81424E+01
1773	0.7	1.7320	-1.81441E+01
1773	0.7	1.7330	-1.81458E+01
1773	0.7	1.7340	-1.81476E+01
1773	0.7	1.7350	-1.81494E+01
1773	0.7	1.7360	-1.81512E+01
1773	0.7	1.7370	-1.81530E+01
1773	0.7	1.7380	-1.81549E+01
1773	0.7	1.7390	-1.81568E+01
1773	0.7	1.7400	-1.81587E+01
1773	0.7	1.7410	-1.81607E+01
1773	0.7	1.7420	-1.81626E+01
1773	0.7	1.7430	-1.81646E+01
1773	0.7	1.7440	-1.81667E+01
1773	0.7	1.7450	-1.81687E+01
1773	0.7	1.7460	-1.81708E+01
1773	0.7	1.7470	-1.81728E+01
1773	0.7	1.7480	-1.81750E+01
1773	0.7	1.7490	-1.81771E+01
1773	0.7	1.7500	-1.81792E+01
1773	0.7	1.7510	-1.81814E+01
1773	0.7	1.7520	-1.81836E+01
1773	0.7	1.7530	-1.81858E+01
1773	0.7	1.7540	-1.81880E+01
1773	0.7	1.7550	-1.81903E+01
1773	0.7	1.7560	-1.81926E+01
1773	0.7	1.7570	-1.81948E+01
1773	0.7	1.7580	-1.81972E+01
1773	0.7	1.7590	-1.81995E+01
1773	0.7	1.7600	-1.82018E+01
1773	0.7	1.7610	-1.82042E+01
1773	0.7	1.7620	-1.82066E+01
1773	0.7	1.7630	-1.82090E+01
1773	0.7	1.7640	-1.82114E+01
1773	0.7	1.7650	-1.82138E+01
1773	0.7	1.7660	-1.82163E+01
1773	0.7	1.7670	-1.82187E+01
1773	0.7	1.7680	-1.82212E+01
1773	0.7	1.7690	-1.82237E+01
1773	0.7	1.7700	-1.82262E+01
1773	0.7	1.7710	-1.82287E+01
1773	0.7	1.7720	-1.82313E+01
1773	0.7	1.7730	-1.82338E+01
1773	0.7	1.7740	-1.82364E+01
1773	0.7	1.7750	-1.82390E+01
1773	0.7	1.7760	-1.82416E+01
1773	0.7	1.7770	-1.82442E+01
1773	0.7	1.7780	-1.82468E+01
1773	0.7	1.7790	-1.82495E+01
1773	0.7	1.7800	-1.82522E+01
1773	0.7	1.7810	-1.82548E+01
1773	0.7	1.7820	-1.82575E+01
1773	0.7	1.7830	-1.82602E+01
1773	0.7	1.7840	-1.82629E+01
1773	0.7	1.7850	-1.82657E+01
1773	0.7	1.7860	-1.82684E+01
1773	0.7	1.7870	-1.82712E+01
1773	0.7	1.7880	-1.82739E+01
1773	0.7	1.7890	-1.82767E+01
1773	0.7	1.7900	-1.82795E+01
1773	0.7	1.7910	-1.82823E+01
1773	0.7	1.7920	-1.82851E+01
1773	0.7	1.7930	-1.82880E+01
1773	0.7	1.7940	-1.82908E+01
1773	0.7	1.7950	-1.82937E+01
1773	0.7	1.7960	-1.82966E+01
1773	0.7	1.7970	-1.82994E+01
1773	0.7	1.7980	-1.83023E+01
1773	0.7	1.7990	-1.83052E+01
1773	0.7	1.8000	-1.83082E+01
1773	0.7	1.8010	-1.83111E+01
1773	0.7	1.8020	-1.83141E+01
1773	0.7	1.8030	-1.83170E+01
1773	0.7	1.8040	-1.83200E+01
1773	0.7	1.8050	-1.83230E+01
1773	0.7	1.8060	-1.83260E+01
1773	0.7	1.8070	-1.83290E+01
1773	0.7	1.8080	-1.83320E+01
1773	0.7	1.8090	-1.83350E+01
1773	0.7	1.8100	-1.83381E+01
1773	0.7	1.8110	-1.83411E+01
1773	0.7	1.8120	-1.83442E+01
1773	0.7	1.8130	-1.83473E+01

1773	0.7	1.8140	-1.83504E+01
1773	0.7	1.8150	-1.83535E+01
1773	0.7	1.8160	-1.83566E+01
1773	0.7	1.8170	-1.83597E+01
1773	0.7	1.8180	-1.83629E+01
1773	0.7	1.8190	-1.83660E+01
1773	0.7	1.8200	-1.83692E+01
1773	0.7	1.8210	-1.83724E+01
1773	0.7	1.8220	-1.83756E+01
1773	0.7	1.8230	-1.83788E+01
1773	0.7	1.8240	-1.83820E+01
1773	0.7	1.8250	-1.83853E+01
1773	0.7	1.8260	-1.83885E+01
1773	0.7	1.8270	-1.83918E+01
1773	0.7	1.8280	-1.83951E+01
1773	0.7	1.8290	-1.83984E+01
1773	0.7	1.8300	-1.84017E+01
1773	0.7	1.8310	-1.84050E+01
1773	0.7	1.8320	-1.84083E+01
1773	0.7	1.8330	-1.84117E+01
1773	0.7	1.8340	-1.84151E+01
1773	0.7	1.8350	-1.84184E+01
1773	0.7	1.8360	-1.84218E+01
1773	0.7	1.8370	-1.84252E+01
1773	0.7	1.8380	-1.84287E+01
1773	0.7	1.8390	-1.84321E+01
1773	0.7	1.8400	-1.84356E+01
1773	0.7	1.8410	-1.84391E+01
1773	0.7	1.8420	-1.84426E+01
1773	0.7	1.8430	-1.84461E+01
1773	0.7	1.8440	-1.84496E+01
1773	0.7	1.8450	-1.84532E+01
1773	0.7	1.8460	-1.84567E+01
1773	0.7	1.8470	-1.84603E+01
1773	0.7	1.8480	-1.84639E+01
1773	0.7	1.8490	-1.84676E+01
1773	0.7	1.8500	-1.84712E+01
1773	0.7	1.8510	-1.84749E+01
1773	0.7	1.8520	-1.84786E+01
1773	0.7	1.8530	-1.84823E+01
1773	0.7	1.8540	-1.84860E+01
1773	0.7	1.8550	-1.84898E+01
1773	0.7	1.8560	-1.84936E+01
1773	0.7	1.8570	-1.84974E+01
1773	0.7	1.8580	-1.85012E+01
1773	0.7	1.8590	-1.85051E+01
1773	0.7	1.8600	-1.85089E+01
1773	0.7	1.8610	-1.85129E+01
1773	0.7	1.8620	-1.85168E+01
1773	0.7	1.8630	-1.85208E+01
1773	0.7	1.8640	-1.85248E+01
1773	0.7	1.8650	-1.85288E+01
1773	0.7	1.8660	-1.85329E+01
1773	0.7	1.8670	-1.85369E+01
1773	0.7	1.8680	-1.85411E+01
1773	0.7	1.8690	-1.85452E+01
1773	0.7	1.8700	-1.85494E+01
1773	0.7	1.8710	-1.85537E+01
1773	0.7	1.8720	-1.85579E+01
1773	0.7	1.8730	-1.85623E+01
1773	0.7	1.8740	-1.85666E+01
1773	0.7	1.8750	-1.85710E+01
1773	0.7	1.8760	-1.85755E+01
1773	0.7	1.8770	-1.85799E+01
1773	0.7	1.8780	-1.85845E+01
1773	0.7	1.8790	-1.85891E+01
1773	0.7	1.8800	-1.85937E+01
1773	0.7	1.8810	-1.85984E+01
1773	0.7	1.8820	-1.86031E+01
1773	0.7	1.8830	-1.86079E+01
1773	0.7	1.8840	-1.86127E+01
1773	0.7	1.8850	-1.86176E+01
1773	0.7	1.8860	-1.86226E+01
1773	0.7	1.8870	-1.86276E+01
1773	0.7	1.8880	-1.86327E+01
1773	0.7	1.8890	-1.86379E+01
1773	0.7	1.8900	-1.86431E+01
1773	0.7	1.8910	-1.86484E+01
1773	0.7	1.8920	-1.86538E+01
1773	0.7	1.8930	-1.86593E+01
1773	0.7	1.8940	-1.86648E+01
1773	0.7	1.8950	-1.86704E+01
1773	0.7	1.8960	-1.86761E+01
1773	0.7	1.8970	-1.86819E+01
1773	0.7	1.8980	-1.86878E+01
1773	0.7	1.8990	-1.86938E+01
1773	0.7	1.9000	-1.86999E+01
1773	0.7	1.9010	-1.87060E+01
1773	0.7	1.9020	-1.87123E+01
1773	0.7	1.9030	-1.87186E+01
1773	0.7	1.9040	-1.87251E+01
1773	0.7	1.9050	-1.87317E+01

1773	0.7	1.9060	-1.87384E+01
1773	0.7	1.9070	-1.87452E+01
1773	0.7	1.9080	-1.87521E+01
1773	0.7	1.9090	-1.87591E+01
1773	0.7	1.9100	-1.87663E+01
1773	0.7	1.9110	-1.87736E+01
1773	0.7	1.9120	-1.87810E+01
1773	0.7	1.9130	-1.87885E+01
1773	0.7	1.9140	-1.87961E+01
1773	0.7	1.9150	-1.88039E+01
1773	0.7	1.9160	-1.88118E+01
1773	0.7	1.9170	-1.88198E+01
1773	0.7	1.9180	-1.88280E+01
1773	0.7	1.9190	-1.88362E+01
1773	0.7	1.9200	-1.88446E+01
1773	0.7	1.9210	-1.88532E+01
1773	0.7	1.9220	-1.88618E+01
1773	0.7	1.9230	-1.88706E+01
1773	0.7	1.9240	-1.88795E+01
1773	0.7	1.9250	-1.88885E+01
1773	0.7	1.9260	-1.88976E+01
1773	0.7	1.9270	-1.89068E+01
1773	0.7	1.9280	-1.89161E+01
1773	0.7	1.9290	-1.89255E+01
1773	0.7	1.9300	-1.89350E+01
1773	0.7	1.9310	-1.89446E+01
1773	0.7	1.9320	-1.89542E+01
1773	0.7	1.9330	-1.89639E+01
1773	0.7	1.9340	-1.89737E+01
1773	0.7	1.9350	-1.89835E+01
1773	0.7	1.9360	-1.89933E+01
1773	0.7	1.9370	-1.90032E+01
1773	0.7	1.9380	-1.90130E+01
1773	0.7	1.9390	-1.90229E+01
1773	0.7	1.9400	-1.90327E+01
1773	0.7	1.9410	-1.90425E+01
1773	0.7	1.9420	-1.90522E+01
1773	0.7	1.9430	-1.90619E+01
1773	0.7	1.9440	-1.90714E+01
1773	0.7	1.9450	-1.90809E+01
1773	0.7	1.9460	-1.90902E+01
1773	0.7	1.9470	-1.90994E+01
1773	0.7	1.9480	-1.91083E+01
1773	0.7	1.9490	-1.91171E+01
1773	0.7	1.9500	-1.91257E+01
1773	0.7	1.9510	-1.91340E+01
1773	0.7	1.9520	-1.91421E+01
1773	0.7	1.9530	-1.91499E+01
1773	0.7	1.9540	-1.91573E+01
1773	0.7	1.9550	-1.91645E+01
1773	0.7	1.9560	-1.91712E+01
1773	0.7	1.9570	-1.91776E+01
1773	0.7	1.9580	-1.91836E+01
1773	0.7	1.9590	-1.91892E+01
1773	0.7	1.9600	-1.91943E+01
1773	0.7	1.9610	-1.91990E+01
1773	0.7	1.9620	-1.92031E+01
1773	0.7	1.9630	-1.92068E+01
1773	0.7	1.9640	-1.92100E+01
1773	0.7	1.9650	-1.92126E+01
1773	0.7	1.9660	-1.92147E+01
1773	0.7	1.9670	-1.92163E+01
1773	0.7	1.9680	-1.92173E+01
1773	0.7	1.9690	-1.92177E+01
1773	0.7	1.9700	-1.92176E+01
1773	0.7	1.9710	-1.92169E+01
1773	0.7		

1773	0.7	1.9980	-1.90018E+01
1773	0.7	1.9990	-1.89879E+01
1773	0.7	2.0000	-1.89725E+01
1773	0.7	2.0010	-1.89530E+01
1773	0.7	2.0020	-1.89320E+01
1773	0.7	2.0030	-1.89107E+01
1773	0.7	2.0040	-1.88890E+01
1773	0.7	2.0050	-1.88671E+01
1773	0.7	2.0060	-1.88449E+01
1773	0.7	2.0070	-1.88224E+01
1773	0.7	2.0080	-1.87997E+01
1773	0.7	2.0090	-1.87768E+01
1773	0.7	2.0100	-1.87537E+01
1773	0.7	2.0110	-1.87304E+01
1773	0.7	2.0120	-1.87069E+01
1773	0.7	2.0130	-1.86831E+01
1773	0.7	2.0140	-1.86592E+01
1773	0.7	2.0150	-1.86351E+01
1773	0.7	2.0160	-1.86109E+01
1773	0.7	2.0170	-1.85864E+01
1773	0.7	2.0180	-1.85618E+01
1773	0.7	2.0190	-1.85370E+01
1773	0.7	2.0200	-1.85121E+01
1773	0.7	2.0210	-1.84870E+01
1773	0.7	2.0220	-1.84617E+01
1773	0.7	2.0230	-1.84363E+01
1773	0.7	2.0240	-1.84107E+01
1773	0.7	2.0250	-1.83849E+01
1773	0.7	2.0260	-1.83590E+01
1773	0.7	2.0270	-1.83330E+01
1773	0.7	2.0280	-1.83067E+01
1773	0.7	2.0290	-1.82804E+01
1773	0.7	2.0300	-1.82538E+01
1773	0.7	2.0310	-1.82272E+01
1773	0.7	2.0320	-1.82003E+01
1773	0.7	2.0330	-1.81734E+01
1773	0.7	2.0340	-1.81462E+01
1773	0.7	2.0350	-1.81189E+01
1773	0.7	2.0360	-1.80915E+01
1773	0.7	2.0370	-1.80639E+01
1773	0.7	2.0380	-1.80362E+01
1773	0.7	2.0390	-1.80083E+01
1773	0.7	2.0400	-1.79802E+01
1773	0.7	2.0410	-1.79520E+01
1773	0.7	2.0420	-1.79236E+01
1773	0.7	2.0430	-1.78951E+01
1773	0.7	2.0440	-1.78664E+01
1773	0.7	2.0450	-1.78376E+01
1773	0.7	2.0460	-1.78086E+01
1773	0.7	2.0470	-1.77795E+01
1773	0.7	2.0480	-1.77502E+01
1773	0.7	2.0490	-1.77207E+01
1773	0.7	2.0500	-1.76911E+01
2273	0.7	1.6400	-1.52079E+01
2273	0.7	1.6410	-1.52070E+01
2273	0.7	1.6420	-1.52060E+01
2273	0.7	1.6430	-1.52050E+01
2273	0.7	1.6440	-1.52039E+01
2273	0.7	1.6450	-1.52027E+01
2273	0.7	1.6460	-1.52015E+01
2273	0.7	1.6470	-1.52002E+01
2273	0.7	1.6480	-1.51988E+01
2273	0.7	1.6490	-1.51973E+01
2273	0.7	1.6500	-1.51958E+01
2273	0.7	1.6510	-1.51942E+01
2273	0.7	1.6520	-1.51926E+01
2273	0.7	1.6530	-1.51909E+01
2273	0.7	1.6540	-1.51892E+01
2273	0.7	1.6550	-1.51875E+01
2273	0.7	1.6560	-1.51857E+01
2273	0.7	1.6570	-1.51839E+01
2273	0.7	1.6580	-1.51821E+01
2273	0.7	1.6590	-1.51803E+01
2273	0.7	1.6600	-1.51786E+01
2273	0.7	1.6610	-1.51768E+01
2273	0.7	1.6620	-1.51751E+01
2273	0.7	1.6630	-1.51734E+01
2273	0.7	1.6640	-1.51718E+01
2273	0.7	1.6650	-1.51701E+01
2273	0.7	1.6660	-1.51686E+01
2273	0.7	1.6670	-1.51670E+01
2273	0.7	1.6680	-1.51656E+01
2273	0.7	1.6690	-1.51641E+01
2273	0.7	1.6700	-1.51628E+01
2273	0.7	1.6710	-1.51614E+01
2273	0.7	1.6720	-1.51602E+01
2273	0.7	1.6730	-1.51589E+01
2273	0.7	1.6740	-1.51578E+01
2273	0.7	1.6750	-1.51567E+01
2273	0.7	1.6760	-1.51556E+01
2273	0.7	1.6770	-1.51546E+01
2273	0.7	1.6780	-1.51537E+01

2273	0.7	1.6790	-1.51528E+01
2273	0.7	1.6800	-1.51520E+01
2273	0.7	1.6810	-1.51512E+01
2273	0.7	1.6820	-1.51505E+01
2273	0.7	1.6830	-1.51498E+01
2273	0.7	1.6840	-1.51492E+01
2273	0.7	1.6850	-1.51487E+01
2273	0.7	1.6860	-1.51482E+01
2273	0.7	1.6870	-1.51477E+01
2273	0.7	1.6880	-1.51473E+01
2273	0.7	1.6890	-1.51469E+01
2273	0.7	1.6900	-1.51466E+01
2273	0.7	1.6910	-1.51464E+01
2273	0.7	1.6920	-1.51461E+01
2273	0.7	1.6930	-1.51460E+01
2273	0.7	1.6940	-1.51459E+01
2273	0.7	1.6950	-1.51458E+01
2273	0.7	1.6960	-1.51458E+01
2273	0.7	1.6970	-1.51458E+01
2273	0.7	1.6980	-1.51458E+01
2273	0.7	1.6990	-1.51459E+01
2273	0.7	1.7000	-1.51461E+01
2273	0.7	1.7010	-1.51462E+01
2273	0.7	1.7020	-1.51465E+01
2273	0.7	1.7030	-1.51467E+01
2273	0.7	1.7040	-1.51470E+01
2273	0.7	1.7050	-1.51474E+01
2273	0.7	1.7060	-1.51478E+01
2273	0.7	1.7070	-1.51482E+01
2273	0.7	1.7080	-1.51486E+01
2273	0.7	1.7090	-1.51491E+01
2273	0.7	1.7100	-1.51496E+01
2273	0.7	1.7110	-1.51502E+01
2273	0.7	1.7120	-1.51508E+01
2273	0.7	1.7130	-1.51514E+01
2273	0.7	1.7140	-1.51521E+01
2273	0.7	1.7150	-1.51528E+01
2273	0.7	1.7160	-1.51535E+01
2273	0.7	1.7170	-1.51543E+01
2273	0.7	1.7180	-1.51551E+01
2273	0.7	1.7190	-1.51559E+01
2273	0.7	1.7200	-1.51568E+01
2273	0.7	1.7210	-1.51576E+01
2273	0.7	1.7220	-1.51586E+01
2273	0.7	1.7230	-1.51595E+01
2273	0.7	1.7240	-1.51605E+01
2273	0.7	1.7250	-1.51615E+01
2273	0.7	1.7260	-1.51625E+01
2273	0.7	1.7270	-1.51636E+01
2273	0.7	1.7280	-1.51647E+01
2273	0.7	1.7290	-1.51658E+01
2273	0.7	1.7300	-1.51669E+01
2273	0.7	1.7310	-1.51681E+01
2273	0.7	1.7320	-1.51693E+01
2273	0.7	1.7330	-1.51705E+01
2273	0.7	1.7340	-1.51718E+01
2273	0.7	1.7350	-1.51730E+01
2273	0.7	1.7360	-1.51743E+01
2273	0.7	1.7370	-1.51756E+01
2273	0.7	1.7380	-1.51770E+01
2273	0.7	1.7390	-1.51784E+01
2273	0.7	1.7400	-1.51797E+01
2273	0.7	1.7410	-1.51812E+01
2273	0.7	1.7420	-1.51826E+01
2273	0.7	1.7430	-1.51841E+01
2273	0.7	1.7440	-1.51856E+01
2273	0.7	1.7450	-1.51871E+01
2273	0.7	1.7460	-1.51886E+01
2273	0.7	1.7470	-1.51901E+01
2273	0.7	1.7480	-1.51917E+01
2273	0.7	1.7490	-1.51933E+01
2273	0.7	1.7500	-1.51949E+01
2273	0.7	1.7510	-1.51966E+01
2273	0.7	1.7520	-1.51982E+01
2273	0.7	1.7530	-1.51999E+01
2273	0.7	1.7540	-1.52016E+01
2273	0.7	1.7550	-1.52033E+01
2273	0.7	1.7560	-1.52051E+01
2273	0.7	1.7570	-1.52068E+01
2273	0.7	1.7580	-1.52086E+01
2273	0.7	1.7590	-1.52104E+01
2273	0.7	1.7600	-1.52122E+01
2273	0.7	1.7610	-1.52140E+01
2273	0.7	1.7620	-1.52159E+01
2273	0.7	1.7630	-1.52178E+01
2273	0.7	1.7640	-1.52197E+01
2273	0.7	1.7650	-1.52216E+01
2273	0.7	1.7660	-1.52235E+01
2273	0.7	1.7670	-1.52255E+01
2273	0.7	1.7680	-1.52274E+01
2273	0.7	1.7690	-1.52294E+01
2273	0.7	1.7700	-1.52314E+01

2273	0.7	1.7710	-1.52334E+01
2273	0.7	1.7720	-1.52355E+01
2273	0.7	1.7730	-1.52375E+01
2273	0.7	1.7740	-1.52396E+01
2273	0.7	1.7750	-1.52417E+01
2273	0.7	1.7760	-1.52438E+01
2273	0.7	1.7770	-1.52459E+01
2273	0.7	1.7780	-1.52481E+01
2273	0.7	1.7790	-1.52502E+01
2273	0.7	1.7800	-1.52524E+01
2273	0.7	1.7810	-1.52546E+01
2273	0.7	1.7820	-1.52568E+01
2273	0.7	1.7830	-1.52590E+01
2273	0.7	1.7840	-1.52613E+01
2273	0.7	1.7850	-1.52635E+01
2273	0.7	1.7860	-1.52658E+01
2273	0.7	1.7870	-1.52681E+01
2273	0.7	1.7880	-1.52704E+01
2273	0.7	1.7890	-1.52727E+01
2273	0.7	1.7900	-1.52751E+01
2273	0.7	1.7910	-1.52774E+01
2273	0.7	1.7920	-1.52798E+01
2273	0.7	1.7930	-1.52822E+01
2273	0.7	1.7940	-1.52846E+01
2273	0.7	1.7950	-1.52870E+01
2273	0.7	1.7960	-1.52895E+01
2273	0.7	1.7970	-1.52919E+01
2273	0.7	1.7980	-1.52944E+01
2273	0.7	1.7990	-1.52969E+01
2273	0.7	1.8000	-1.52994E+01
2273	0.7	1.8010	-1.53019E+01
2273	0.7	1.8020	-1.53044E+01
2273	0.7	1.8030	-1.53070E+01
2273	0.7	1.8040	-1.53096E+01
2273	0.7	1.8050	-1.53121E+01
2273	0.7	1.8060	-1.53147E+01
2273	0.7	1.8070	-1.53174E+01
2273	0.7	1.8080	-1.53200E+01
2273	0.7	1.8090	-1.53227E+01
2273	0.7	1.8100	-1.53253E+01
2273	0.7	1.8110	-1.53280E+01
2273	0.7	1.8120	-1.53307E+01
2273	0.7	1.8130	-1.53334E+01
2273	0.7	1.8140	-1.53362E+01
2273	0.7	1.8150	-1.53389E+01
2273	0.7	1.8160	-1.53417E+01
2273	0.7	1.8170	-1.53445E+01
2273	0.7	1.8180	-1.53473E+01
2273	0.7	1.8190	-1.53501E+01
2273	0.7	1.8200	-1.53530E+01
2273	0.7	1.8210	-1.53558E+01
2273	0.7	1.8220	-1.53587E+01
2273	0.7	1.8230	-1.53616E+01
2273	0.7	1.8240	-1.53646E+01
2273	0.7	1.8250	-1.53675E+01
2273	0.7	1.8260	-1.53704E+01
2273	0.7	1.8270	-1.53734E+01
2273	0.7	1.8280	-1.53764E+01
2273	0.7	1.8290	-1.53794E+01
2273	0.7	1.8300	-1.53825E+01
2273	0.7	1.8310	-1.53855E+01
2273	0.7	1.8320	-1.53886E+01
2273	0.7	1.8330	-1.53917E+01
2273	0.7	1.8340	-1.53948E+01
2273	0.7	1.8350	-1.53980E+01
2273	0.7	1.8360	-1.54012E+01
2273	0.7		

2273	0.7	1.8630	-1.54966E+01
2273	0.7	1.8640	-1.55006E+01
2273	0.7	1.8650	-1.55047E+01
2273	0.7	1.8660	-1.55087E+01
2273	0.7	1.8670	-1.55128E+01
2273	0.7	1.8680	-1.55170E+01
2273	0.7	1.8690	-1.55211E+01
2273	0.7	1.8700	-1.55254E+01
2273	0.7	1.8710	-1.55296E+01
2273	0.7	1.8720	-1.55339E+01
2273	0.7	1.8730	-1.55383E+01
2273	0.7	1.8740	-1.55427E+01
2273	0.7	1.8750	-1.55471E+01
2273	0.7	1.8760	-1.55516E+01
2273	0.7	1.8770	-1.55562E+01
2273	0.7	1.8780	-1.55608E+01
2273	0.7	1.8790	-1.55654E+01
2273	0.7	1.8800	-1.55701E+01
2273	0.7	1.8810	-1.55748E+01
2273	0.7	1.8820	-1.55796E+01
2273	0.7	1.8830	-1.55845E+01
2273	0.7	1.8840	-1.55894E+01
2273	0.7	1.8850	-1.55943E+01
2273	0.7	1.8860	-1.55993E+01
2273	0.7	1.8870	-1.56044E+01
2273	0.7	1.8880	-1.56095E+01
2273	0.7	1.8890	-1.56146E+01
2273	0.7	1.8900	-1.56198E+01
2273	0.7	1.8910	-1.56251E+01
2273	0.7	1.8920	-1.56304E+01
2273	0.7	1.8930	-1.56358E+01
2273	0.7	1.8940	-1.56412E+01
2273	0.7	1.8950	-1.56467E+01
2273	0.7	1.8960	-1.56522E+01
2273	0.7	1.8970	-1.56577E+01
2273	0.7	1.8980	-1.56634E+01
2273	0.7	1.8990	-1.56690E+01
2273	0.7	1.9000	-1.56747E+01
2273	0.7	1.9010	-1.56805E+01
2273	0.7	1.9020	-1.56863E+01
2273	0.7	1.9030	-1.56921E+01
2273	0.7	1.9040	-1.56980E+01
2273	0.7	1.9050	-1.57039E+01
2273	0.7	1.9060	-1.57099E+01
2273	0.7	1.9070	-1.57158E+01
2273	0.7	1.9080	-1.57218E+01
2273	0.7	1.9090	-1.57279E+01
2273	0.7	1.9100	-1.57339E+01
2273	0.7	1.9110	-1.57400E+01
2273	0.7	1.9120	-1.57460E+01
2273	0.7	1.9130	-1.57521E+01
2273	0.7	1.9140	-1.57582E+01

2273	0.7	1.9150	-1.57642E+01
2273	0.7	1.9160	-1.57703E+01
2273	0.7	1.9170	-1.57763E+01
2273	0.7	1.9180	-1.57823E+01
2273	0.7	1.9190	-1.57883E+01
2273	0.7	1.9200	-1.57942E+01
2273	0.7	1.9210	-1.58001E+01
2273	0.7	1.9220	-1.58060E+01
2273	0.7	1.9230	-1.58117E+01
2273	0.7	1.9240	-1.58174E+01
2273	0.7	1.9250	-1.58231E+01
2273	0.7	1.9260	-1.58286E+01
2273	0.7	1.9270	-1.58341E+01
2273	0.7	1.9280	-1.58394E+01
2273	0.7	1.9290	-1.58446E+01
2273	0.7	1.9300	-1.58497E+01
2273	0.7	1.9310	-1.58547E+01
2273	0.7	1.9320	-1.58595E+01
2273	0.7	1.9330	-1.58642E+01
2273	0.7	1.9340	-1.58687E+01
2273	0.7	1.9350	-1.58730E+01
2273	0.7	1.9360	-1.58771E+01
2273	0.7	1.9370	-1.58811E+01
2273	0.7	1.9380	-1.58848E+01
2273	0.7	1.9390	-1.58884E+01
2273	0.7	1.9400	-1.58917E+01
2273	0.7	1.9410	-1.58947E+01
2273	0.7	1.9420	-1.58975E+01
2273	0.7	1.9430	-1.59001E+01
2273	0.7	1.9440	-1.59024E+01
2273	0.7	1.9450	-1.59045E+01
2273	0.7	1.9460	-1.59062E+01
2273	0.7	1.9470	-1.59077E+01
2273	0.7	1.9480	-1.59089E+01
2273	0.7	1.9490	-1.59098E+01
2273	0.7	1.9500	-1.59104E+01
2273	0.7	1.9510	-1.59107E+01
2273	0.7	1.9520	-1.59107E+01
2273	0.7	1.9530	-1.59104E+01
2273	0.7	1.9540	-1.59097E+01
2273	0.7	1.9550	-1.59088E+01
2273	0.7	1.9560	-1.59075E+01
2273	0.7	1.9570	-1.59058E+01
2273	0.7	1.9580	-1.59039E+01
2273	0.7	1.9590	-1.59016E+01
2273	0.7	1.9600	-1.58990E+01
2273	0.7	1.9610	-1.58961E+01
2273	0.7	1.9620	-1.58929E+01
2273	0.7	1.9630	-1.58893E+01
2273	0.7	1.9640	-1.58854E+01
2273	0.7	1.9650	-1.58812E+01
2273	0.7	1.9660	-1.58767E+01

2273	0.7	1.9670	-1.58719E+01
2273	0.7	1.9680	-1.58667E+01
2273	0.7	1.9690	-1.58613E+01
2273	0.7	1.9700	-1.58556E+01
2273	0.7	1.9710	-1.58495E+01
2273	0.7	1.9720	-1.58432E+01
2273	0.7	1.9730	-1.58366E+01
2273	0.7	1.9740	-1.58297E+01
2273	0.7	1.9750	-1.58225E+01
2273	0.7	1.9760	-1.58151E+01
2273	0.7	1.9770	-1.58074E+01
2273	0.7	1.9780	-1.57994E+01
2273	0.7	1.9790	-1.57911E+01
2273	0.7	1.9800	-1.57826E+01
2273	0.7	1.9810	-1.57739E+01
2273	0.7	1.9820	-1.57649E+01
2273	0.7	1.9830	-1.57557E+01
2273	0.7	1.9840	-1.57462E+01
2273	0.7	1.9850	-1.57365E+01
2273	0.7	1.9860	-1.57266E+01
2273	0.7	1.9870	-1.57164E+01
2273	0.7	1.9880	-1.57060E+01
2273	0.7	1.9890	-1.56954E+01
2273	0.7	1.9900	-1.56846E+01
2273	0.7	1.9910	-1.56735E+01
2273	0.7	1.9920	-1.56622E+01
2273	0.7	1.9930	-1.56506E+01
2273	0.7	1.9940	-1.56388E+01
2273	0.7	1.9950	-1.56267E+01
2273	0.7	1.9960	-1.56142E+01
2273	0.7	1.9970	-1.56014E+01
2273	0.7	1.9980	-1.55881E+01
2273	0.7	1.9990	-1.55742E+01
2273	0.7	2.0000	-1.55595E+01
2273	0.7	2.0010	-1.55440E+01
2273	0.7	2.0020	-1.55278E+01
2273	0.7	2.0030	-1.55109E+01
2273	0.7	2.0040	-1.54936E+01
2273	0.7	2.0050	-1.54759E+01
2273	0.7	2.0060	-1.54579E+01
2273	0.7	2.0070	-1.54396E+01
2273	0.7	2.0080	-1.54212E+01
2273	0.7	2.0090	-1.54025E+01
2273	0.7	2.0100	-1.53837E+01

A.2.8. $(U_{0.2}Pu_{0.8})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D _{Pu} (m ² /s)
1273	0.8	1.6100	-2.29149E+01
1273	0.8	1.6110	-2.29065E+01
1273	0.8	1.6120	-2.28985E+01
1273	0.8	1.6130	-2.28909E+01
1273	0.8	1.6140	-2.28837E+01
1273	0.8	1.6150	-2.28768E+01
1273	0.8	1.6160	-2.28703E+01
1273	0.8	1.6170	-2.28641E+01
1273	0.8	1.6180	-2.28582E+01
1273	0.8	1.6190	-2.28526E+01
1273	0.8	1.6200	-2.28473E+01
1273	0.8	1.6210	-2.28422E+01
1273	0.8	1.6220	-2.28374E+01
1273	0.8	1.6230	-2.28328E+01
1273	0.8	1.6240	-2.28285E+01
1273	0.8	1.6250	-2.28244E+01
1273	0.8	1.6260	-2.28204E+01
1273	0.8	1.6270	-2.28167E+01
1273	0.8	1.6280	-2.28132E+01
1273	0.8	1.6290	-2.28098E+01
1273	0.8	1.6300	-2.28066E+01
1273	0.8	1.6310	-2.28036E+01
1273	0.8	1.6320	-2.28008E+01
1273	0.8	1.6330	-2.27981E+01
1273	0.8	1.6340	-2.27956E+01
1273	0.8	1.6350	-2.27932E+01
1273	0.8	1.6360	-2.27909E+01
1273	0.8	1.6370	-2.27888E+01
1273	0.8	1.6380	-2.27869E+01
1273	0.8	1.6390	-2.27850E+01
1273	0.8	1.6400	-2.27833E+01

1273	0.8	1.6410	-2.27817E+01
1273	0.8	1.6420	-2.27802E+01
1273	0.8	1.6430	-2.27788E+01
1273	0.8	1.6440	-2.27775E+01
1273	0.8	1.6450	-2.27763E+01
1273	0.8	1.6460	-2.27753E+01
1273	0.8	1.6470	-2.27743E+01
1273	0.8	1.6480	-2.27734E+01
1273	0.8	1.6490	-2.27726E+01
1273	0.8	1.6500	-2.27719E+01
1273	0.8	1.6510	-2.27713E+01
1273	0.8	1.6520	-2.27708E+01
1273	0.8	1.6530	-2.27704E+01
1273	0.8	1.6540	-2.27700E+01
1273	0.8	1.6550	-2.27697E+01
1273	0.8	1.6560	-2.27695E+01
1273	0.8	1.6570	-2.27694E+01
1273	0.8	1.6580	-2.27694E+01
1273	0.8	1.6590	-2.27694E+01
1273	0.8	1.6600	-2.27695E+01
1273	0.8	1.6610	-2.27696E+01
1273	0.8	1.6620	-2.27698E+01
1273	0.8	1.6630	-2.27701E+01
1273	0.8	1.6640	-2.27705E+01
1273	0.8	1.6650	-2.27709E+01
1273	0.8	1.6660	-2.27714E+01
1273	0.8	1.6670	-2.27719E+01
1273	0.8	1.6680	-2.27725E+01
1273	0.8	1.6690	-2.27731E+01
1273	0.8	1.6700	-2.27738E+01
1273	0.8	1.6710	-2.27745E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D _{Pu} (m ² /s)
1273	0.8	1.6740	-2.27771E+01
1273	0.8	1.6750	-2.27778E+01
1273	0.8	1.6760	-2.27790E+01
1273	0.8	1.6770	-2.27801E+01
1273	0.8	1.6780	-2.27812E+01
1273	0.8	1.6790	-2.27823E+01
1273	0.8	1.6800	-2.27835E+01
1273	0.8	1.6810	-2.27847E+01
1273	0.8	1.6820	-2.27860E+01
1273	0.8	1.6830	-2.27873E+01
1273	0.8	1.6840	-2.27886E+01
1273	0.8	1.6850	-2.27900E+01
1273	0.8	1.6860	-2.27914E+01
1273	0.8	1.6870	-2.27929E+01
1273	0.8	1.6880	-2.27944E+01
1273	0.8	1.6890	-2.27959E+01
1273	0.8	1.6900	-2.27975E+01
1273	0.8	1.6910	-2.27991E+01
1273	0.8	1.6920	-2.28008E+01
1273	0.8	1.6930	-2.28024E+01
1273	0.8	1.6940	-2.28042E+01
1273	0.8	1.6950	-2.28059E+01
1273	0.8	1.6960	-2.28077E+01
1273	0.8	1.6970	-2.28095E+01
1273	0.8	1.6980	-2.28113E+01
1273	0.8	1.6990	-2.28132E+01
1273	0.8	1.7000	-2.28151E+01
1273	0.8	1.7010	-2.28170E+01
1273	0.8	1.7020	-2.28190E+01
1273	0.8	1.7030	-2.28210E+01
1273	0.8	1.7040	-2.28230E+01
1273	0.8	1.7050	-2.28250E+01
1273	0.8	1.7060	-2.28271E+01
12			

1273	0.8	1.7090	-2.28334E+01
1273	0.8	1.7100	-2.28356E+01
1273	0.8	1.7110	-2.28378E+01
1273	0.8	1.7120	-2.28400E+01
1273	0.8	1.7130	-2.28423E+01
1273	0.8	1.7140	-2.28445E+01
1273	0.8	1.7150	-2.28468E+01
1273	0.8	1.7160	-2.28491E+01
1273	0.8	1.7170	-2.28515E+01
1273	0.8	1.7180	-2.28538E+01
1273	0.8	1.7190	-2.28562E+01
1273	0.8	1.7200	-2.28586E+01
1273	0.8	1.7210	-2.28610E+01
1273	0.8	1.7220	-2.28635E+01
1273	0.8	1.7230	-2.28659E+01
1273	0.8	1.7240	-2.28684E+01
1273	0.8	1.7250	-2.28709E+01
1273	0.8	1.7260	-2.28734E+01
1273	0.8	1.7270	-2.28760E+01
1273	0.8	1.7280	-2.28785E+01
1273	0.8	1.7290	-2.28811E+01
1273	0.8	1.7300	-2.28837E+01
1273	0.8	1.7310	-2.28863E+01
1273	0.8	1.7320	-2.28889E+01
1273	0.8	1.7330	-2.28916E+01
1273	0.8	1.7340	-2.28943E+01
1273	0.8	1.7350	-2.28969E+01
1273	0.8	1.7360	-2.28996E+01
1273	0.8	1.7370	-2.29024E+01
1273	0.8	1.7380	-2.29051E+01
1273	0.8	1.7390	-2.29078E+01
1273	0.8	1.7400	-2.29106E+01
1273	0.8	1.7410	-2.29134E+01
1273	0.8	1.7420	-2.29162E+01
1273	0.8	1.7430	-2.29190E+01
1273	0.8	1.7440	-2.29218E+01
1273	0.8	1.7450	-2.29246E+01
1273	0.8	1.7460	-2.29275E+01
1273	0.8	1.7470	-2.29304E+01
1273	0.8	1.7480	-2.29332E+01
1273	0.8	1.7490	-2.29361E+01
1273	0.8	1.7500	-2.29390E+01
1273	0.8	1.7510	-2.29420E+01
1273	0.8	1.7520	-2.29449E+01
1273	0.8	1.7530	-2.29478E+01
1273	0.8	1.7540	-2.29508E+01
1273	0.8	1.7550	-2.29538E+01
1273	0.8	1.7560	-2.29568E+01
1273	0.8	1.7570	-2.29598E+01
1273	0.8	1.7580	-2.29628E+01
1273	0.8	1.7590	-2.29658E+01
1273	0.8	1.7600	-2.29688E+01
1273	0.8	1.7610	-2.29719E+01
1273	0.8	1.7620	-2.29749E+01
1273	0.8	1.7630	-2.29780E+01
1273	0.8	1.7640	-2.29811E+01
1273	0.8	1.7650	-2.29842E+01
1273	0.8	1.7660	-2.29873E+01
1273	0.8	1.7670	-2.29904E+01
1273	0.8	1.7680	-2.29935E+01
1273	0.8	1.7690	-2.29967E+01
1273	0.8	1.7700	-2.29998E+01
1273	0.8	1.7710	-2.30030E+01
1273	0.8	1.7720	-2.30061E+01
1273	0.8	1.7730	-2.30093E+01
1273	0.8	1.7740	-2.30125E+01
1273	0.8	1.7750	-2.30157E+01
1273	0.8	1.7760	-2.30189E+01
1273	0.8	1.7770	-2.30221E+01
1273	0.8	1.7780	-2.30254E+01
1273	0.8	1.7790	-2.30286E+01
1273	0.8	1.7800	-2.30318E+01
1273	0.8	1.7810	-2.30351E+01
1273	0.8	1.7820	-2.30384E+01
1273	0.8	1.7830	-2.30416E+01
1273	0.8	1.7840	-2.30449E+01
1273	0.8	1.7850	-2.30482E+01
1273	0.8	1.7860	-2.30515E+01
1273	0.8	1.7870	-2.30548E+01
1273	0.8	1.7880	-2.30582E+01
1273	0.8	1.7890	-2.30615E+01
1273	0.8	1.7900	-2.30648E+01
1273	0.8	1.7910	-2.30682E+01
1273	0.8	1.7920	-2.30716E+01
1273	0.8	1.7930	-2.30749E+01
1273	0.8	1.7940	-2.30783E+01
1273	0.8	1.7950	-2.30817E+01
1273	0.8	1.7960	-2.30851E+01
1273	0.8	1.7970	-2.30885E+01
1273	0.8	1.7980	-2.30919E+01
1273	0.8	1.7990	-2.30953E+01
1273	0.8	1.8000	-2.30988E+01

1273	0.8	1.8010	-2.31022E+01
1273	0.8	1.8020	-2.31056E+01
1273	0.8	1.8030	-2.31091E+01
1273	0.8	1.8040	-2.31126E+01
1273	0.8	1.8050	-2.31160E+01
1273	0.8	1.8060	-2.31195E+01
1273	0.8	1.8070	-2.31230E+01
1273	0.8	1.8080	-2.31265E+01
1273	0.8	1.8090	-2.31300E+01
1273	0.8	1.8100	-2.31335E+01
1273	0.8	1.8110	-2.31371E+01
1273	0.8	1.8120	-2.31406E+01
1273	0.8	1.8130	-2.31441E+01
1273	0.8	1.8140	-2.31477E+01
1273	0.8	1.8150	-2.31513E+01
1273	0.8	1.8160	-2.31548E+01
1273	0.8	1.8170	-2.31584E+01
1273	0.8	1.8180	-2.31620E+01
1273	0.8	1.8190	-2.31656E+01
1273	0.8	1.8200	-2.31692E+01
1273	0.8	1.8210	-2.31728E+01
1273	0.8	1.8220	-2.31765E+01
1273	0.8	1.8230	-2.31801E+01
1273	0.8	1.8240	-2.31837E+01
1273	0.8	1.8250	-2.31874E+01
1273	0.8	1.8260	-2.31910E+01
1273	0.8	1.8270	-2.31947E+01
1273	0.8	1.8280	-2.31984E+01
1273	0.8	1.8290	-2.32021E+01
1273	0.8	1.8300	-2.32058E+01
1273	0.8	1.8310	-2.32095E+01
1273	0.8	1.8320	-2.32132E+01
1273	0.8	1.8330	-2.32170E+01
1273	0.8	1.8340	-2.32207E+01
1273	0.8	1.8350	-2.32245E+01
1273	0.8	1.8360	-2.32282E+01
1273	0.8	1.8370	-2.32320E+01
1273	0.8	1.8380	-2.32358E+01
1273	0.8	1.8390	-2.32396E+01
1273	0.8	1.8400	-2.32434E+01
1273	0.8	1.8410	-2.32472E+01
1273	0.8	1.8420	-2.32510E+01
1273	0.8	1.8430	-2.32549E+01
1273	0.8	1.8440	-2.32587E+01
1273	0.8	1.8450	-2.32626E+01
1273	0.8	1.8460	-2.32665E+01
1273	0.8	1.8470	-2.32704E+01
1273	0.8	1.8480	-2.32743E+01
1273	0.8	1.8490	-2.32782E+01
1273	0.8	1.8500	-2.32821E+01
1273	0.8	1.8510	-2.32861E+01
1273	0.8	1.8520	-2.32900E+01
1273	0.8	1.8530	-2.32940E+01
1273	0.8	1.8540	-2.32980E+01
1273	0.8	1.8550	-2.33019E+01
1273	0.8	1.8560	-2.33060E+01
1273	0.8	1.8570	-2.33100E+01
1273	0.8	1.8580	-2.33140E+01
1273	0.8	1.8590	-2.33181E+01
1273	0.8	1.8600	-2.33221E+01
1273	0.8	1.8610	-2.33262E+01
1273	0.8	1.8620	-2.33303E+01
1273	0.8	1.8630	-2.33344E+01
1273	0.8	1.8640	-2.33386E+01
1273	0.8	1.8650	-2.33427E+01
1273	0.8	1.8660	-2.33469E+01
1273	0.8	1.8670	-2.33511E+01
1273	0.8	1.8680	-2.33553E+01
1273	0.8	1.8690	-2.33595E+01
1273	0.8	1.8700	-2.33638E+01
1273	0.8	1.8710	-2.33680E+01
1273	0.8	1.8720	-2.33723E+01
1273	0.8	1.8730	-2.33766E+01
1273	0.8	1.8740	-2.33809E+01
1273	0.8	1.8750	-2.33853E+01
1273	0.8	1.8760	-2.33896E+01
1273	0.8	1.8770	-2.33940E+01
1273	0.8	1.8780	-2.33984E+01
1273	0.8	1.8790	-2.34029E+01
1273	0.8	1.8800	-2.34073E+01
1273	0.8	1.8810	-2.34118E+01
1273	0.8	1.8820	-2.34163E+01
1273	0.8	1.8830	-2.34209E+01
1273	0.8	1.8840	-2.34254E+01
1273	0.8	1.8850	-2.34300E+01
1273	0.8	1.8860	-2.34347E+01
1273	0.8	1.8870	-2.34393E+01
1273	0.8	1.8880	-2.34440E+01
1273	0.8	1.8890	-2.34487E+01
1273	0.8	1.8900	-2.34535E+01
1273	0.8	1.8910	-2.34583E+01
1273	0.8	1.8920	-2.34631E+01

1273	0.8	1.8930	-2.34679E+01
1273	0.8	1.8940	-2.34728E+01
1273	0.8	1.8950	-2.34778E+01
1273	0.8	1.8960	-2.34828E+01
1273	0.8	1.8970	-2.34878E+01
1273	0.8	1.8980	-2.34928E+01
1273	0.8	1.8990	-2.34979E+01
1273	0.8	1.9000	-2.35031E+01
1273	0.8	1.9010	-2.35083E+01
1273	0.8	1.9020	-2.35136E+01
1273	0.8	1.9030	-2.35189E+01
1273	0.8	1.9040	-2.35242E+01
1273	0.8	1.9050	-2.35296E+01
1273	0.8	1.9060	-2.35351E+01
1273	0.8	1.9070	-2.35407E+01
1273	0.8	1.9080	-2.35463E+01
1273	0.8	1.9090	-2.35519E+01
1273	0.8	1.9100	-2.35577E+01
1273	0.8	1.9110	-2.35635E+01
1273	0.8	1.9120	-2.35694E+01
1273	0.8	1.9130	-2.35753E+01
1273	0.8	1.9140	-2.35814E+01
1273	0.8	1.9150	-2.35875E+01
1273	0.8	1.9160	-2.35937E+01
1273	0.8	1.9170	-2.36000E+01
1273	0.8	1.9180	-2.36064E+01
1273	0.8	1.9190	-2.36129E+01
1273	0.8	1.9200	-2.36195E+01
1273	0.8	1.9210	-2.36262E+01
1273	0.8	1.9220	-2.36330E+01
1273	0.8	1.9230	-2.36399E+01
1273	0.8	1.9240	-2.36469E+01
1273	0.8	1.9250	-2.36540E+01
1273	0.8	1.9260	-2.36613E+01
1273	0.8	1.9270	-2.36687E+01
1273	0.8	1.9280	-2.36762E+01
1273	0.8	1.9290	-2.36838E+01
1273	0.8	1.9300	-2.36915E+01
1273	0.8	1.9310	-2.36994E+01
1273	0.8	1.9320	-2.37074E+01
1273	0.8	1.9330	-2.37155E+01
1273	0.8	1.9340	-2.37238E+01
1273	0.8	1.9350	-2.37321E+01
1273	0.8	1.9360	-2.37406E+01
1273	0.8	1.9370	-2.37492E+01
1273	0.8	1.9380	-2.37579E+01
1273	0.8	1.9390	-2.37667E+01
1273	0.8	1.9400	-2.37756E+01
1273	0.8	1.9410	-2.37845E+01
1273	0.8	1.9420	-2.37936E+01
1273	0.8	1.9430	-2.38026E+01
1273	0.8	1.9440	-2.38118E+01
1273	0.8	1.9450	-2.38209E+01
1273	0.8	1.9460	-2.38300E+01
1273	0.8	1.9470	-2.38392E+01
1273	0.8	1.9480	-2.38484E+01
1273	0.8	1.9490	-2.38572E+01
1273	0.8	1.9500	-2.38661E+01
1273	0.8	1.9510	-2.38749E+01
1273	0.8	1.9520	-2.38835E+01
1273	0.8	1.9530	-2.38919E+01
1273	0.8	1.9540	-2.39000E+01
1273	0.8	1.9550	-2.39079E+01
1273	0.8	1.9560	-2.39155E+01
1273	0.8	1.9570	-2.39227E+01
1273	0.8	1.9580	-2.39295E+01
1273	0.8		

1273	0.8	1.9850	-2.38496E+01
1273	0.8	1.9860	-2.38356E+01
1273	0.8	1.9870	-2.38209E+01
1273	0.8	1.9880	-2.38055E+01
1273	0.8	1.9890	-2.37896E+01
1273	0.8	1.9900	-2.37730E+01
1273	0.8	1.9910	-2.37558E+01
1273	0.8	1.9920	-2.37381E+01
1273	0.8	1.9930	-2.37198E+01
1273	0.8	1.9940	-2.37010E+01
1273	0.8	1.9950	-2.36816E+01
1273	0.8	1.9960	-2.36618E+01
1273	0.8	1.9970	-2.36415E+01
1273	0.8	1.9980	-2.36207E+01
1273	0.8	1.9990	-2.35994E+01
1273	0.8	2.0000	-2.35776E+01
1273	0.8	2.0010	-2.35478E+01
1273	0.8	2.0020	-2.35175E+01
1273	0.8	2.0030	-2.34869E+01
1273	0.8	2.0040	-2.34558E+01
1273	0.8	2.0050	-2.34244E+01
1273	0.8	2.0060	-2.33927E+01
1273	0.8	2.0070	-2.33606E+01
1273	0.8	2.0080	-2.33283E+01
1273	0.8	2.0090	-2.32956E+01
1273	0.8	2.0100	-2.32626E+01
1273	0.8	2.0110	-2.32293E+01
1273	0.8	2.0120	-2.31957E+01
1273	0.8	2.0130	-2.31618E+01
1273	0.8	2.0140	-2.31277E+01
1273	0.8	2.0150	-2.30933E+01
1273	0.8	2.0160	-2.30586E+01
1273	0.8	2.0170	-2.30236E+01
1273	0.8	2.0180	-2.29884E+01
1273	0.8	2.0190	-2.29529E+01
1273	0.8	2.0200	-2.29172E+01
1273	0.8	2.0210	-2.28812E+01
1273	0.8	2.0220	-2.28449E+01
1273	0.8	2.0230	-2.28083E+01
1273	0.8	2.0240	-2.27715E+01
1273	0.8	2.0250	-2.27345E+01
1273	0.8	2.0260	-2.26971E+01
1273	0.8	2.0270	-2.26595E+01
1273	0.8	2.0280	-2.26217E+01
1273	0.8	2.0290	-2.25835E+01
1273	0.8	2.0300	-2.25451E+01
1273	0.8	2.0310	-2.25064E+01
1273	0.8	2.0320	-2.24674E+01
1273	0.8	2.0330	-2.24282E+01
1273	0.8	2.0340	-2.23887E+01
1273	0.8	2.0350	-2.23489E+01
1273	0.8	2.0360	-2.23088E+01
1273	0.8	2.0370	-2.22684E+01
1273	0.8	2.0380	-2.22278E+01
1273	0.8	2.0390	-2.21868E+01
1273	0.8	2.0400	-2.21455E+01
1273	0.8	2.0410	-2.21040E+01
1273	0.8	2.0420	-2.20621E+01
1273	0.8	2.0430	-2.20200E+01
1273	0.8	2.0440	-2.19775E+01
1273	0.8	2.0450	-2.19348E+01
1273	0.8	2.0460	-2.18917E+01
1273	0.8	2.0470	-2.18483E+01
1273	0.8	2.0480	-2.18046E+01
1273	0.8	2.0490	-2.17606E+01
1273	0.8	2.0500	-2.17163E+01
1273	0.8	2.0510	-2.16717E+01
1273	0.8	2.0520	-2.16268E+01
1273	0.8	2.0530	-2.15815E+01
1273	0.8	2.0540	-2.15360E+01
1273	0.8	2.0550	-2.14901E+01
1273	0.8	2.0560	-2.14439E+01
1273	0.8	2.0570	-2.13975E+01
1273	0.8	2.0580	-2.13507E+01
1273	0.8	2.0590	-2.13036E+01
1273	0.8	2.0600	-2.12562E+01
1273	0.8	2.0610	-2.12086E+01
1273	0.8	2.0620	-2.11607E+01
1273	0.8	2.0630	-2.11124E+01
1273	0.8	2.0640	-2.10640E+01
1273	0.8	2.0650	-2.10152E+01
1273	0.8	2.0660	-2.09662E+01
1273	0.8	2.0670	-2.09170E+01
1273	0.8	2.0680	-2.08675E+01
1273	0.8	2.0690	-2.08177E+01
1273	0.8	2.0700	-2.07678E+01
1273	0.8	2.0710	-2.07176E+01
1273	0.8	2.0720	-2.06673E+01
1273	0.8	2.0730	-2.06167E+01
1273	0.8	2.0740	-2.05660E+01
1273	0.8	2.0750	-2.05151E+01
1273	0.8	2.0760	-2.04640E+01

1273	0.8	2.0770	-2.04127E+01
1273	0.8	2.0780	-2.03614E+01
1273	0.8	2.0790	-2.03098E+01
1273	0.8	2.0800	-2.02582E+01
1273	0.8	1.6100	-1.78799E+01
1273	0.8	1.6110	-1.78749E+01
1273	0.8	1.6120	-1.78701E+01
1273	0.8	1.6130	-1.78653E+01
1273	0.8	1.6140	-1.78608E+01
1273	0.8	1.6150	-1.78564E+01
1273	0.8	1.6160	-1.78521E+01
1273	0.8	1.6170	-1.78480E+01
1273	0.8	1.6180	-1.78440E+01
1273	0.8	1.6190	-1.78402E+01
1273	0.8	1.6200	-1.78365E+01
1273	0.8	1.6210	-1.78329E+01
1273	0.8	1.6220	-1.78294E+01
1273	0.8	1.6230	-1.78261E+01
1273	0.8	1.6240	-1.78229E+01
1273	0.8	1.6250	-1.78198E+01
1273	0.8	1.6260	-1.78168E+01
1273	0.8	1.6270	-1.78139E+01
1273	0.8	1.6280	-1.78111E+01
1273	0.8	1.6290	-1.78084E+01
1273	0.8	1.6300	-1.78058E+01
1273	0.8	1.6310	-1.78034E+01
1273	0.8	1.6320	-1.78010E+01
1273	0.8	1.6330	-1.77987E+01
1273	0.8	1.6340	-1.77965E+01
1273	0.8	1.6350	-1.77944E+01
1273	0.8	1.6360	-1.77923E+01
1273	0.8	1.6370	-1.77904E+01
1273	0.8	1.6380	-1.77885E+01
1273	0.8	1.6390	-1.77867E+01
1273	0.8	1.6400	-1.77850E+01
1273	0.8	1.6410	-1.77834E+01
1273	0.8	1.6420	-1.77818E+01
1273	0.8	1.6430	-1.77803E+01
1273	0.8	1.6440	-1.77789E+01
1273	0.8	1.6450	-1.77775E+01
1273	0.8	1.6460	-1.77763E+01
1273	0.8	1.6470	-1.77750E+01
1273	0.8	1.6480	-1.77739E+01
1273	0.8	1.6490	-1.77728E+01
1273	0.8	1.6500	-1.77717E+01
1273	0.8	1.6510	-1.77708E+01
1273	0.8	1.6520	-1.77698E+01
1273	0.8	1.6530	-1.77690E+01
1273	0.8	1.6540	-1.77682E+01
1273	0.8	1.6550	-1.77674E+01
1273	0.8	1.6560	-1.77667E+01
1273	0.8	1.6570	-1.77661E+01
1273	0.8	1.6580	-1.77655E+01
1273	0.8	1.6590	-1.77650E+01
1273	0.8	1.6600	-1.77645E+01
1273	0.8	1.6610	-1.77640E+01
1273	0.8	1.6620	-1.77636E+01
1273	0.8	1.6630	-1.77633E+01
1273	0.8	1.6640	-1.77630E+01
1273	0.8	1.6650	-1.77627E+01
1273	0.8	1.6660	-1.77625E+01
1273	0.8	1.6670	-1.77623E+01
1273	0.8	1.6680	-1.77622E+01
1273	0.8	1.6690	-1.77621E+01
1273	0.8	1.6700	-1.77621E+01
1273	0.8	1.6710	-1.77621E+01
1273	0.8	1.6720	-1.77621E+01
1273	0.8	1.6730	-1.77622E+01
1273	0.8	1.6740	-1.77623E+01
1273	0.8	1.6750	-1.77625E+01
1273	0.8	1.6760	-1.77627E+01
1273	0.8	1.6770	-1.77629E+01
1273	0.8	1.6780	-1.77632E+01
1273	0.8	1.6790	-1.77635E+01
1273	0.8	1.6800	-1.77638E+01
1273	0.8	1.6810	-1.77642E+01
1273	0.8	1.6820	-1.77646E+01
1273	0.8	1.6830	-1.77650E+01
1273	0.8	1.6840	-1.77655E+01
1273	0.8	1.6850	-1.77660E+01
1273	0.8	1.6860	-1.77665E+01
1273	0.8	1.6870	-1.77671E+01
1273	0.8	1.6880	-1.77676E+01
1273	0.8	1.6890	-1.77683E+01
1273	0.8	1.6900	-1.77689E+01
1273	0.8	1.6910	-1.77696E+01
1273	0.8	1.6920	-1.77703E+01
1273	0.8	1.6930	-1.77711E+01
1273	0.8	1.6940	-1.77718E+01
1273	0.8	1.6950	-1.77726E+01
1273	0.8	1.6960	-1.77735E+01
1273	0.8	1.6970	-1.77743E+01

1773	0.8	1.6980	-1.77752E+01
1773	0.8	1.6990	-1.77761E+01
1773	0.8	1.7000	-1.77770E+01
1773	0.8	1.7010	-1.77780E+01
1773	0.8	1.7020	-1.77790E+01
1773	0.8	1.7030	-1.77800E+01
1773	0.8	1.7040	-1.77810E+01
1773	0.8	1.7050	-1.77821E+01
1773	0.8	1.7060	-1.77832E+01
1773	0.8	1.7070	-1.77843E+01
1773	0.8	1.7080	-1.77854E+01
1773	0.8	1.7090	-1.77866E+01
1773	0.8	1.7100	-1.77877E+01
1773	0.8	1.7110	-1.77889E+01
1773	0.8	1.7120	-1.77902E+01
1773	0.8	1.7130	-1.77914E+01
1773	0.8	1.7140	-1.77927E+01
1773	0.8	1.7150	-1.77940E+01
1773	0.8	1.7160	-1.77953E+01
1773	0.8	1.7170	-1.77966E+01
1773	0.8	1.7180	-1.77980E+01
1773	0.8	1.7190	-1.77993E+01
1773	0.8	1.7200	-1.78007E+01
1773	0.8	1.7210	-1.78021E+01
1773	0.8	1.7220	-1.78036E+01
1773	0.8	1.7230	-1.78050E+01
1773	0.8	1.7240	-1.78065E+01
1773	0.8	1.7250	-1.78080E+01
1773	0.8	1.7260	-1.78095E+01
1773	0.8	1.7270	-1.78110E+01
1773	0.8	1.7280	-1.78126E+01
1773	0.8	1.7290	-1.78142E+01
1773	0.8	1.7300	-1.78158E+01
1773	0.8	1.7310	-1.78174E+01
1773	0.8	1.7320	-1.78190E+01
1773	0.8	1.7330	-1.78206E+01
1773	0.8	1.7340	-1.78223E+01
1773	0.8	1.7350	-1.78240E+01
1773	0.8	1.7360	-1.78257E+01
1773	0.8	1.7370	-1.78274E+01
1773	0.8	1.7380	-1.78291E+01
1773	0.8	1.7390	-1.78309E+01
1773	0.8	1.7400	-1.78327E+01
1773	0.8	1.7410	-1.78344E+01
1773	0.8	1.7420	-1.78362E+01
1773	0.8	1.7430	-1.78381E+01
1773	0.8	1.7440	-1.78399E+01
1773	0.8	1.7450	-1.78417E+01
1773	0.8	1.7460	-1.78436E+01
1773	0.8	1.7470	-1.78455E+01
1773	0.8	1.7480	-1.78474E+01
1773	0.8	1.7490	-1.78493E+01
1773	0.8	1.7500	-1.78512E+01
1773	0.8	1.7510	-1.78532E+01
1773	0.8	1.7520	-1.78552E+01
1773	0.8	1.7530	-1.78571E+01
1773	0.8	1.7540	-1.78591E+01
1773	0.8	1.7550	-1.78611E+01
1773	0.8	1.7560	-1.78632E+01
1773	0.8	1.7570	-1.78652E+01
1773	0.8	1.7580	-1.78672E+01
1773	0.8	1.7590	-1.78693E+01
1773	0.8	1.7600	-1.78714E+01
1773	0.8	1.7610	-1.78735E+01
1773	0.8	1.7620	-1.78756E+01
1773	0.8	1.7630	-1.78777E+01
1773	0.8		

1773	0.8	1.7900	-1.79404E+01
1773	0.8	1.7910	-1.79429E+01
1773	0.8	1.7920	-1.79454E+01
1773	0.8	1.7930	-1.79480E+01
1773	0.8	1.7940	-1.79505E+01
1773	0.8	1.7950	-1.79531E+01
1773	0.8	1.7960	-1.79556E+01
1773	0.8	1.7970	-1.79582E+01
1773	0.8	1.7980	-1.79608E+01
1773	0.8	1.7990	-1.79634E+01
1773	0.8	1.8000	-1.79661E+01
1773	0.8	1.8010	-1.79687E+01
1773	0.8	1.8020	-1.79713E+01
1773	0.8	1.8030	-1.79740E+01
1773	0.8	1.8040	-1.79767E+01
1773	0.8	1.8050	-1.79794E+01
1773	0.8	1.8060	-1.79821E+01
1773	0.8	1.8070	-1.79848E+01
1773	0.8	1.8080	-1.79875E+01
1773	0.8	1.8090	-1.79903E+01
1773	0.8	1.8100	-1.79930E+01
1773	0.8	1.8110	-1.79958E+01
1773	0.8	1.8120	-1.79986E+01
1773	0.8	1.8130	-1.80014E+01
1773	0.8	1.8140	-1.80042E+01
1773	0.8	1.8150	-1.80070E+01
1773	0.8	1.8160	-1.80098E+01
1773	0.8	1.8170	-1.80127E+01
1773	0.8	1.8180	-1.80155E+01
1773	0.8	1.8190	-1.80184E+01
1773	0.8	1.8200	-1.80213E+01
1773	0.8	1.8210	-1.80242E+01
1773	0.8	1.8220	-1.80271E+01
1773	0.8	1.8230	-1.80300E+01
1773	0.8	1.8240	-1.80330E+01
1773	0.8	1.8250	-1.80359E+01
1773	0.8	1.8260	-1.80389E+01
1773	0.8	1.8270	-1.80419E+01
1773	0.8	1.8280	-1.80449E+01
1773	0.8	1.8290	-1.80479E+01
1773	0.8	1.8300	-1.80509E+01
1773	0.8	1.8310	-1.80540E+01
1773	0.8	1.8320	-1.80570E+01
1773	0.8	1.8330	-1.80601E+01
1773	0.8	1.8340	-1.80632E+01
1773	0.8	1.8350	-1.80663E+01
1773	0.8	1.8360	-1.80694E+01
1773	0.8	1.8370	-1.80725E+01
1773	0.8	1.8380	-1.80756E+01
1773	0.8	1.8390	-1.80788E+01
1773	0.8	1.8400	-1.80820E+01
1773	0.8	1.8410	-1.80852E+01
1773	0.8	1.8420	-1.80884E+01
1773	0.8	1.8430	-1.80916E+01
1773	0.8	1.8440	-1.80948E+01
1773	0.8	1.8450	-1.80981E+01
1773	0.8	1.8460	-1.81013E+01
1773	0.8	1.8470	-1.81046E+01
1773	0.8	1.8480	-1.81079E+01
1773	0.8	1.8490	-1.81112E+01
1773	0.8	1.8500	-1.81146E+01
1773	0.8	1.8510	-1.81179E+01
1773	0.8	1.8520	-1.81213E+01
1773	0.8	1.8530	-1.81247E+01
1773	0.8	1.8540	-1.81281E+01
1773	0.8	1.8550	-1.81315E+01
1773	0.8	1.8560	-1.81349E+01
1773	0.8	1.8570	-1.81384E+01
1773	0.8	1.8580	-1.81419E+01
1773	0.8	1.8590	-1.81454E+01
1773	0.8	1.8600	-1.81489E+01
1773	0.8	1.8610	-1.81524E+01
1773	0.8	1.8620	-1.81560E+01
1773	0.8	1.8630	-1.81596E+01
1773	0.8	1.8640	-1.81631E+01
1773	0.8	1.8650	-1.81668E+01
1773	0.8	1.8660	-1.81704E+01
1773	0.8	1.8670	-1.81741E+01
1773	0.8	1.8680	-1.81777E+01
1773	0.8	1.8690	-1.81814E+01
1773	0.8	1.8700	-1.81852E+01
1773	0.8	1.8710	-1.81889E+01
1773	0.8	1.8720	-1.81927E+01
1773	0.8	1.8730	-1.81965E+01
1773	0.8	1.8740	-1.82003E+01
1773	0.8	1.8750	-1.82041E+01
1773	0.8	1.8760	-1.82080E+01
1773	0.8	1.8770	-1.82119E+01
1773	0.8	1.8780	-1.82158E+01
1773	0.8	1.8790	-1.82197E+01
1773	0.8	1.8800	-1.82237E+01
1773	0.8	1.8810	-1.82277E+01

1773	0.8	1.8820	-1.82317E+01
1773	0.8	1.8830	-1.82357E+01
1773	0.8	1.8840	-1.82398E+01
1773	0.8	1.8850	-1.82439E+01
1773	0.8	1.8860	-1.82480E+01
1773	0.8	1.8870	-1.82522E+01
1773	0.8	1.8880	-1.82563E+01
1773	0.8	1.8890	-1.82605E+01
1773	0.8	1.8900	-1.82648E+01
1773	0.8	1.8910	-1.82691E+01
1773	0.8	1.8920	-1.82733E+01
1773	0.8	1.8930	-1.82777E+01
1773	0.8	1.8940	-1.82820E+01
1773	0.8	1.8950	-1.82864E+01
1773	0.8	1.8960	-1.82908E+01
1773	0.8	1.8970	-1.82953E+01
1773	0.8	1.8980	-1.82997E+01
1773	0.8	1.8990	-1.83042E+01
1773	0.8	1.9000	-1.83087E+01
1773	0.8	1.9010	-1.83133E+01
1773	0.8	1.9020	-1.83179E+01
1773	0.8	1.9030	-1.83225E+01
1773	0.8	1.9040	-1.83271E+01
1773	0.8	1.9050	-1.83317E+01
1773	0.8	1.9060	-1.83364E+01
1773	0.8	1.9070	-1.83411E+01
1773	0.8	1.9080	-1.83458E+01
1773	0.8	1.9090	-1.83505E+01
1773	0.8	1.9100	-1.83552E+01
1773	0.8	1.9110	-1.83600E+01
1773	0.8	1.9120	-1.83647E+01
1773	0.8	1.9130	-1.83694E+01
1773	0.8	1.9140	-1.83742E+01
1773	0.8	1.9150	-1.83789E+01
1773	0.8	1.9160	-1.83837E+01
1773	0.8	1.9170	-1.83884E+01
1773	0.8	1.9180	-1.83931E+01
1773	0.8	1.9190	-1.83978E+01
1773	0.8	1.9200	-1.84024E+01
1773	0.8	1.9210	-1.84071E+01
1773	0.8	1.9220	-1.84116E+01
1773	0.8	1.9230	-1.84161E+01
1773	0.8	1.9240	-1.84206E+01
1773	0.8	1.9250	-1.84250E+01
1773	0.8	1.9260	-1.84293E+01
1773	0.8	1.9270	-1.84336E+01
1773	0.8	1.9280	-1.84377E+01
1773	0.8	1.9290	-1.84418E+01
1773	0.8	1.9300	-1.84457E+01
1773	0.8	1.9310	-1.84495E+01
1773	0.8	1.9320	-1.84531E+01
1773	0.8	1.9330	-1.84567E+01
1773	0.8	1.9340	-1.84600E+01
1773	0.8	1.9350	-1.84632E+01
1773	0.8	1.9360	-1.84662E+01
1773	0.8	1.9370	-1.84690E+01
1773	0.8	1.9380	-1.84716E+01
1773	0.8	1.9390	-1.84740E+01
1773	0.8	1.9400	-1.84761E+01
1773	0.8	1.9410	-1.84780E+01
1773	0.8	1.9420	-1.84797E+01
1773	0.8	1.9430	-1.84811E+01
1773	0.8	1.9440	-1.84821E+01
1773	0.8	1.9450	-1.84829E+01
1773	0.8	1.9460	-1.84834E+01
1773	0.8	1.9470	-1.84836E+01
1773	0.8	1.9480	-1.84834E+01
1773	0.8	1.9490	-1.84830E+01
1773	0.8	1.9500	-1.84821E+01
1773	0.8	1.9510	-1.84809E+01
1773	0.8	1.9520	-1.84794E+01
1773	0.8	1.9530	-1.84775E+01
1773	0.8	1.9540	-1.84752E+01
1773	0.8	1.9550	-1.84725E+01
1773	0.8	1.9560	-1.84695E+01
1773	0.8	1.9570	-1.84660E+01
1773	0.8	1.9580	-1.84622E+01
1773	0.8	1.9590	-1.84580E+01
1773	0.8	1.9600	-1.84534E+01
1773	0.8	1.9610	-1.84484E+01
1773	0.8	1.9620	-1.84430E+01
1773	0.8	1.9630	-1.84373E+01
1773	0.8	1.9640	-1.84311E+01
1773	0.8	1.9650	-1.84245E+01
1773	0.8	1.9660	-1.84176E+01
1773	0.8	1.9670	-1.84103E+01
1773	0.8	1.9680	-1.84026E+01
1773	0.8	1.9690	-1.83945E+01
1773	0.8	1.9700	-1.83861E+01
1773	0.8	1.9710	-1.83773E+01
1773	0.8	1.9720	-1.83682E+01
1773	0.8	1.9730	-1.83587E+01

1773	0.8	1.9740	-1.83488E+01
1773	0.8	1.9750	-1.83387E+01
1773	0.8	1.9760	-1.83282E+01
1773	0.8	1.9770	-1.83173E+01
1773	0.8	1.9780	-1.83062E+01
1773	0.8	1.9790	-1.82947E+01
1773	0.8	1.9800	-1.82829E+01
1773	0.8	1.9810	-1.82708E+01
1773	0.8	1.9820	-1.82584E+01
1773	0.8	1.9830	-1.82457E+01
1773	0.8	1.9840	-1.82327E+01
1773	0.8	1.9850	-1.82195E+01
1773	0.8	1.9860	-1.82060E+01
1773	0.8	1.9870	-1.81921E+01
1773	0.8	1.9880	-1.81781E+01
1773	0.8	1.9890	-1.81637E+01
1773	0.8	1.9900	-1.81491E+01
1773	0.8	1.9910	-1.81342E+01
1773	0.8	1.9920	-1.81191E+01
1773	0.8	1.9930	-1.81037E+01
1773	0.8	1.9940	-1.80880E+01
1773	0.8	1.9950	-1.80721E+01
1773	0.8	1.9960	-1.80560E+01
1773	0.8	1.9970	-1.80395E+01
1773	0.8	1.9980	-1.80228E+01
1773	0.8	1.9990	-1.80058E+01
1773	0.8	2.0000	-1.79875E+01
1773	0.8	2.0010	-1.79660E+01
1773	0.8	2.0020	-1.79434E+01
1773	0.8	2.0030	-1.79204E+01
1773	0.8	2.0040	-1.78971E+01
1773	0.8	2.0050	-1.78737E+01
1773	0.8	2.0060	-1.78501E+01
1773	0.8	2.0070	-1.78263E+01
1773	0.8	2.0080	-1.78023E+01
1773	0.8	2.0090	-1.77781E+01
1773	0.8	2.0100	-1.77537E+01
1773	0.8	2.0110	-1.77292E+01
1773	0.8	2.0120	-1.77045E+01
1773	0.8	2.0130	-1.76796E+01
1773	0.8	2.0140	-1.76546E+01
1773	0.8	2.0150	-1.76294E+01
1773	0.8	2.0160	-1.76040E+01
1773	0.8	2.0170	-1.75785E+01
1773	0.8	2.0180	-1.75527E+01
1773	0.8	2.0190	-1.75269E+01
1773	0.8	2.0200	-1.75008E+01
1773	0.8	2.0210	-1.74746E+01
1773	0.8	2.0220	-1.74483E+01
1773	0.8	2.0230	-1.74217E+01
1773	0.8	2.0240	-1.73951E+01
1773	0.8	2.0250	-1.73682E+01
1773	0.8	2.0260	-1.73412E+01
1773	0.8	2.0270	-1.73140E+01
1773	0.8	2.0280	-1.72867E+01
1773	0.8	2.0290	-1.72591E+01
1773	0.8	2.0300	-1.72315E+01
1773	0.8	2.0310	-1.72036E+01
1773	0.8	2.0320	-1.71756E+01
1773	0.8	2.0330	-1.71474E+01
1773	0.8	2.0340	-1.71191E+01
1773	0.8	2.0350	-1.70906E+01
1773	0.8	2.0360	-1.70619E+01
1773	0.8	2.0370	-1.70330E+01
1773	0.8	2.0380	-1.70040E+01
1773	0.8	2.0390	-1.69748E+01
1773	0.8		

2273	0.8	1.6250	-1.49751E+01
2273	0.8	1.6260	-1.49729E+01
2273	0.8	1.6270	-1.49707E+01
2273	0.8	1.6280	-1.49686E+01
2273	0.8	1.6290	-1.49665E+01
2273	0.8	1.6300	-1.49645E+01
2273	0.8	1.6310	-1.49625E+01
2273	0.8	1.6320	-1.49606E+01
2273	0.8	1.6330	-1.49587E+01
2273	0.8	1.6340	-1.49569E+01
2273	0.8	1.6350	-1.49552E+01
2273	0.8	1.6360	-1.49535E+01
2273	0.8	1.6370	-1.49518E+01
2273	0.8	1.6380	-1.49502E+01
2273	0.8	1.6390	-1.49487E+01
2273	0.8	1.6400	-1.49472E+01
2273	0.8	1.6410	-1.49457E+01
2273	0.8	1.6420	-1.49443E+01
2273	0.8	1.6430	-1.49430E+01
2273	0.8	1.6440	-1.49417E+01
2273	0.8	1.6450	-1.49404E+01
2273	0.8	1.6460	-1.49392E+01
2273	0.8	1.6470	-1.49380E+01
2273	0.8	1.6480	-1.49369E+01
2273	0.8	1.6490	-1.49358E+01
2273	0.8	1.6500	-1.49348E+01
2273	0.8	1.6510	-1.49338E+01
2273	0.8	1.6520	-1.49328E+01
2273	0.8	1.6530	-1.49319E+01
2273	0.8	1.6540	-1.49310E+01
2273	0.8	1.6550	-1.49302E+01
2273	0.8	1.6560	-1.49294E+01
2273	0.8	1.6570	-1.49286E+01
2273	0.8	1.6580	-1.49279E+01
2273	0.8	1.6590	-1.49272E+01
2273	0.8	1.6600	-1.49266E+01
2273	0.8	1.6610	-1.49259E+01
2273	0.8	1.6620	-1.49254E+01
2273	0.8	1.6630	-1.49248E+01
2273	0.8	1.6640	-1.49243E+01
2273	0.8	1.6650	-1.49238E+01
2273	0.8	1.6660	-1.49234E+01
2273	0.8	1.6670	-1.49230E+01
2273	0.8	1.6680	-1.49226E+01
2273	0.8	1.6690	-1.49223E+01
2273	0.8	1.6700	-1.49220E+01
2273	0.8	1.6710	-1.49217E+01
2273	0.8	1.6720	-1.49214E+01
2273	0.8	1.6730	-1.49212E+01
2273	0.8	1.6740	-1.49210E+01
2273	0.8	1.6750	-1.49209E+01
2273	0.8	1.6760	-1.49207E+01
2273	0.8	1.6770	-1.49206E+01
2273	0.8	1.6780	-1.49206E+01
2273	0.8	1.6790	-1.49205E+01
2273	0.8	1.6800	-1.49205E+01
2273	0.8	1.6810	-1.49205E+01
2273	0.8	1.6820	-1.49205E+01
2273	0.8	1.6830	-1.49206E+01
2273	0.8	1.6840	-1.49207E+01
2273	0.8	1.6850	-1.49208E+01
2273	0.8	1.6860	-1.49210E+01
2273	0.8	1.6870	-1.49211E+01
2273	0.8	1.6880	-1.49213E+01
2273	0.8	1.6890	-1.49216E+01
2273	0.8	1.6900	-1.49218E+01
2273	0.8	1.6910	-1.49221E+01
2273	0.8	1.6920	-1.49224E+01
2273	0.8	1.6930	-1.49227E+01
2273	0.8	1.6940	-1.49230E+01
2273	0.8	1.6950	-1.49234E+01
2273	0.8	1.6960	-1.49238E+01
2273	0.8	1.6970	-1.49242E+01
2273	0.8	1.6980	-1.49246E+01
2273	0.8	1.6990	-1.49251E+01
2273	0.8	1.7000	-1.49256E+01
2273	0.8	1.7010	-1.49261E+01
2273	0.8	1.7020	-1.49266E+01
2273	0.8	1.7030	-1.49271E+01
2273	0.8	1.7040	-1.49277E+01
2273	0.8	1.7050	-1.49283E+01
2273	0.8	1.7060	-1.49289E+01
2273	0.8	1.7070	-1.49295E+01
2273	0.8	1.7080	-1.49302E+01
2273	0.8	1.7090	-1.49308E+01
2273	0.8	1.7100	-1.49315E+01
2273	0.8	1.7110	-1.49322E+01
2273	0.8	1.7120	-1.49330E+01
2273	0.8	1.7130	-1.49337E+01
2273	0.8	1.7140	-1.49345E+01
2273	0.8	1.7150	-1.49353E+01
2273	0.8	1.7160	-1.49361E+01

2273	0.8	1.7170	-1.49369E+01
2273	0.8	1.7180	-1.49377E+01
2273	0.8	1.7190	-1.49386E+01
2273	0.8	1.7200	-1.49395E+01
2273	0.8	1.7210	-1.49404E+01
2273	0.8	1.7220	-1.49413E+01
2273	0.8	1.7230	-1.49422E+01
2273	0.8	1.7240	-1.49432E+01
2273	0.8	1.7250	-1.49441E+01
2273	0.8	1.7260	-1.49451E+01
2273	0.8	1.7270	-1.49461E+01
2273	0.8	1.7280	-1.49472E+01
2273	0.8	1.7290	-1.49482E+01
2273	0.8	1.7300	-1.49493E+01
2273	0.8	1.7310	-1.49503E+01
2273	0.8	1.7320	-1.49514E+01
2273	0.8	1.7330	-1.49525E+01
2273	0.8	1.7340	-1.49536E+01
2273	0.8	1.7350	-1.49548E+01
2273	0.8	1.7360	-1.49559E+01
2273	0.8	1.7370	-1.49571E+01
2273	0.8	1.7380	-1.49583E+01
2273	0.8	1.7390	-1.49595E+01
2273	0.8	1.7400	-1.49607E+01
2273	0.8	1.7410	-1.49620E+01
2273	0.8	1.7420	-1.49632E+01
2273	0.8	1.7430	-1.49645E+01
2273	0.8	1.7440	-1.49658E+01
2273	0.8	1.7450	-1.49671E+01
2273	0.8	1.7460	-1.49684E+01
2273	0.8	1.7470	-1.49697E+01
2273	0.8	1.7480	-1.49710E+01
2273	0.8	1.7490	-1.49724E+01
2273	0.8	1.7500	-1.49738E+01
2273	0.8	1.7510	-1.49752E+01
2273	0.8	1.7520	-1.49766E+01
2273	0.8	1.7530	-1.49780E+01
2273	0.8	1.7540	-1.49794E+01
2273	0.8	1.7550	-1.49809E+01
2273	0.8	1.7560	-1.49823E+01
2273	0.8	1.7570	-1.49838E+01
2273	0.8	1.7580	-1.49853E+01
2273	0.8	1.7590	-1.49868E+01
2273	0.8	1.7600	-1.49883E+01
2273	0.8	1.7610	-1.49898E+01
2273	0.8	1.7620	-1.49914E+01
2273	0.8	1.7630	-1.49930E+01
2273	0.8	1.7640	-1.49945E+01
2273	0.8	1.7650	-1.49961E+01
2273	0.8	1.7660	-1.49977E+01
2273	0.8	1.7670	-1.49993E+01
2273	0.8	1.7680	-1.50010E+01
2273	0.8	1.7690	-1.50026E+01
2273	0.8	1.7700	-1.50043E+01
2273	0.8	1.7710	-1.50059E+01
2273	0.8	1.7720	-1.50076E+01
2273	0.8	1.7730	-1.50093E+01
2273	0.8	1.7740	-1.50110E+01
2273	0.8	1.7750	-1.50128E+01
2273	0.8	1.7760	-1.50145E+01
2273	0.8	1.7770	-1.50163E+01
2273	0.8	1.7780	-1.50180E+01
2273	0.8	1.7790	-1.50198E+01
2273	0.8	1.7800	-1.50216E+01
2273	0.8	1.7810	-1.50234E+01
2273	0.8	1.7820	-1.50252E+01
2273	0.8	1.7830	-1.50271E+01
2273	0.8	1.7840	-1.50289E+01
2273	0.8	1.7850	-1.50308E+01
2273	0.8	1.7860	-1.50326E+01
2273	0.8	1.7870	-1.50345E+01
2273	0.8	1.7880	-1.50364E+01
2273	0.8	1.7890	-1.50383E+01
2273	0.8	1.7900	-1.50403E+01
2273	0.8	1.7910	-1.50422E+01
2273	0.8	1.7920	-1.50442E+01
2273	0.8	1.7930	-1.50461E+01
2273	0.8	1.7940	-1.50481E+01
2273	0.8	1.7950	-1.50501E+01
2273	0.8	1.7960	-1.50521E+01
2273	0.8	1.7970	-1.50541E+01
2273	0.8	1.7980	-1.50562E+01
2273	0.8	1.7990	-1.50582E+01
2273	0.8	1.8000	-1.50603E+01
2273	0.8	1.8010	-1.50623E+01
2273	0.8	1.8020	-1.50644E+01
2273	0.8	1.8030	-1.50665E+01
2273	0.8	1.8040	-1.50686E+01
2273	0.8	1.8050	-1.50707E+01
2273	0.8	1.8060	-1.50729E+01
2273	0.8	1.8070	-1.50750E+01
2273	0.8	1.8080	-1.50772E+01

2273	0.8	1.8090	-1.50794E+01
2273	0.8	1.8100	-1.50816E+01
2273	0.8	1.8110	-1.50838E+01
2273	0.8	1.8120	-1.50860E+01
2273	0.8	1.8130	-1.50882E+01
2273	0.8	1.8140	-1.50904E+01
2273	0.8	1.8150	-1.50927E+01
2273	0.8	1.8160	-1.50950E+01
2273	0.8	1.8170	-1.50973E+01
2273	0.8	1.8180	-1.50996E+01
2273	0.8	1.8190	-1.51019E+01
2273	0.8	1.8200	-1.51042E+01
2273	0.8	1.8210	-1.51065E+01
2273	0.8	1.8220	-1.51089E+01
2273	0.8	1.8230	-1.51112E+01
2273	0.8	1.8240	-1.51136E+01
2273	0.8	1.8250	-1.51160E+01
2273	0.8	1.8260	-1.51184E+01
2273	0.8	1.8270	-1.51208E+01
2273	0.8	1.8280	-1.51233E+01
2273	0.8	1.8290	-1.51257E+01
2273	0.8	1.8300	-1.51282E+01
2273	0.8	1.8310	-1.51307E+01
2273	0.8	1.8320	-1.51332E+01
2273	0.8	1.8330	-1.51357E+01
2273	0.8	1.8340	-1.51382E+01
2273	0.8	1.8350	-1.51407E+01
2273	0.8	1.8360	-1.51433E+01
2273	0.8	1.8370	-1.51458E+01
2273	0.8	1.8380	-1.51484E+01
2273	0.8	1.8390	-1.51510E+01
2273	0.8	1.8400	-1.51536E+01
2273	0.8	1.8410	-1.51562E+01
2273	0.8	1.8420	-1.51588E+01
2273	0.8	1.8430	-1.51615E+01
2273	0.8	1.8440	-1.51641E+01
2273	0.8	1.8450	-1.51668E+01
2273	0.8	1.8460	-1.51695E+01
2273	0.8	1.8470	-1.51722E+01
2273	0.8	1.8480	-1.51749E+01
2273	0.8	1.8490	-1.51777E+01
2273	0.8	1.8500	-1.51804E+01
2273	0.8	1.8510	-1.51832E+01
2273	0.8	1.8520	-1.51860E+01
2273	0.8	1.8530	-1.51888E+01
2273	0.8	1.8540	-1.51916E+01
2273	0.8	1.8550	-1.51944E+01
2273	0.8	1.8560	-1.51972E+01
2273	0.8	1.8570	-1.52001E+01
2273	0.8	1.8580	-1.52030E+01
2273	0.8	1.8590	-1.52059E+01
2273	0.8	1.8600	-1.52088E+01
2273	0.8	1.8610	-1.52117E+01
2273	0.8	1.8620	-1.52146E+01
2273	0.8	1.8630	-1.52175E+01
2273	0.8	1.8640	-1.52205E+01
2273	0.8	1.8650	-1.52235E+01
2273	0.8	1.8660	-1.52264E+01
2273	0.8	1.8670	-1.52294E+01
2273	0.8	1.8680	-1.52324E+01
2273	0.8	1.8690	-1.52355E+01
2273	0.8	1.8700	-1.52385E+01
2273	0.8	1.8710	-1.52415E+01
2273	0.8	1.8720	-1.52446E+01
2273	0.8	1.8730	-1.52477E+01
2273	0.8	1.8740	-1.52507E+01
2273	0.8		

2273	0.8	1.9010	-1.53346E+01
2273	0.8	1.9020	-1.53375E+01
2273	0.8	1.9030	-1.53404E+01
2273	0.8	1.9040	-1.53432E+01
2273	0.8	1.9050	-1.53460E+01
2273	0.8	1.9060	-1.53487E+01
2273	0.8	1.9070	-1.53514E+01
2273	0.8	1.9080	-1.53540E+01
2273	0.8	1.9090	-1.53566E+01
2273	0.8	1.9100	-1.53591E+01
2273	0.8	1.9110	-1.53615E+01
2273	0.8	1.9120	-1.53638E+01
2273	0.8	1.9130	-1.53661E+01
2273	0.8	1.9140	-1.53683E+01
2273	0.8	1.9150	-1.53704E+01
2273	0.8	1.9160	-1.53724E+01
2273	0.8	1.9170	-1.53742E+01
2273	0.8	1.9180	-1.53760E+01
2273	0.8	1.9190	-1.53777E+01
2273	0.8	1.9200	-1.53792E+01
2273	0.8	1.9210	-1.53807E+01
2273	0.8	1.9220	-1.53820E+01
2273	0.8	1.9230	-1.53831E+01
2273	0.8	1.9240	-1.53841E+01
2273	0.8	1.9250	-1.53850E+01
2273	0.8	1.9260	-1.53857E+01
2273	0.8	1.9270	-1.53863E+01
2273	0.8	1.9280	-1.53867E+01
2273	0.8	1.9290	-1.53869E+01
2273	0.8	1.9300	-1.53870E+01
2273	0.8	1.9310	-1.53868E+01
2273	0.8	1.9320	-1.53865E+01
2273	0.8	1.9330	-1.53860E+01
2273	0.8	1.9340	-1.53853E+01
2273	0.8	1.9350	-1.53844E+01
2273	0.8	1.9360	-1.53833E+01
2273	0.8	1.9370	-1.53820E+01
2273	0.8	1.9380	-1.53804E+01
2273	0.8	1.9390	-1.53787E+01

2273	0.8	1.9400	-1.53767E+01
2273	0.8	1.9410	-1.53745E+01
2273	0.8	1.9420	-1.53721E+01
2273	0.8	1.9430	-1.53695E+01
2273	0.8	1.9440	-1.53666E+01
2273	0.8	1.9450	-1.53635E+01
2273	0.8	1.9460	-1.53601E+01
2273	0.8	1.9470	-1.53566E+01
2273	0.8	1.9480	-1.53527E+01
2273	0.8	1.9490	-1.53487E+01
2273	0.8	1.9500	-1.53444E+01
2273	0.8	1.9510	-1.53399E+01
2273	0.8	1.9520	-1.53351E+01
2273	0.8	1.9530	-1.53301E+01
2273	0.8	1.9540	-1.53249E+01
2273	0.8	1.9550	-1.53194E+01
2273	0.8	1.9560	-1.53137E+01
2273	0.8	1.9570	-1.53077E+01
2273	0.8	1.9580	-1.53015E+01
2273	0.8	1.9590	-1.52951E+01
2273	0.8	1.9600	-1.52884E+01
2273	0.8	1.9610	-1.52816E+01
2273	0.8	1.9620	-1.52745E+01
2273	0.8	1.9630	-1.52671E+01
2273	0.8	1.9640	-1.52596E+01
2273	0.8	1.9650	-1.52518E+01
2273	0.8	1.9660	-1.52438E+01
2273	0.8	1.9670	-1.52356E+01
2273	0.8	1.9680	-1.52271E+01
2273	0.8	1.9690	-1.52185E+01
2273	0.8	1.9700	-1.52096E+01
2273	0.8	1.9710	-1.52006E+01
2273	0.8	1.9720	-1.51913E+01
2273	0.8	1.9730	-1.51818E+01
2273	0.8	1.9740	-1.51722E+01
2273	0.8	1.9750	-1.51623E+01
2273	0.8	1.9760	-1.51522E+01
2273	0.8	1.9770	-1.51419E+01
2273	0.8	1.9780	-1.51315E+01

2273	0.8	1.9790	-1.51208E+01
2273	0.8	1.9800	-1.51100E+01
2273	0.8	1.9810	-1.50989E+01
2273	0.8	1.9820	-1.50877E+01
2273	0.8	1.9830	-1.50763E+01
2273	0.8	1.9840	-1.50647E+01
2273	0.8	1.9850	-1.50529E+01
2273	0.8	1.9860	-1.50409E+01
2273	0.8	1.9870	-1.50288E+01
2273	0.8	1.9880	-1.50164E+01
2273	0.8	1.9890	-1.50039E+01
2273	0.8	1.9900	-1.49912E+01
2273	0.8	1.9910	-1.49782E+01
2273	0.8	1.9920	-1.49651E+01
2273	0.8	1.9930	-1.49518E+01
2273	0.8	1.9940	-1.49382E+01
2273	0.8	1.9950	-1.49244E+01
2273	0.8	1.9960	-1.49103E+01
2273	0.8	1.9970	-1.48959E+01
2273	0.8	1.9980	-1.48810E+01
2273	0.8	1.9990	-1.48657E+01
2273	0.8	2.0000	-1.48497E+01
2273	0.8	2.0010	-1.48332E+01
2273	0.8	2.0020	-1.48160E+01
2273	0.8	2.0030	-1.47983E+01
2273	0.8	2.0040	-1.47802E+01
2273	0.8	2.0050	-1.47618E+01
2273	0.8	2.0060	-1.47431E+01
2273	0.8	2.0070	-1.47242E+01
2273	0.8	2.0080	-1.47051E+01
2273	0.8	2.0090	-1.46859E+01
2273	0.8	2.0100	-1.46665E+01

A.2.9. $(U_{0.1}Pu_{0.9})O_{2+x}$:

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)
1273	0.9	1.6000	-2.21775E+01
1273	0.9	1.6010	-2.21743E+01
1273	0.9	1.6020	-2.21712E+01
1273	0.9	1.6030	-2.21682E+01
1273	0.9	1.6040	-2.21652E+01
1273	0.9	1.6050	-2.21623E+01
1273	0.9	1.6060	-2.21595E+01
1273	0.9	1.6070	-2.21568E+01
1273	0.9	1.6080	-2.21542E+01
1273	0.9	1.6090	-2.21516E+01
1273	0.9	1.6100	-2.21491E+01
1273	0.9	1.6110	-2.21467E+01
1273	0.9	1.6120	-2.21444E+01
1273	0.9	1.6130	-2.21421E+01
1273	0.9	1.6140	-2.21399E+01
1273	0.9	1.6150	-2.21377E+01
1273	0.9	1.6160	-2.21356E+01
1273	0.9	1.6170	-2.21336E+01
1273	0.9	1.6180	-2.21316E+01
1273	0.9	1.6190	-2.21297E+01
1273	0.9	1.6200	-2.21279E+01
1273	0.9	1.6210	-2.21261E+01
1273	0.9	1.6220	-2.21244E+01
1273	0.9	1.6230	-2.21227E+01
1273	0.9	1.6240	-2.21211E+01
1273	0.9	1.6250	-2.21195E+01
1273	0.9	1.6260	-2.21180E+01
1273	0.9	1.6270	-2.21165E+01
1273	0.9	1.6280	-2.21151E+01
1273	0.9	1.6290	-2.21137E+01
1273	0.9	1.6300	-2.21124E+01
1273	0.9	1.6310	-2.21111E+01
1273	0.9	1.6320	-2.21099E+01
1273	0.9	1.6330	-2.21087E+01
1273	0.9	1.6340	-2.21075E+01
1273	0.9	1.6350	-2.21064E+01
1273	0.9	1.6360	-2.21054E+01
1273	0.9	1.6370	-2.21044E+01
1273	0.9	1.6380	-2.21034E+01
1273	0.9	1.6390	-2.21024E+01
1273	0.9	1.6400	-2.21016E+01
1273	0.9	1.6410	-2.21007E+01
1273	0.9	1.6420	-2.20999E+01
1273	0.9	1.6430	-2.20991E+01
1273	0.9	1.6440	-2.20984E+01

			(m ² /s)
1273	0.9	1.6450	-2.20977E+01
1273	0.9	1.6460	-2.20970E+01
1273	0.9	1.6470	-2.20964E+01
1273	0.9	1.6480	-2.20958E+01
1273	0.9	1.6490	-2.20952E+01
1273	0.9	1.6500	-2.20947E+01
1273	0.9	1.6510	-2.20942E+01
1273	0.9	1.6520	-2.20937E+01
1273	0.9	1.6530	-2.20933E+01
1273	0.9	1.6540	-2.20929E+01
1273	0.9	1.6550	-2.20925E+01
1273	0.9	1.6560	-2.20922E+01
1273	0.9	1.6570	-2.20919E+01
1273	0.9	1.6580	-2.20916E+01
1273	0.9	1.6590	-2.20914E+01
1273	0.9	1.6600	-2.20912E+01
1273	0.9	1.6610	-2.20910E+01
1273	0.9	1.6620	-2.20908E+01
1273	0.9	1.6630	-2.20907E+01
1273	0.9	1.6640	-2.20906E+01
1273	0.9	1.6650	-2.20905E+01
1273	0.9	1.6660	-2.20905E+01
1273	0.9	1.6670	-2.20905E+01
1273	0.9	1.6680	-2.20905E+01
1273	0.9	1.6690	-2.20905E+01
1273	0.9	1.6700	-2.20906E+01
1273	0.9	1.6710	-2.20907E+01
1273	0.9	1.6720	-2.20908E+01
1273	0.9	1.6730	-2.20909E+01
1273	0.9	1.6740	-2.20911E+01
1273	0.9	1.6750	-2.20913E+01
1273	0.9	1.6760	-2.20915E+01
1273	0.9	1.6770	-2.20917E+01
1273	0.9	1.6780	-2.20920E+01
1273	0.9	1.6790	-2.20923E+01
1273	0.9	1.6800	-2.20926E+01
1273	0.9	1.6810	-2.20929E+01
1273	0.9	1.6820	-2.20933E+01
1273	0.9	1.6830	-2.20936E+01
1273	0.9	1.6840	-2.20940E+01
1273	0.9	1.6850	-2.20944E+01
1273	0.9	1.6860	-2.20949E+01
1273	0.9	1.6870	-2.20953E+01
1273	0.9	1.6880	-2.20958E+01
1273	0.9	1.6890	-2.20963E+01

T (K)	Pu/M	O/(U+Pu)	Log ₁₀ D ² _{Pu} (m ² /s)
1273	0.9	1.6900	-2.20968E+01
1273	0.9	1.6910	-2.20974E+01
1273	0.9	1.6920	-2.20979E+01
1273	0.9	1.6930	-2.20985E+01
1273	0.9	1.6940	-2.20991E+01
1273	0.9	1.6950	-2.20998E+01
1273	0.9	1.6960	-2.21004E+01
1273	0.9	1.6970	-2.21011E+01
1273	0.9	1.6980	-2.21017E+01
1273	0.9	1.6990	-2.21024E+01
1273	0.9	1.7000	-2.21032E+01
1273	0.9	1.7010	-2.21039E+01
1273	0.9	1.7020	-2.21046E+01
1273	0.9	1.7030	-2.21054E+01
1273	0.9	1.7040	-2.21062E+01
1273	0.9	1.7050	-2.21070E+01
1273	0.9	1.7060	-2.21078E+01
1273	0.9	1.7070	-2.21087E+01
1273	0.9	1.7080	-2.21096E+01
1273	0.9	1.7090	-2.21104E+01
1273	0.9	1.7100	-2.21113E+01
1273	0.9	1.7110	-2.21122E+01
1273	0.9	1.7120	-2.21132E+01
1273	0.9	1.7130	-2.21141E+01
1273	0.9	1.7140	-2.21151E+01
1273	0.9	1.7150	-2.21161E+01
1273	0.9	1.7160	-2.21171E+01
1273	0.9	1.7170	-2.21181E+01
1273	0.9	1.7180	-2.21191E+01
1273	0.9	1.7190	-2.21202E+01
1273	0.9	1.7200	-2.21212E+01
1273	0.9	1.7210	-2.21223E+01
1273	0.9	1.7220	-2.21234E+01
1273	0.9	1.7230	-2.21245E+01
1273	0.9	1.7240	-2.21256E+01
1273	0.9	1.7250	-2.21268E+01
1273	0.9	1.7260	-2.21279E+01
1273	0.9	1.7270	-2.21291E+01
1273	0.9	1.7280	-2.21303E+01
1273	0.9	1.7290	-2.21315E+01
1273	0.9	1.7300	-2.21327E+01
1273	0.9	1.7310	-2.21339E+01

1273	0.9	1.7380	-2.21429E+01
1273	0.9	1.7390	-2.21442E+01
1273	0.9	1.7400	-2.21456E+01
1273	0.9	1.7410	-2.21470E+01
1273	0.9	1.7420	-2.21483E+01
1273	0.9	1.7430	-2.21497E+01
1273	0.9	1.7440	-2.21511E+01
1273	0.9	1.7450	-2.21526E+01
1273	0.9	1.7460	-2.21540E+01
1273	0.9	1.7470	-2.21554E+01
1273	0.9	1.7480	-2.21569E+01
1273	0.9	1.7490	-2.21584E+01
1273	0.9	1.7500	-2.21599E+01
1273	0.9	1.7510	-2.21614E+01
1273	0.9	1.7520	-2.21629E+01
1273	0.9	1.7530	-2.21644E+01
1273	0.9	1.7540	-2.21660E+01
1273	0.9	1.7550	-2.21675E+01
1273	0.9	1.7560	-2.21691E+01
1273	0.9	1.7570	-2.21706E+01
1273	0.9	1.7580	-2.21722E+01
1273	0.9	1.7590	-2.21738E+01
1273	0.9	1.7600	-2.21755E+01
1273	0.9	1.7610	-2.21771E+01
1273	0.9	1.7620	-2.21787E+01
1273	0.9	1.7630	-2.21804E+01
1273	0.9	1.7640	-2.21820E+01
1273	0.9	1.7650	-2.21837E+01
1273	0.9	1.7660	-2.21854E+01
1273	0.9	1.7670	-2.21871E+01
1273	0.9	1.7680	-2.21888E+01
1273	0.9	1.7690	-2.21905E+01
1273	0.9	1.7700	-2.21923E+01
1273	0.9	1.7710	-2.21940E+01
1273	0.9	1.7720	-2.21958E+01
1273	0.9	1.7730	-2.21975E+01
1273	0.9	1.7740	-2.21993E+01
1273	0.9	1.7750	-2.22011E+01
1273	0.9	1.7760	-2.22029E+01
1273	0.9	1.7770	-2.22047E+01
1273	0.9	1.7780	-2.22065E+01
1273	0.9	1.7790	-2.22084E+01
1273	0.9	1.7800	-2.22102E+01
1273	0.9	1.7810	-2.22121E+01
1273	0.9	1.7820	-2.22140E+01
1273	0.9	1.7830	-2.22158E+01
1273	0.9	1.7840	-2.22177E+01
1273	0.9	1.7850	-2.22196E+01
1273	0.9	1.7860	-2.22216E+01
1273	0.9	1.7870	-2.22235E+01
1273	0.9	1.7880	-2.22254E+01
1273	0.9	1.7890	-2.22274E+01
1273	0.9	1.7900	-2.22293E+01
1273	0.9	1.7910	-2.22313E+01
1273	0.9	1.7920	-2.22333E+01
1273	0.9	1.7930	-2.22353E+01
1273	0.9	1.7940	-2.22373E+01
1273	0.9	1.7950	-2.22393E+01
1273	0.9	1.7960	-2.22413E+01
1273	0.9	1.7970	-2.22434E+01
1273	0.9	1.7980	-2.22454E+01
1273	0.9	1.7990	-2.22475E+01
1273	0.9	1.8000	-2.22495E+01
1273	0.9	1.8010	-2.22516E+01
1273	0.9	1.8020	-2.22537E+01
1273	0.9	1.8030	-2.22558E+01
1273	0.9	1.8040	-2.22579E+01
1273	0.9	1.8050	-2.22600E+01
1273	0.9	1.8060	-2.22622E+01
1273	0.9	1.8070	-2.22643E+01
1273	0.9	1.8080	-2.22665E+01
1273	0.9	1.8090	-2.22686E+01
1273	0.9	1.8100	-2.22708E+01
1273	0.9	1.8110	-2.22730E+01
1273	0.9	1.8120	-2.22752E+01
1273	0.9	1.8130	-2.22774E+01
1273	0.9	1.8140	-2.22796E+01
1273	0.9	1.8150	-2.22818E+01
1273	0.9	1.8160	-2.22841E+01
1273	0.9	1.8170	-2.22863E+01
1273	0.9	1.8180	-2.22886E+01
1273	0.9	1.8190	-2.22908E+01
1273	0.9	1.8200	-2.22931E+01
1273	0.9	1.8210	-2.22954E+01
1273	0.9	1.8220	-2.22977E+01
1273	0.9	1.8230	-2.23000E+01
1273	0.9	1.8240	-2.23023E+01
1273	0.9	1.8250	-2.23047E+01
1273	0.9	1.8260	-2.23070E+01
1273	0.9	1.8270	-2.23094E+01
1273	0.9	1.8280	-2.23117E+01
1273	0.9	1.8290	-2.23141E+01

1273	0.9	1.8300	-2.23165E+01
1273	0.9	1.8310	-2.23189E+01
1273	0.9	1.8320	-2.23213E+01
1273	0.9	1.8330	-2.23237E+01
1273	0.9	1.8340	-2.23261E+01
1273	0.9	1.8350	-2.23285E+01
1273	0.9	1.8360	-2.23310E+01
1273	0.9	1.8370	-2.23334E+01
1273	0.9	1.8380	-2.23359E+01
1273	0.9	1.8390	-2.23384E+01
1273	0.9	1.8400	-2.23409E+01
1273	0.9	1.8410	-2.23434E+01
1273	0.9	1.8420	-2.23459E+01
1273	0.9	1.8430	-2.23484E+01
1273	0.9	1.8440	-2.23509E+01
1273	0.9	1.8450	-2.23534E+01
1273	0.9	1.8460	-2.23560E+01
1273	0.9	1.8470	-2.23586E+01
1273	0.9	1.8480	-2.23611E+01
1273	0.9	1.8490	-2.23637E+01
1273	0.9	1.8500	-2.23663E+01
1273	0.9	1.8510	-2.23689E+01
1273	0.9	1.8520	-2.23715E+01
1273	0.9	1.8530	-2.23741E+01
1273	0.9	1.8540	-2.23768E+01
1273	0.9	1.8550	-2.23794E+01
1273	0.9	1.8560	-2.23820E+01
1273	0.9	1.8570	-2.23847E+01
1273	0.9	1.8580	-2.23874E+01
1273	0.9	1.8590	-2.23901E+01
1273	0.9	1.8600	-2.23928E+01
1273	0.9	1.8610	-2.23955E+01
1273	0.9	1.8620	-2.23982E+01
1273	0.9	1.8630	-2.24009E+01
1273	0.9	1.8640	-2.24036E+01
1273	0.9	1.8650	-2.24064E+01
1273	0.9	1.8660	-2.24091E+01
1273	0.9	1.8670	-2.24119E+01
1273	0.9	1.8680	-2.24147E+01
1273	0.9	1.8690	-2.24174E+01
1273	0.9	1.8700	-2.24202E+01
1273	0.9	1.8710	-2.24230E+01
1273	0.9	1.8720	-2.24259E+01
1273	0.9	1.8730	-2.24287E+01
1273	0.9	1.8740	-2.24315E+01
1273	0.9	1.8750	-2.24344E+01
1273	0.9	1.8760	-2.24372E+01
1273	0.9	1.8770	-2.24401E+01
1273	0.9	1.8780	-2.24429E+01
1273	0.9	1.8790	-2.24458E+01
1273	0.9	1.8800	-2.24487E+01
1273	0.9	1.8810	-2.24516E+01
1273	0.9	1.8820	-2.24545E+01
1273	0.9	1.8830	-2.24574E+01
1273	0.9	1.8840	-2.24604E+01
1273	0.9	1.8850	-2.24633E+01
1273	0.9	1.8860	-2.24662E+01
1273	0.9	1.8870	-2.24692E+01
1273	0.9	1.8880	-2.24721E+01
1273	0.9	1.8890	-2.24751E+01
1273	0.9	1.8900	-2.24780E+01
1273	0.9	1.8910	-2.24810E+01
1273	0.9	1.8920	-2.24840E+01
1273	0.9	1.8930	-2.24870E+01
1273	0.9	1.8940	-2.24900E+01
1273	0.9	1.8950	-2.24929E+01
1273	0.9	1.8960	-2.24959E+01
1273	0.9	1.8970	-2.24989E+01
1273	0.9	1.8980	-2.25019E+01
1273	0.9	1.8990	-2.25049E+01
1273	0.9	1.9000	-2.25079E+01
1273	0.9	1.9010	-2.25109E+01
1273	0.9	1.9020	-2.25139E+01
1273	0.9	1.9030	-2.25168E+01
1273	0.9	1.9040	-2.25198E+01
1273	0.9	1.9050	-2.25228E+01
1273	0.9	1.9060	-2.25257E+01
1273	0.9	1.9070	-2.25287E+01
1273	0.9	1.9080	-2.25316E+01
1273	0.9	1.9090	-2.25346E+01
1273	0.9	1.9100	-2.25375E+01
1273	0.9	1.9110	-2.25404E+01
1273	0.9	1.9120	-2.25432E+01
1273	0.9	1.9130	-2.25461E+01
1273	0.9	1.9140	-2.25489E+01
1273	0.9	1.9150	-2.25517E+01
1273	0.9	1.9160	-2.25545E+01
1273	0.9	1.9170	-2.25571E+01
1273	0.9	1.9180	-2.25598E+01
1273	0.9	1.9190	-2.25624E+01
1273	0.9	1.9200	-2.25650E+01
1273	0.9	1.9210	-2.25675E+01

1273	0.9	1.9220	-2.25700E+01
1273	0.9	1.9230	-2.25724E+01
1273	0.9	1.9240	-2.25747E+01
1273	0.9	1.9250	-2.25770E+01
1273	0.9	1.9260	-2.25791E+01
1273	0.9	1.9270	-2.25812E+01
1273	0.9	1.9280	-2.25832E+01
1273	0.9	1.9290	-2.25850E+01
1273	0.9	1.9300	-2.25868E+01
1273	0.9	1.9310	-2.25884E+01
1273	0.9	1.9320	-2.25898E+01
1273	0.9	1.9330	-2.25912E+01
1273	0.9	1.9340	-2.25923E+01
1273	0.9	1.9350	-2.25933E+01
1273	0.9	1.9360	-2.25941E+01
1273	0.9	1.9370	-2.25948E+01
1273	0.9	1.9380	-2.25952E+01
1273	0.9	1.9390	-2.25954E+01
1273	0.9	1.9400	-2.25953E+01
1273	0.9	1.9410	-2.25951E+01
1273	0.9	1.9420	-2.25945E+01
1273	0.9	1.9430	-2.25937E+01
1273	0.9	1.9440	-2.25926E+01
1273	0.9	1.9450	-2.25912E+01
1273	0.9	1.9460	-2.25895E+01
1273	0.9	1.9470	-2.25874E+01
1273	0.9	1.9480	-2.25850E+01
1273	0.9	1.9490	-2.25823E+01
1273	0.9	1.9500	-2.25791E+01
1273	0.9	1.9510	-2.25756E+01
1273	0.9	1.9520	-2.25717E+01
1273	0.9	1.9530	-2.25674E+01
1273	0.9	1.9540	-2.25626E+01
1273	0.9	1.9550	-2.25575E+01
1273	0.9	1.9560	-2.25519E+01
1273	0.9	1.9570	-2.25458E+01
1273	0.9	1.9580	-2.25393E+01
1273	0.9	1.9590	-2.25323E+01
1273	0.9	1.9600	-2.25249E+01
1273	0.9	1.9610	-2.25169E+01
1273	0.9	1.9620	-2.25085E+01
1273	0.9	1.9630	-2.24997E+01
1273	0.9	1.9640	-2.24903E+01
1273	0.9	1.9650	-2.24805E+01
1273	0.9	1.9660	-2.24701E+01
1273	0.9	1.9670	-2.24593E+01
1273	0.9	1.9680	-2.24480E+01
1273	0.9	1.9690	-2.24363E+01
1273	0.9	1.9700	-2.24240E+01
1273	0.9	1.9710	-2.24113E+01
1273	0.9	1.9720	-2.23981E+01
1273	0.9	1.9730	-2.23845E+01
1273	0.9	1.9740	-2.23704E+01
1273	0.9	1.9750	-2.23558E+01
1273	0.9	1.9760	-2.23408E+01
1273	0.9	1.9770	-2.23253E+01
1273	0.9	1.9780	-2.23094E+01
1273	0.9	1.9790	-2.22931E+01
1273	0.9	1.9800	-2.22764E+01
1273	0.9	1.9810	-2.22592E+01
1273	0.9	1.9820	-2.22416E+01
1273	0.9	1.9830	-2.22235E+01
1273	0.9	1.9840	-2.22051E+01
1273	0.9	1.9850	-2.21863E+01
1273	0.9	1.9860	-2.21670E+01
1273	0.9	1.9870	-2.21474E+01
1273	0.9		

1273	0.9	2.0140	-2.14060E+01
1273	0.9	2.0150	-2.13716E+01
1273	0.9	2.0160	-2.13370E+01
1273	0.9	2.0170	-2.13021E+01
1273	0.9	2.0180	-2.12669E+01
1273	0.9	2.0190	-2.12314E+01
1273	0.9	2.0200	-2.11956E+01
1273	0.9	2.0210	-2.11595E+01
1273	0.9	2.0220	-2.11231E+01
1273	0.9	2.0230	-2.10864E+01
1273	0.9	2.0240	-2.10494E+01
1273	0.9	2.0250	-2.10121E+01
1273	0.9	2.0260	-2.09744E+01
1273	0.9	2.0270	-2.09364E+01
1273	0.9	2.0280	-2.08981E+01
1273	0.9	2.0290	-2.08594E+01
1273	0.9	2.0300	-2.08203E+01
1273	0.9	2.0310	-2.07809E+01
1273	0.9	2.0320	-2.07411E+01
1273	0.9	2.0330	-2.07009E+01
1273	0.9	2.0340	-2.06603E+01
1273	0.9	2.0350	-2.06193E+01
1273	0.9	2.0360	-2.05778E+01
1273	0.9	2.0370	-2.05359E+01
1273	0.9	2.0380	-2.04936E+01
1273	0.9	2.0390	-2.04507E+01
1273	0.9	2.0400	-2.04075E+01
1273	0.9	2.0410	-2.03637E+01
1273	0.9	2.0420	-2.03194E+01
1273	0.9	2.0430	-2.02746E+01
1273	0.9	2.0440	-2.02292E+01
1273	0.9	2.0450	-2.01834E+01
1273	0.9	2.0460	-2.01369E+01
1273	0.9	2.0470	-2.00899E+01
1273	0.9	2.0480	-2.00424E+01
1273	0.9	2.0490	-1.99943E+01
1273	0.9	2.0500	-1.99460E+01
1273	0.9	1.5800	-1.74904E+01
1273	0.9	1.5810	-1.74860E+01
1273	0.9	1.5820	-1.74818E+01
1273	0.9	1.5830	-1.74777E+01
1273	0.9	1.5840	-1.74736E+01
1273	0.9	1.5850	-1.74696E+01
1273	0.9	1.5860	-1.74657E+01
1273	0.9	1.5870	-1.74619E+01
1273	0.9	1.5880	-1.74582E+01
1273	0.9	1.5890	-1.74546E+01
1273	0.9	1.5900	-1.74510E+01
1273	0.9	1.5910	-1.74475E+01
1273	0.9	1.5920	-1.74441E+01
1273	0.9	1.5930	-1.74408E+01
1273	0.9	1.5940	-1.74375E+01
1273	0.9	1.5950	-1.74343E+01
1273	0.9	1.5960	-1.74312E+01
1273	0.9	1.5970	-1.74281E+01
1273	0.9	1.5980	-1.74251E+01
1273	0.9	1.5990	-1.74221E+01
1273	0.9	1.6000	-1.74192E+01
1273	0.9	1.6010	-1.74164E+01
1273	0.9	1.6020	-1.74137E+01
1273	0.9	1.6030	-1.74109E+01
1273	0.9	1.6040	-1.74083E+01
1273	0.9	1.6050	-1.74057E+01
1273	0.9	1.6060	-1.74031E+01
1273	0.9	1.6070	-1.74007E+01
1273	0.9	1.6080	-1.73982E+01
1273	0.9	1.6090	-1.73958E+01
1273	0.9	1.6100	-1.73935E+01
1273	0.9	1.6110	-1.73912E+01
1273	0.9	1.6120	-1.73890E+01
1273	0.9	1.6130	-1.73868E+01
1273	0.9	1.6140	-1.73846E+01
1273	0.9	1.6150	-1.73825E+01
1273	0.9	1.6160	-1.73804E+01
1273	0.9	1.6170	-1.73784E+01
1273	0.9	1.6180	-1.73764E+01
1273	0.9	1.6190	-1.73745E+01
1273	0.9	1.6200	-1.73726E+01
1273	0.9	1.6210	-1.73708E+01
1273	0.9	1.6220	-1.73690E+01
1273	0.9	1.6230	-1.73672E+01
1273	0.9	1.6240	-1.73654E+01
1273	0.9	1.6250	-1.73638E+01
1273	0.9	1.6260	-1.73621E+01
1273	0.9	1.6270	-1.73605E+01
1273	0.9	1.6280	-1.73589E+01
1273	0.9	1.6290	-1.73573E+01
1273	0.9	1.6300	-1.73558E+01
1273	0.9	1.6310	-1.73543E+01
1273	0.9	1.6320	-1.73529E+01
1273	0.9	1.6330	-1.73515E+01
1273	0.9	1.6340	-1.73501E+01

1773	0.9	1.6350	-1.73487E+01
1773	0.9	1.6360	-1.73474E+01
1773	0.9	1.6370	-1.73461E+01
1773	0.9	1.6380	-1.73449E+01
1773	0.9	1.6390	-1.73437E+01
1773	0.9	1.6400	-1.73425E+01
1773	0.9	1.6410	-1.73413E+01
1773	0.9	1.6420	-1.73402E+01
1773	0.9	1.6430	-1.73391E+01
1773	0.9	1.6440	-1.73380E+01
1773	0.9	1.6450	-1.73369E+01
1773	0.9	1.6460	-1.73359E+01
1773	0.9	1.6470	-1.73349E+01
1773	0.9	1.6480	-1.73340E+01
1773	0.9	1.6490	-1.73330E+01
1773	0.9	1.6500	-1.73321E+01
1773	0.9	1.6510	-1.73312E+01
1773	0.9	1.6520	-1.73304E+01
1773	0.9	1.6530	-1.73295E+01
1773	0.9	1.6540	-1.73287E+01
1773	0.9	1.6550	-1.73279E+01
1773	0.9	1.6560	-1.73271E+01
1773	0.9	1.6570	-1.73264E+01
1773	0.9	1.6580	-1.73257E+01
1773	0.9	1.6590	-1.73250E+01
1773	0.9	1.6600	-1.73243E+01
1773	0.9	1.6610	-1.73237E+01
1773	0.9	1.6620	-1.73231E+01
1773	0.9	1.6630	-1.73225E+01
1773	0.9	1.6640	-1.73219E+01
1773	0.9	1.6650	-1.73213E+01
1773	0.9	1.6660	-1.73208E+01
1773	0.9	1.6670	-1.73203E+01
1773	0.9	1.6680	-1.73198E+01
1773	0.9	1.6690	-1.73193E+01
1773	0.9	1.6700	-1.73189E+01
1773	0.9	1.6710	-1.73184E+01
1773	0.9	1.6720	-1.73180E+01
1773	0.9	1.6730	-1.73176E+01
1773	0.9	1.6740	-1.73172E+01
1773	0.9	1.6750	-1.73169E+01
1773	0.9	1.6760	-1.73166E+01
1773	0.9	1.6770	-1.73162E+01
1773	0.9	1.6780	-1.73160E+01
1773	0.9	1.6790	-1.73157E+01
1773	0.9	1.6800	-1.73154E+01
1773	0.9	1.6810	-1.73152E+01
1773	0.9	1.6820	-1.73150E+01
1773	0.9	1.6830	-1.73148E+01
1773	0.9	1.6840	-1.73146E+01
1773	0.9	1.6850	-1.73144E+01
1773	0.9	1.6860	-1.73143E+01
1773	0.9	1.6870	-1.73141E+01
1773	0.9	1.6880	-1.73140E+01
1773	0.9	1.6890	-1.73139E+01
1773	0.9	1.6900	-1.73139E+01
1773	0.9	1.6910	-1.73138E+01
1773	0.9	1.6920	-1.73137E+01
1773	0.9	1.6930	-1.73137E+01
1773	0.9	1.6940	-1.73137E+01
1773	0.9	1.6950	-1.73137E+01
1773	0.9	1.6960	-1.73137E+01
1773	0.9	1.6970	-1.73138E+01
1773	0.9	1.6980	-1.73138E+01
1773	0.9	1.6990	-1.73139E+01
1773	0.9	1.7000	-1.73140E+01
1773	0.9	1.7010	-1.73141E+01
1773	0.9	1.7020	-1.73142E+01
1773	0.9	1.7030	-1.73143E+01
1773	0.9	1.7040	-1.73144E+01
1773	0.9	1.7050	-1.73146E+01
1773	0.9	1.7060	-1.73148E+01
1773	0.9	1.7070	-1.73150E+01
1773	0.9	1.7080	-1.73152E+01
1773	0.9	1.7090	-1.73154E+01
1773	0.9	1.7100	-1.73156E+01
1773	0.9	1.7110	-1.73159E+01
1773	0.9	1.7120	-1.73161E+01
1773	0.9	1.7130	-1.73164E+01
1773	0.9	1.7140	-1.73167E+01
1773	0.9	1.7150	-1.73170E+01
1773	0.9	1.7160	-1.73173E+01
1773	0.9	1.7170	-1.73176E+01
1773	0.9	1.7180	-1.73180E+01
1773	0.9	1.7190	-1.73183E+01
1773	0.9	1.7200	-1.73187E+01
1773	0.9	1.7210	-1.73191E+01
1773	0.9	1.7220	-1.73195E+01
1773	0.9	1.7230	-1.73199E+01
1773	0.9	1.7240	-1.73203E+01
1773	0.9	1.7250	-1.73207E+01
1773	0.9	1.7260	-1.73212E+01

1773	0.9	1.7270	-1.73217E+01
1773	0.9	1.7280	-1.73221E+01
1773	0.9	1.7290	-1.73226E+01
1773	0.9	1.7300	-1.73231E+01
1773	0.9	1.7310	-1.73236E+01
1773	0.9	1.7320	-1.73242E+01
1773	0.9	1.7330	-1.73247E+01
1773	0.9	1.7340	-1.73252E+01
1773	0.9	1.7350	-1.73258E+01
1773	0.9	1.7360	-1.73264E+01
1773	0.9	1.7370	-1.73270E+01
1773	0.9	1.7380	-1.73275E+01
1773	0.9	1.7390	-1.73282E+01
1773	0.9	1.7400	-1.73288E+01
1773	0.9	1.7410	-1.73294E+01
1773	0.9	1.7420	-1.73301E+01
1773	0.9	1.7430	-1.73307E+01
1773	0.9	1.7440	-1.73314E+01
1773	0.9	1.7450	-1.73321E+01
1773	0.9	1.7460	-1.73327E+01
1773	0.9	1.7470	-1.73334E+01
1773	0.9	1.7480	-1.73342E+01
1773	0.9	1.7490	-1.73349E+01
1773	0.9	1.7500	-1.73356E+01
1773	0.9	1.7510	-1.73364E+01
1773	0.9	1.7520	-1.73371E+01
1773	0.9	1.7530	-1.73379E+01
1773	0.9	1.7540	-1.73387E+01
1773	0.9	1.7550	-1.73394E+01
1773	0.9	1.7560	-1.73402E+01
1773	0.9	1.7570	-1.73411E+01
1773	0.9	1.7580	-1.73419E+01
1773	0.9	1.7590	-1.73427E+01
1773	0.9	1.7600	-1.73436E+01
1773	0.9	1.7610	-1.73444E+01
1773	0.9	1.7620	-1.73453E+01
1773	0.9	1.7630	-1.73462E+01
1773	0.9	1.7640	-1.73470E+01
1773	0.9	1.7650	-1.73479E+01
1773	0.9	1.7660	-1.73488E+01
1773	0.9	1.7670	-1.73498E+01
1773	0.9	1.7680	-1.73507E+01
1773	0.9	1.7690	-1.73516E+01
1773	0.9	1.7700	-1.73526E+01
1773	0.9	1.7710	-1.73535E+01
1773	0.9	1.7720	-1.73545E+01
1773	0.9	1.7730	-1.73555E+01
1773	0.9	1.7740	-1.73565E+01
1773	0.9	1.7750	-1.73575E+01
1773	0.9	1.7760	-1.73585E+01
1773	0.9	1.7770	-1.73595E+01
1773	0.9	1.7780	-1.73605E+01
1773	0.9	1.7790	-1.73615E+01
1773	0.9	1.7800	-1.73626E+01
1773	0.9	1.7810	-1.73636E+01
1773	0.9	1.7820	-1.73647E+01
1773	0.9	1.7830	-1.73658E+01
1773	0.9	1.7840	-1.73669E+01
1773	0.9	1.7850	-1.73680E+01
1773	0.9	1.7860	-1.73691E+01
1773	0.9	1.7870	-1.73702E+01
1773	0.9	1.7880	-1.73713E+01
1773	0.9	1.7890	-1.73725E+01
1773	0.9	1.7900	-1.73736E+01
1773	0.9	1.7910	-1.73747E+01
1773	0.9	1.7920	-1.73759E+01
1773	0.9		

1773	0.9	1.8190	-1.74108E+01
1773	0.9	1.8200	-1.74122E+01
1773	0.9	1.8210	-1.74136E+01
1773	0.9	1.8220	-1.74150E+01
1773	0.9	1.8230	-1.74165E+01
1773	0.9	1.8240	-1.74179E+01
1773	0.9	1.8250	-1.74194E+01
1773	0.9	1.8260	-1.74208E+01
1773	0.9	1.8270	-1.74223E+01
1773	0.9	1.8280	-1.74238E+01
1773	0.9	1.8290	-1.74253E+01
1773	0.9	1.8300	-1.74268E+01
1773	0.9	1.8310	-1.74283E+01
1773	0.9	1.8320	-1.74298E+01
1773	0.9	1.8330	-1.74313E+01
1773	0.9	1.8340	-1.74329E+01
1773	0.9	1.8350	-1.74344E+01
1773	0.9	1.8360	-1.74360E+01
1773	0.9	1.8370	-1.74375E+01
1773	0.9	1.8380	-1.74391E+01
1773	0.9	1.8390	-1.74406E+01
1773	0.9	1.8400	-1.74422E+01
1773	0.9	1.8410	-1.74438E+01
1773	0.9	1.8420	-1.74454E+01
1773	0.9	1.8430	-1.74470E+01
1773	0.9	1.8440	-1.74486E+01
1773	0.9	1.8450	-1.74502E+01
1773	0.9	1.8460	-1.74518E+01
1773	0.9	1.8470	-1.74535E+01
1773	0.9	1.8480	-1.74551E+01
1773	0.9	1.8490	-1.74568E+01
1773	0.9	1.8500	-1.74584E+01
1773	0.9	1.8510	-1.74601E+01
1773	0.9	1.8520	-1.74617E+01
1773	0.9	1.8530	-1.74634E+01
1773	0.9	1.8540	-1.74651E+01
1773	0.9	1.8550	-1.74667E+01
1773	0.9	1.8560	-1.74684E+01
1773	0.9	1.8570	-1.74701E+01
1773	0.9	1.8580	-1.74718E+01
1773	0.9	1.8590	-1.74735E+01
1773	0.9	1.8600	-1.74752E+01
1773	0.9	1.8610	-1.74769E+01
1773	0.9	1.8620	-1.74786E+01
1773	0.9	1.8630	-1.74804E+01
1773	0.9	1.8640	-1.74821E+01
1773	0.9	1.8650	-1.74838E+01
1773	0.9	1.8660	-1.74855E+01
1773	0.9	1.8670	-1.74873E+01
1773	0.9	1.8680	-1.74890E+01
1773	0.9	1.8690	-1.74907E+01
1773	0.9	1.8700	-1.74925E+01
1773	0.9	1.8710	-1.74942E+01
1773	0.9	1.8720	-1.74959E+01
1773	0.9	1.8730	-1.74977E+01
1773	0.9	1.8740	-1.74994E+01
1773	0.9	1.8750	-1.75011E+01
1773	0.9	1.8760	-1.75029E+01
1773	0.9	1.8770	-1.75046E+01
1773	0.9	1.8780	-1.75063E+01
1773	0.9	1.8790	-1.75080E+01
1773	0.9	1.8800	-1.75098E+01
1773	0.9	1.8810	-1.75115E+01
1773	0.9	1.8820	-1.75132E+01
1773	0.9	1.8830	-1.75149E+01
1773	0.9	1.8840	-1.75166E+01
1773	0.9	1.8850	-1.75182E+01
1773	0.9	1.8860	-1.75199E+01
1773	0.9	1.8870	-1.75216E+01
1773	0.9	1.8880	-1.75232E+01
1773	0.9	1.8890	-1.75248E+01
1773	0.9	1.8900	-1.75264E+01
1773	0.9	1.8910	-1.75280E+01
1773	0.9	1.8920	-1.75296E+01
1773	0.9	1.8930	-1.75312E+01
1773	0.9	1.8940	-1.75327E+01
1773	0.9	1.8950	-1.75342E+01
1773	0.9	1.8960	-1.75357E+01
1773	0.9	1.8970	-1.75372E+01
1773	0.9	1.8980	-1.75386E+01
1773	0.9	1.8990	-1.75400E+01
1773	0.9	1.9000	-1.75413E+01
1773	0.9	1.9010	-1.75427E+01
1773	0.9	1.9020	-1.75439E+01
1773	0.9	1.9030	-1.75452E+01
1773	0.9	1.9040	-1.75464E+01
1773	0.9	1.9050	-1.75475E+01
1773	0.9	1.9060	-1.75486E+01
1773	0.9	1.9070	-1.75497E+01
1773	0.9	1.9080	-1.75507E+01
1773	0.9	1.9090	-1.75516E+01
1773	0.9	1.9100	-1.75524E+01

1773	0.9	1.9110	-1.75532E+01
1773	0.9	1.9120	-1.75540E+01
1773	0.9	1.9130	-1.75546E+01
1773	0.9	1.9140	-1.75552E+01
1773	0.9	1.9150	-1.75556E+01
1773	0.9	1.9160	-1.75560E+01
1773	0.9	1.9170	-1.75563E+01
1773	0.9	1.9180	-1.75565E+01
1773	0.9	1.9190	-1.75566E+01
1773	0.9	1.9200	-1.75566E+01
1773	0.9	1.9210	-1.75564E+01
1773	0.9	1.9220	-1.75562E+01
1773	0.9	1.9230	-1.75558E+01
1773	0.9	1.9240	-1.75553E+01
1773	0.9	1.9250	-1.75546E+01
1773	0.9	1.9260	-1.75538E+01
1773	0.9	1.9270	-1.75529E+01
1773	0.9	1.9280	-1.75518E+01
1773	0.9	1.9290	-1.75505E+01
1773	0.9	1.9300	-1.75491E+01
1773	0.9	1.9310	-1.75475E+01
1773	0.9	1.9320	-1.75457E+01
1773	0.9	1.9330	-1.75437E+01
1773	0.9	1.9340	-1.75416E+01
1773	0.9	1.9350	-1.75393E+01
1773	0.9	1.9360	-1.75367E+01
1773	0.9	1.9370	-1.75340E+01
1773	0.9	1.9380	-1.75310E+01
1773	0.9	1.9390	-1.75278E+01
1773	0.9	1.9400	-1.75244E+01
1773	0.9	1.9410	-1.75208E+01
1773	0.9	1.9420	-1.75170E+01
1773	0.9	1.9430	-1.75129E+01
1773	0.9	1.9440	-1.75086E+01
1773	0.9	1.9450	-1.75040E+01
1773	0.9	1.9460	-1.74992E+01
1773	0.9	1.9470	-1.74941E+01
1773	0.9	1.9480	-1.74888E+01
1773	0.9	1.9490	-1.74832E+01
1773	0.9	1.9500	-1.74774E+01
1773	0.9	1.9510	-1.74713E+01
1773	0.9	1.9520	-1.74650E+01
1773	0.9	1.9530	-1.74584E+01
1773	0.9	1.9540	-1.74515E+01
1773	0.9	1.9550	-1.74444E+01
1773	0.9	1.9560	-1.74370E+01
1773	0.9	1.9570	-1.74293E+01
1773	0.9	1.9580	-1.74214E+01
1773	0.9	1.9590	-1.74132E+01
1773	0.9	1.9600	-1.74048E+01
1773	0.9	1.9610	-1.73960E+01
1773	0.9	1.9620	-1.73870E+01
1773	0.9	1.9630	-1.73778E+01
1773	0.9	1.9640	-1.73683E+01
1773	0.9	1.9650	-1.73585E+01
1773	0.9	1.9660	-1.73484E+01
1773	0.9	1.9670	-1.73381E+01
1773	0.9	1.9680	-1.73276E+01
1773	0.9	1.9690	-1.73168E+01
1773	0.9	1.9700	-1.73057E+01
1773	0.9	1.9710	-1.72944E+01
1773	0.9	1.9720	-1.72828E+01
1773	0.9	1.9730	-1.72710E+01
1773	0.9	1.9740	-1.72589E+01
1773	0.9	1.9750	-1.72466E+01
1773	0.9	1.9760	-1.72340E+01
1773	0.9	1.9770	-1.72212E+01
1773	0.9	1.9780	-1.72081E+01
1773	0.9	1.9790	-1.71948E+01
1773	0.9	1.9800	-1.71813E+01
1773	0.9	1.9810	-1.71675E+01
1773	0.9	1.9820	-1.71535E+01
1773	0.9	1.9830	-1.71393E+01
1773	0.9	1.9840	-1.71248E+01
1773	0.9	1.9850	-1.71101E+01
1773	0.9	1.9860	-1.70951E+01
1773	0.9	1.9870	-1.70800E+01
1773	0.9	1.9880	-1.70645E+01
1773	0.9	1.9890	-1.70489E+01
1773	0.9	1.9900	-1.70330E+01
1773	0.9	1.9910	-1.70169E+01
1773	0.9	1.9920	-1.70006E+01
1773	0.9	1.9930	-1.69840E+01
1773	0.9	1.9940	-1.69672E+01
1773	0.9	1.9950	-1.69502E+01
1773	0.9	1.9960	-1.69329E+01
1773	0.9	1.9970	-1.69154E+01
1773	0.9	1.9980	-1.68976E+01
1773	0.9	1.9990	-1.68795E+01
1773	0.9	2.0000	-1.68605E+01
1773	0.9	2.0010	-1.68395E+01
1773	0.9	2.0020	-1.68176E+01

1773	0.9	2.0030	-1.67954E+01
1773	0.9	2.0040	-1.67730E+01
1773	0.9	2.0050	-1.67505E+01
1773	0.9	2.0060	-1.67278E+01
1773	0.9	2.0070	-1.67049E+01
1773	0.9	2.0080	-1.66818E+01
1773	0.9	2.0090	-1.66585E+01
1773	0.9	2.0100	-1.66351E+01
1773	0.9	2.0110	-1.66115E+01
1773	0.9	2.0120	-1.65878E+01
1773	0.9	2.0130	-1.65639E+01
1773	0.9	2.0140	-1.65398E+01
1773	0.9	2.0150	-1.65156E+01
1773	0.9	2.0160	-1.64912E+01
1773	0.9	2.0170	-1.64666E+01
1773	0.9	2.0180	-1.64418E+01
1773	0.9	2.0190	-1.64169E+01
1773	0.9	2.0200	-1.63919E+01
2273	0.9	1.5800	-1.47719E+01
2273	0.9	1.5810	-1.47684E+01
2273	0.9	1.5820	-1.47651E+01
2273	0.9	1.5830	-1.47617E+01
2273	0.9	1.5840	-1.47585E+01
2273	0.9	1.5850	-1.47553E+01
2273	0.9	1.5860	-1.47521E+01
2273	0.9	1.5870	-1.47490E+01
2273	0.9	1.5880	-1.47459E+01
2273	0.9	1.5890	-1.47429E+01
2273	0.9	1.5900	-1.47400E+01
2273	0.9	1.5910	-1.47370E+01
2273	0.9	1.5920	-1.47342E+01
2273	0.9	1.5930	-1.47314E+01
2273	0.9	1.5940	-1.47286E+01
2273	0.9	1.5950	-1.47259E+01
2273	0.9	1.5960	-1.47232E+01
2273	0.9	1.5970	-1.47206E+01
2273	0.9	1.5980	-1.47180E+01
2273	0.9	1.5990	-1.47154E+01
2273	0.9	1.6000	-1.47129E+01
2273	0.9	1.6010	-1.47105E+01
2273	0.9	1.6020	-1.47080E+01
2273	0.9	1.6030	-1.47056E+01
2273	0.9	1.6040	-1.47033E+01
2273	0.9	1.6050	-1.47010E+01
2273	0.9	1.6060	-1.46987E+01
2273	0.9	1.6070	-1.46965E+01
2273	0.9	1.6080	-1.46943E+01
2273	0.9	1.6090	-1.46921E+01
2273	0.9	1.6100	-1.46900E+01
2273	0.9	1.6110	-1.46879E+01
2273	0.9	1.6120	-1.46859E+01
2273	0.9	1.6130	-1.46839E+01
2273	0.9	1.6140	-1.46819E+01
2273	0.9	1.6150	-1.46799E+01
2273	0.9	1.6160	-1.46780E+01
2273	0.9	1.6170	-1.46761E+01
2273	0.9	1.6180	-1.46743E+01
2273	0.9	1.6190	-1.46724E+01
2273	0.9	1.6200	-1.46707E+01
2273	0.9	1.6210	-1.46689E+01
2273	0.9	1.6220	-1.46672E+01
2273	0.9	1.6230	-1.46655E+01
2273	0.9	1.6240	-1.46638E+01
2273	0.9	1.6250	-1.46621E+01
2273	0.9	1.6260	-1.46605E+01
2273	0.9	1.6270	-1.46589E+01
2273	0.9		

2273	0.9	1.6540	-1.46254E+01
2273	0.9	1.6550	-1.46244E+01
2273	0.9	1.6560	-1.46235E+01
2273	0.9	1.6570	-1.46226E+01
2273	0.9	1.6580	-1.46217E+01
2273	0.9	1.6590	-1.46209E+01
2273	0.9	1.6600	-1.46200E+01
2273	0.9	1.6610	-1.46192E+01
2273	0.9	1.6620	-1.46184E+01
2273	0.9	1.6630	-1.46176E+01
2273	0.9	1.6640	-1.46169E+01
2273	0.9	1.6650	-1.46161E+01
2273	0.9	1.6660	-1.46154E+01
2273	0.9	1.6670	-1.46147E+01
2273	0.9	1.6680	-1.46140E+01
2273	0.9	1.6690	-1.46133E+01
2273	0.9	1.6700	-1.46126E+01
2273	0.9	1.6710	-1.46120E+01
2273	0.9	1.6720	-1.46114E+01
2273	0.9	1.6730	-1.46108E+01
2273	0.9	1.6740	-1.46102E+01
2273	0.9	1.6750	-1.46096E+01
2273	0.9	1.6760	-1.46090E+01
2273	0.9	1.6770	-1.46085E+01
2273	0.9	1.6780	-1.46079E+01
2273	0.9	1.6790	-1.46074E+01
2273	0.9	1.6800	-1.46069E+01
2273	0.9	1.6810	-1.46064E+01
2273	0.9	1.6820	-1.46060E+01
2273	0.9	1.6830	-1.46055E+01
2273	0.9	1.6840	-1.46051E+01
2273	0.9	1.6850	-1.46046E+01
2273	0.9	1.6860	-1.46042E+01
2273	0.9	1.6870	-1.46038E+01
2273	0.9	1.6880	-1.46035E+01
2273	0.9	1.6890	-1.46031E+01
2273	0.9	1.6900	-1.46027E+01
2273	0.9	1.6910	-1.46024E+01
2273	0.9	1.6920	-1.46021E+01
2273	0.9	1.6930	-1.46018E+01
2273	0.9	1.6940	-1.46015E+01
2273	0.9	1.6950	-1.46012E+01
2273	0.9	1.6960	-1.46009E+01
2273	0.9	1.6970	-1.46007E+01
2273	0.9	1.6980	-1.46004E+01
2273	0.9	1.6990	-1.46002E+01
2273	0.9	1.7000	-1.46000E+01
2273	0.9	1.7010	-1.45998E+01
2273	0.9	1.7020	-1.45996E+01
2273	0.9	1.7030	-1.45994E+01
2273	0.9	1.7040	-1.45992E+01
2273	0.9	1.7050	-1.45991E+01
2273	0.9	1.7060	-1.45989E+01
2273	0.9	1.7070	-1.45988E+01
2273	0.9	1.7080	-1.45987E+01
2273	0.9	1.7090	-1.45986E+01
2273	0.9	1.7100	-1.45985E+01
2273	0.9	1.7110	-1.45984E+01
2273	0.9	1.7120	-1.45984E+01
2273	0.9	1.7130	-1.45983E+01
2273	0.9	1.7140	-1.45983E+01
2273	0.9	1.7150	-1.45982E+01
2273	0.9	1.7160	-1.45982E+01
2273	0.9	1.7170	-1.45982E+01
2273	0.9	1.7180	-1.45982E+01
2273	0.9	1.7190	-1.45982E+01
2273	0.9	1.7200	-1.45983E+01
2273	0.9	1.7210	-1.45983E+01
2273	0.9	1.7220	-1.45984E+01
2273	0.9	1.7230	-1.45984E+01
2273	0.9	1.7240	-1.45985E+01
2273	0.9	1.7250	-1.45986E+01
2273	0.9	1.7260	-1.45987E+01
2273	0.9	1.7270	-1.45988E+01
2273	0.9	1.7280	-1.45989E+01
2273	0.9	1.7290	-1.45990E+01
2273	0.9	1.7300	-1.45992E+01
2273	0.9	1.7310	-1.45993E+01
2273	0.9	1.7320	-1.45995E+01
2273	0.9	1.7330	-1.45996E+01
2273	0.9	1.7340	-1.45998E+01
2273	0.9	1.7350	-1.46000E+01
2273	0.9	1.7360	-1.46002E+01
2273	0.9	1.7370	-1.46004E+01
2273	0.9	1.7380	-1.46006E+01
2273	0.9	1.7390	-1.46009E+01
2273	0.9	1.7400	-1.46011E+01
2273	0.9	1.7410	-1.46014E+01
2273	0.9	1.7420	-1.46016E+01
2273	0.9	1.7430	-1.46019E+01
2273	0.9	1.7440	-1.46022E+01
2273	0.9	1.7450	-1.46025E+01

2273	0.9	1.7460	-1.46028E+01
2273	0.9	1.7470	-1.46031E+01
2273	0.9	1.7480	-1.46034E+01
2273	0.9	1.7490	-1.46037E+01
2273	0.9	1.7500	-1.46041E+01
2273	0.9	1.7510	-1.46044E+01
2273	0.9	1.7520	-1.46048E+01
2273	0.9	1.7530	-1.46052E+01
2273	0.9	1.7540	-1.46056E+01
2273	0.9	1.7550	-1.46059E+01
2273	0.9	1.7560	-1.46063E+01
2273	0.9	1.7570	-1.46067E+01
2273	0.9	1.7580	-1.46072E+01
2273	0.9	1.7590	-1.46076E+01
2273	0.9	1.7600	-1.46080E+01
2273	0.9	1.7610	-1.46085E+01
2273	0.9	1.7620	-1.46089E+01
2273	0.9	1.7630	-1.46094E+01
2273	0.9	1.7640	-1.46099E+01
2273	0.9	1.7650	-1.46103E+01
2273	0.9	1.7660	-1.46108E+01
2273	0.9	1.7670	-1.46113E+01
2273	0.9	1.7680	-1.46118E+01
2273	0.9	1.7690	-1.46124E+01
2273	0.9	1.7700	-1.46129E+01
2273	0.9	1.7710	-1.46134E+01
2273	0.9	1.7720	-1.46140E+01
2273	0.9	1.7730	-1.46145E+01
2273	0.9	1.7740	-1.46151E+01
2273	0.9	1.7750	-1.46156E+01
2273	0.9	1.7760	-1.46162E+01
2273	0.9	1.7770	-1.46168E+01
2273	0.9	1.7780	-1.46174E+01
2273	0.9	1.7790	-1.46180E+01
2273	0.9	1.7800	-1.46186E+01
2273	0.9	1.7810	-1.46192E+01
2273	0.9	1.7820	-1.46198E+01
2273	0.9	1.7830	-1.46205E+01
2273	0.9	1.7840	-1.46211E+01
2273	0.9	1.7850	-1.46218E+01
2273	0.9	1.7860	-1.46224E+01
2273	0.9	1.7870	-1.46231E+01
2273	0.9	1.7880	-1.46238E+01
2273	0.9	1.7890	-1.46245E+01
2273	0.9	1.7900	-1.46252E+01
2273	0.9	1.7910	-1.46259E+01
2273	0.9	1.7920	-1.46266E+01
2273	0.9	1.7930	-1.46273E+01
2273	0.9	1.7940	-1.46280E+01
2273	0.9	1.7950	-1.46287E+01
2273	0.9	1.7960	-1.46295E+01
2273	0.9	1.7970	-1.46302E+01
2273	0.9	1.7980	-1.46310E+01
2273	0.9	1.7990	-1.46317E+01
2273	0.9	1.8000	-1.46325E+01
2273	0.9	1.8010	-1.46333E+01
2273	0.9	1.8020	-1.46341E+01
2273	0.9	1.8030	-1.46349E+01
2273	0.9	1.8040	-1.46357E+01
2273	0.9	1.8050	-1.46365E+01
2273	0.9	1.8060	-1.46373E+01
2273	0.9	1.8070	-1.46381E+01
2273	0.9	1.8080	-1.46389E+01
2273	0.9	1.8090	-1.46398E+01
2273	0.9	1.8100	-1.46406E+01
2273	0.9	1.8110	-1.46415E+01
2273	0.9	1.8120	-1.46423E+01
2273	0.9	1.8130	-1.46432E+01
2273	0.9	1.8140	-1.46440E+01
2273	0.9	1.8150	-1.46449E+01
2273	0.9	1.8160	-1.46458E+01
2273	0.9	1.8170	-1.46467E+01
2273	0.9	1.8180	-1.46476E+01
2273	0.9	1.8190	-1.46485E+01
2273	0.9	1.8200	-1.46494E+01
2273	0.9	1.8210	-1.46503E+01
2273	0.9	1.8220	-1.46512E+01
2273	0.9	1.8230	-1.46522E+01
2273	0.9	1.8240	-1.46531E+01
2273	0.9	1.8250	-1.46540E+01
2273	0.9	1.8260	-1.46550E+01
2273	0.9	1.8270	-1.46559E+01
2273	0.9	1.8280	-1.46569E+01
2273	0.9	1.8290	-1.46578E+01
2273	0.9	1.8300	-1.46588E+01
2273	0.9	1.8310	-1.46598E+01
2273	0.9	1.8320	-1.46608E+01
2273	0.9	1.8330	-1.46617E+01
2273	0.9	1.8340	-1.46627E+01
2273	0.9	1.8350	-1.46637E+01
2273	0.9	1.8360	-1.46647E+01
2273	0.9	1.8370	-1.46657E+01

2273	0.9	1.8380	-1.46667E+01
2273	0.9	1.8390	-1.46677E+01
2273	0.9	1.8400	-1.46687E+01
2273	0.9	1.8410	-1.46697E+01
2273	0.9	1.8420	-1.46707E+01
2273	0.9	1.8430	-1.46718E+01
2273	0.9	1.8440	-1.46728E+01
2273	0.9	1.8450	-1.46738E+01
2273	0.9	1.8460	-1.46748E+01
2273	0.9	1.8470	-1.46759E+01
2273	0.9	1.8480	-1.46769E+01
2273	0.9	1.8490	-1.46779E+01
2273	0.9	1.8500	-1.46790E+01
2273	0.9	1.8510	-1.46800E+01
2273	0.9	1.8520	-1.46810E+01
2273	0.9	1.8530	-1.46821E+01
2273	0.9	1.8540	-1.46831E+01
2273	0.9	1.8550	-1.46841E+01
2273	0.9	1.8560	-1.46851E+01
2273	0.9	1.8570	-1.46862E+01
2273	0.9	1.8580	-1.46872E+01
2273	0.9	1.8590	-1.46882E+01
2273	0.9	1.8600	-1.46892E+01
2273	0.9	1.8610	-1.46903E+01
2273	0.9	1.8620	-1.46913E+01
2273	0.9	1.8630	-1.46923E+01
2273	0.9	1.8640	-1.46933E+01
2273	0.9	1.8650	-1.46943E+01
2273	0.9	1.8660	-1.46953E+01
2273	0.9	1.8670	-1.46963E+01
2273	0.9	1.8680	-1.46972E+01
2273	0.9	1.8690	-1.46982E+01
2273	0.9	1.8700	-1.46992E+01
2273	0.9	1.8710	-1.47001E+01
2273	0.9	1.8720	-1.47010E+01
2273	0.9	1.8730	-1.47020E+01
2273	0.9	1.8740	-1.47029E+01
2273	0.9	1.8750	-1.47038E+01
2273	0.9	1.8760	-1.47047E+01
2273	0.9	1.8770	-1.47055E+01
2273	0.9	1.8780	-1.47064E+01
2273	0.9	1.8790	-1.47072E+01
2273	0.9	1.8800	-1.47080E+01
2273	0.9	1.8810	-1.47088E+01
2273	0.9	1.8820	-1.47096E+01
2273	0.9	1.8830	-1.47103E+01
2273	0.9	1.8840	-1.47110E+01
2273	0.9	1.8850	-1.47117E+01
2273	0.9	1.8860	-1.47124E+01
2273	0.9	1.8870	-1.47130E+01
2273	0.9	1.8880	-1.47137E+01
2273	0.9	1.8890	-1.47142E+01
2273	0.9	1.8900	-1.47148E+01
2273	0.9	1.8910	-1.47153E+01
2273	0.9	1.8920	-1.47157E+01
2273	0.9	1.8930	-1.47162E+01
2273	0.9	1.8940	-1.47166E+01
2273	0.9	1.8950	-1.47169E+01
2273	0.9	1.8960	-1.47172E+01
2273	0.9	1.8970	-1.47175E+01
2273	0.9	1.8980	-1.47177E+01
2273	0.9	1.8990	-1.47178E+01
2273	0.9	1.9000	-1.47179E+01
2273	0.9	1.9010	-1.47179E+01
2273	0.9	1.9020	-1.47179E+01
2273	0.9	1.9030	-1.47178E+01
2273	0.9		

2273	0.9	1.9300	-1.46815E+01
2273	0.9	1.9310	-1.46785E+01
2273	0.9	1.9320	-1.46753E+01
2273	0.9	1.9330	-1.46720E+01
2273	0.9	1.9340	-1.46686E+01
2273	0.9	1.9350	-1.46650E+01
2273	0.9	1.9360	-1.46612E+01
2273	0.9	1.9370	-1.46573E+01
2273	0.9	1.9380	-1.46532E+01
2273	0.9	1.9390	-1.46489E+01
2273	0.9	1.9400	-1.46445E+01
2273	0.9	1.9410	-1.46399E+01
2273	0.9	1.9420	-1.46352E+01
2273	0.9	1.9430	-1.46303E+01
2273	0.9	1.9440	-1.46252E+01
2273	0.9	1.9450	-1.46200E+01
2273	0.9	1.9460	-1.46145E+01
2273	0.9	1.9470	-1.46089E+01
2273	0.9	1.9480	-1.46032E+01
2273	0.9	1.9490	-1.45972E+01
2273	0.9	1.9500	-1.45911E+01
2273	0.9	1.9510	-1.45848E+01
2273	0.9	1.9520	-1.45783E+01
2273	0.9	1.9530	-1.45717E+01
2273	0.9	1.9540	-1.45649E+01
2273	0.9	1.9550	-1.45579E+01
2273	0.9	1.9560	-1.45507E+01
2273	0.9	1.9570	-1.45434E+01

2273	0.9	1.9580	-1.45358E+01
2273	0.9	1.9590	-1.45281E+01
2273	0.9	1.9600	-1.45203E+01
2273	0.9	1.9610	-1.45122E+01
2273	0.9	1.9620	-1.45040E+01
2273	0.9	1.9630	-1.44956E+01
2273	0.9	1.9640	-1.44870E+01
2273	0.9	1.9650	-1.44783E+01
2273	0.9	1.9660	-1.44693E+01
2273	0.9	1.9670	-1.44603E+01
2273	0.9	1.9680	-1.44510E+01
2273	0.9	1.9690	-1.44416E+01
2273	0.9	1.9700	-1.44320E+01
2273	0.9	1.9710	-1.44222E+01
2273	0.9	1.9720	-1.44122E+01
2273	0.9	1.9730	-1.44021E+01
2273	0.9	1.9740	-1.43918E+01
2273	0.9	1.9750	-1.43814E+01
2273	0.9	1.9760	-1.43708E+01
2273	0.9	1.9770	-1.43600E+01
2273	0.9	1.9780	-1.43490E+01
2273	0.9	1.9790	-1.43379E+01
2273	0.9	1.9800	-1.43266E+01
2273	0.9	1.9810	-1.43152E+01
2273	0.9	1.9820	-1.43036E+01
2273	0.9	1.9830	-1.42918E+01
2273	0.9	1.9840	-1.42798E+01
2273	0.9	1.9850	-1.42677E+01

2273	0.9	1.9860	-1.42554E+01
2273	0.9	1.9870	-1.42430E+01
2273	0.9	1.9880	-1.42303E+01
2273	0.9	1.9890	-1.42175E+01
2273	0.9	1.9900	-1.42046E+01
2273	0.9	1.9910	-1.41914E+01
2273	0.9	1.9920	-1.41781E+01
2273	0.9	1.9930	-1.41645E+01
2273	0.9	1.9940	-1.41508E+01
2273	0.9	1.9950	-1.41369E+01
2273	0.9	1.9960	-1.41227E+01
2273	0.9	1.9970	-1.41082E+01
2273	0.9	1.9980	-1.40935E+01
2273	0.9	1.9990	-1.40783E+01
2273	0.9	2.0000	-1.40628E+01
2273	0.9	2.0010	-1.40468E+01
2273	0.9	2.0020	-1.40304E+01
2273	0.9	2.0030	-1.40136E+01
2273	0.9	2.0040	-1.39966E+01
2273	0.9	2.0050	-1.39793E+01
2273	0.9	2.0060	-1.39618E+01
2273	0.9	2.0070	-1.39441E+01
2273	0.9	2.0080	-1.39262E+01
2273	0.9	2.0090	-1.39082E+01
2273	0.9	2.0100	-1.38901E+01

Titre : Développement d'un modèle thermo-cinétique pour la diffusion du plutonium dans l'oxyde mixte (U,Pu)O₂

Mots clés : Oxyde mixte (U, Pu)O₂, Oxyde de Plutonium, Combustible MOx, diffusion du Pu, DICTRA, cBΩ

Résumé : L'oxyde mixte d'uranium et de plutonium est utilisé dans les réacteurs REP et RNR-Na. Lors de sa synthèse, les conditions de frittage sont à optimiser pour obtenir les teneurs visées en plutonium et en oxygène ainsi qu'une bonne homogénéité. En réacteur, les pastilles de combustible subissent un fort gradient thermique radial induisant la redistribution du plutonium qui affecte leur comportement. Pour prédire les propriétés thermo-cinétiques de l'oxyde (U,Pu)O_{2+x}, la diffusion du plutonium est modélisée sur la base d'un modèle thermodynamique de type CALPHAD sur l'oxyde mixte.

Les données de la littérature sur la diffusion du plutonium dans (U,Pu)O_{2+x} ont été analysées. Les données expérimentales sont rares et parfois incohérentes entre elles. Ce manque de données a été compensé par l'utilisation du modèle cBΩ pour estimer la diffusion du plutonium dans PuO₂. À partir de notre sélection de données expérimentales et des résultats cBΩ, un modèle DICTRA a été développé sur la diffusion du plutonium dans l'oxyde mixte. Ce modèle permet de calculer le coefficient de diffusion du plutonium pour toute température, teneur en plutonium et stoechiométrie en oxygène.

Title : Development of a thermo-kinetic model for plutonium diffusion in the mixed oxide (U,Pu)O₂

Keywords : mixed oxide of (U, Pu)O₂, Plutonium oxide, MOx fuel, Pu diffusion, DICTRA, cBΩ

Abstract : The uranium and plutonium mixed oxide fuel (U,Pu)O_{2+x} is used in both LWR and SFR reactors. During its synthesis process by sintering, the conditions have to be optimized to get appropriate plutonium content, oxygen stoichiometry and homogeneity. During reactor operation, the fuel pellet experiences high thermal radial gradient resulting in redistribution of plutonium affecting the fuel behavior. In order to develop a better understanding and prediction of the thermo-kinetic properties of mixed oxide (U,Pu)O_{2+x} for both sintering synthesis and in-pile fuel behavior, this work focuses on modelling the plutonium diffusion based on the reliable CALPHAD thermodynamic model for mixed oxide fuel.

We first analyzed the available literature plutonium diffusion data in (U,Pu)O_{2+x} mixed oxide. The scarcity and inconsistency of the experimental data was observed. This lack of data was then complemented by the use of cBΩ model for the estimation of plutonium diffusion in PuO₂. Based on our selection of experimental data and the cBΩ results, a DICTRA based diffusion model was developed for plutonium diffusion in mixed oxide fuel. This model is able to compute the plutonium diffusion coefficient at any temperature, plutonium composition and oxygen stoichiometry.