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Density and viscosity correlations and thermodynamic properties in post-combustion CO_2 capture processes

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Summary:

Physicochemical properties such as density and viscosity are critical in the design of process equipment in the post combustion amine-based CO_2 capture process because they appear in the majority of the mass transfer and interfacial area correlations of the random and structured packing in the absorption column.

Potential absorbents' density and viscosity have been tested and published in the literature at various amine concentrations and temperatures. The Gibbs free energy as molar properties is derived using observed viscosity and density from the literature and fitted to the empirical correlations to reflect the data and equations that may be used to determine other physical characteristics. Estimated coefficients from the correlation fitted data, used to develop a new correlation for the free energy of activation and excess free energy of activation.

The maximum deviation *AARD* of the Redlich and Kister correlation which used for data fitting was less than 4% which is acceptable, and the *AARD* of the new correlation developed in this work was under 1% which shows a quite good accuracy.

The influence of pressure on the trend changes of the free energy of activation and excess free energy of activation might be fascinating in this task because it was done using measured data under atmospheric conditions.

Contents

Nomenclature

symbols	explanations	units
ΔG^{*}	Free energy of activation for viscous flow	J/mol
ΔG^{E*}	Excess free energy of activation for viscous flow	J/mol
h	Planck's constant	J/Hz
i, j, k	Any component	-
M	Molecular weight	kg/mol
N	Total number of polymer and solvent moles	-
N_A	Avogadro's number	$mol{-1}$
η	Viscosity	$mPa{\cdot}s$
ρ	Density	$kg/m3$
R	Universal gas constant	$J{\cdot}K{-1}\ mol{-1}$
T	Temperature	-
τ	Interaction energy between different species	-
V	Molar volume	m^3/mol
V^E	Excess molar volume	m^3/mol
w	Mass ratio	-
x_i	Mole fraction of component	-

Abbreviations

AARD	Average absolute relative deviation
AMD	Absolute maximum deviation
DMEA	N-Dimethylethanolamine
DEEA	N-Diethylethanolamine
MEA	Monoethanolamine
MDEA	N-Methyldiethanolamine

1 Introduction

This study looks at calculating different molar properties like molar volume and free energy of activation for viscous flow from density and viscosity data for binary aqueous amine mixtures, as well as investigating partial molar properties and excess molar properties, and developing correlations to represent partial molar properties and excess molar properties of different amine mixtures.

1.1 Background

Separation and collection of CO_2 from gas streams is now possible using a variety of methods. They are based on absorption, adsorption, membranes, and cryogenics, among other physical and chemical processes. Amine-based methods are notable among CO_2 collection technologies. Because of their reversible interactions with CO_2, amines are useful for separating CO_2 from a variety of CO_2-containing gases, including flue gas. In recent decades, post-combustion CO_2 capture (PCC) employing absorption and desorption has gotten a lot of interest, and numerous amines have been studied for their absorption effectiveness. Monoethanolamide (MEA, IUPAC name:2-aminoethanol) has been utilized in acid gas treatment since 1930. It serves as a standard amine for comparing the performance of different amines in terms of CO_2 capture efficiency, reaction rates, energy demand, and corrosion resistance. [1]

1.2 CO_2 capture technology

CO_2 is captured at atmospheric pressure in exhaust systems during CO_2 capture process. This procedure is more difficult to accomplish in exhaust systems than in natural gas separation due to low CO_2 partial pressure and low concentration in raw flue gas. A gas turbine's flue gas is transported via an absorption column during post combustion capture (PCC). The gas passes through a liquid absorption solvent as it travels from the bottom intake to the top output. The amine solvent interacts with CO_2 in this situation, cleaning the gas before it is released into the environment. The CO_2 rich amine is then sent via a stripper column, where a linked reboiler raises the temperature. The amine releases CO_2 through the top of the column due to the high temperature. The regeneration method allows the lean amine to be reused in the absorption column. CO_2 from the exit stream may now be chilled, compressed, and delivered offshore to be stored in seabed formations. Figure 1.1 illustrates an example of this mechanism. The graphic also demonstrates how the process might be improved by cooling regenerated lean amine with rich amine. [2] [3]

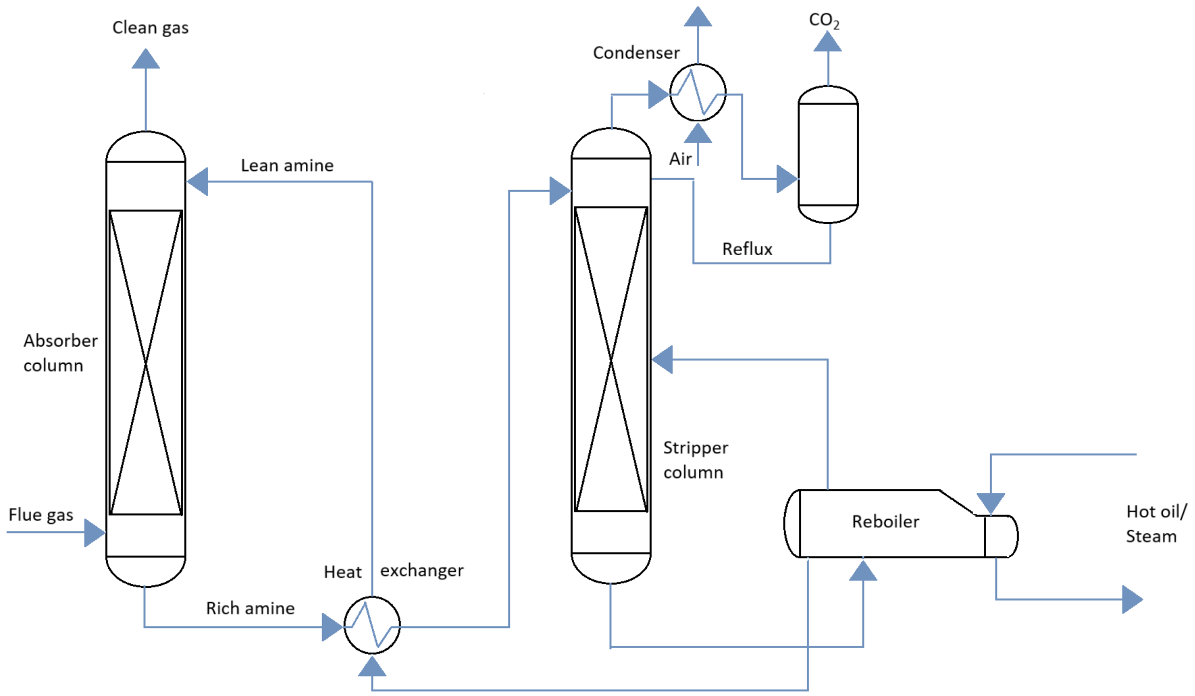

Figure 1.1: CO_2 capture process in a brief based on Larsen et al [3]

1.3 Objectives

In this work, first Eyring viscosity model applied to partial free activation energy of different amines solutions for various flow. Then the excess free energy of activation was calculated. In the meantime, different model developed and $\overline{G_1}$ and $\overline{G_2}$ were calculated based on estimated parameter from Redlich and Kister Correlation by curve fitting method. Then the accuracy of the model has been checked and new correlation for $\overline{G_1}$ and $\overline{G_2}$ in different molar fraction and temperature was developed and it is objective to check the accuracy.

1.4 Outline

The first chapter gives and overview of CO_2 capture technology.
Partially molar qualities and excess molar properties are defined in Chapter 2.
Chapter 3 Conduct a literature search for density and viscosity correlations for pure liquids and liquid mixes that are based on observed data, as well as difficulties with calculations and outcomes.
Chapter 4 gives an overview of correlations and evaluation of correlations.
In Chapter 5, we look at existing and new mathematical correlations for the Gibbs excess free energy to represent the nonideal term in Eyring's viscosity model, as well as the results of our calculations. Curve fitting was used to fit the Gibbs excess free energy to empirical and novel correlation models.
The findings of curve fitting models are discussed in Chapter 6.
Chapter 7 includes the conclusion of applied models and possible further work.

2 Background theory

The goal of this chapter is to set the theoretical basis for using thermodynamics to study gas mixtures and liquid solutions and introduce partial properties, a type of thermodynamic property specified theoretically to distribute total mixture attributes across individual species in a mixture. These are composition-dependent and different from pure species' molar characteristics.

2.1 Relationship of essential property

Equation 2.1 defines the total Gibbs energy of every closed system in terms of its canonical variables, temperature, and pressure. [4]

$$d(nG) = (nV)dP - (nS)dT \tag{2.1}$$

where *n* is the system's total number of moles. It refers to a closed system with a single-phase fluid and no chemical processes.

In the more general scenario of a single-phase, *open* system, material can enter and exit, and *nG* becomes a function of the amount of moles of the chemical species present. It is still a function of *T* and *P*; thus, we can express the functional connection as follows: [4]

$$nG = g(P, T, n_1, n_2, \dots, n_i, \dots)$$

where n_i is the number of moles of species *i*. The entire differential of *nG* is therefore indicated in equation 2.2.

$$d(nG) = \left[\frac{\partial(nG)}{\partial P}\right]_{T,n} dP + \left[\frac{\partial(nG)}{\partial T}\right]_{P,n} dT + \sum_i \left[\frac{\partial(nG)}{\partial n_i}\right]_{P,T,n_j} dn_i \tag{2.2}$$

The total is calculated for all species present, with the subscript n_j indicating that all mole counts except the i^{th} are maintained constant. The derivative gets its own symbol and name in the final term. Thus, the chemical potential of species *i* in the combination follows equation (2.3) by definition. [4]

$$\mu_i \equiv \left[\frac{\partial(nG)}{\partial n_i}\right]_{P,T,n_j} \tag{2.3}$$

3 Theory and literatures

This chapter reviews the literature for theoretical and empirical models of physicochemical properties such as density and viscosity, which are important in the design of process equipment in the post-combustion amine-based CO_2 capture process because they appear in most mass transfer and interfacial area correlations of random and structured packing in the absorption column. The density and viscosity of possible absorbents have been studied and reported in the literature under various amine concentrations and temperatures to represent data that can be used to determine other physical qualities by fitting the measured values to empirical correlations. [3]

3.1 Amines

Organic molecules with the same level of oxidation as ammonia are called ammonia derivatives. When one, two, or three hydrogen atoms are replaced by organic carbon groups, these derivatives are known as amines. Primary amines (RNH_2) have one carbon group connected to nitrogen atom (N), while secondary amines (R_2NH) have two. Three carbon groups are found in tertiary amines (R_3N). Methylamine, methylethanolamine, and triphenylamine are examples of these three forms of amines. [5]

3.2 Partial properties

3.2.1 Partial molar properties

Eq. (2.3) defines the chemical potential as the mole-number derivative of *nG*, implying that additional mole-number derivatives may be relevant in solution thermodynamics. As a result, equation 3.1 is used to represent the partial molar property $\bar{M}_i$ of species *i* in solution. [4]

$$\bar{M}_i \equiv \left[\frac{\partial(nM)}{\partial n_i}\right]_{P,T,n_j} \tag{3.1}$$

On a unit-mass as well as a molar basis, the generic symbols *M* and $\bar{M}_i$ can be used to represent solution characteristics. Equation (3.1) is the same as before, except that *n*, the number of moles, is substituted by *m*, the mass, and partial specific attributes are obtained instead of partial molar qualities. Partially properties can be used to accommodate either. The focus here is on solutions, with molar characteristics denoted by the letter *M*. An overbar with a subscript to indicate the species is used to express partial qualities; the sign is therefore $\bar{M}_i$. Furthermore, just a subscript is used to identify the characteristics of particular species in their pure state at *T* and *P* in the solution, and the sign is M_i. [4]

The chemical potential and the partial molar Gibbs energy are equal, as shown in Eq. (3.2) by the comparison of Eq. (2.3) with Eq. (3.1) stated for the Gibbs energy. [4]

$$\mu_i \equiv \bar{G}_i \tag{3.2}$$

3.2.2 Partial properties in Binary solutions

The equation of partial properties as a function of composition can be derived from the equation of properties of the solution by directly applying Eq. (3.1). However, for binary systems, another method may be more convenient. A sum-relationship expression written for a binary solution looks like Eq. (3.3) [4]

$$M = x_1\bar{M}_1 + x_2\bar{M}_2 \tag{3.3}$$

And in differential form become as:

$$dM = x_1 d\bar{M}_1 + \bar{M}_1 dx_1 + x_2 d\bar{M}_2 + \bar{M}_2 dx_2 \tag{3.4}$$

Eq. (3.5) is the proper version of the Gibbs/Duhem equation when M is known as a function of x_1 at constant T and P. [4]

$$x_1 d\bar{M}_1 + x_2 d\bar{M}_2 = 0 \tag{3.5}$$

$dx_1 = dx_2$ arises from the fact that $x_1 + x_2 = 1$. When x_1 and x_2 are removed independently, two equivalent versions of Eq. (3.3) are obtained. When Eq. (3.5) is used, the result is: [4]

$$\bar{M}_1 = M + x_2\frac{dM}{dx_1} \quad and \quad \bar{M}_2 = M - x_1\frac{dM}{dx_1} \tag{3.6}$$

The partial properties of binary systems may thus be determined directly from a formula for the solution property as a function of composition at constant T and P.

3.2.3 Excess properties

Experimental PVT measurements are closely connected to the residual Gibbs energy and the fugacity coefficient. Where such data can be appropriately connected by equations of state, residual properties can easily offer thermodynamic-property information. Liquid solutions, on the other hand, are frequently dealt with using qualities that quantify deviations from ideal-solution behavior rather than ideal-gas-state behavior. [4]

Excess properties have a mathematical formalism that is similar to residual properties, but it is based on ideal-solution behavior rather than ideal-gas-state behavior. If *M* is the molar (or unit-mass) value of any broad thermodynamic attribute (*e.g., V, U, H, S, G, etc.*), The difference between a solution's actual property value and the value it would have if it were an ideal solution at the same temperature, pressure, and composition is known as M^E. [4]

Thus,

$$M^E \equiv M - M^{id} \tag{3.7}$$

3.3 Density

A substance's density is defined as its mass per unit volume. Understanding how the density of pure and liquid mixtures is affected by pressure and temperature is crucial. Density usually rises as pressure rises and falls as temperature rises.

Due to intermolecular interaction between component molecules, the density of an actual liquid mixture differs from an ideal liquid combination. Excess molar volume V^E of the liquid combination is used to describe this divergence. The density of the combination is then characterized using surplus molar volumes and pure substance molar volumes, as shown in Eq (3.8) [6]

$$\rho = \frac{\sum_1^2 x_i.M_i}{V^E + \sum_1^2 \frac{x_i.M_i}{\rho_i}} \tag{3.8}$$

The thermodynamics-based mathematical formula for excess molar volumes allows for the analysis of observed density under various solution compositions. The excess molar volume, abbreviated as V^E, is defined as: [6]

$$V^E = V - (x_1V_1 + x_2V_2) \tag{3.9}$$

3.4 Viscosity

Internal fluid friction or resistance to deformation by applied stress is referred to as viscosity. The viscosity of fluid molecules is defined by their collisions and interactions, making it challenging to develop a generalized theoretical model that fits all cases. Poling, et al. [7] claimed that there is no equivalent theoretical foundation for estimating liquid viscosity, and that experimental evidence should be used to calculate liquid viscosity. [6]

The notion of viscosity was first proposed by Isaac Newton (1643-1727) by linking the shear stress and velocity gradient of fluid. [8] As demonstrated in Eq. (3.11), it is the ratio of shear stress per unit area to velocity gradient. [6]

$$\tau_{yx} = -\eta \frac{d\vartheta_x}{d_y} \tag{3.10}$$

The viscosity coefficient is found in heat and mass transfer correlations of packing materials used in absorption column design as well as heat transfer correlations used in heat exchanger design. [6]

Many studies have been conducted on the measurement and correlation of solution amine densities for various amine systems with loaded and unloaded CO_2, as well as the use of these data to analyze their thermodynamic properties using correlation and prediction approaches. A review and presentation of some previously published literature on this topic is provided. [6]

3.5 Correlation and prediction

The correlation and prediction approach are a crucial tool in explaining the behavior of a real mixture using the attributes of its pure components and existing experimental data in thermodynamics and phase equilibria of fluid mixtures. Because they are based on the use of equilibrium models, these approaches may save a lot of money and time when it comes to performing trials. They are, however, constrained by the availability of experimental data. [9] It's crucial to pick the right experimental data models, because mistakes caused by bad models can have a big influence on chemical process design and optimization.

3.6 correlation and prediction classification

There are three types of correlation and prediction approaches. Empirical, theoretical, and semi-theoretical correlation approaches are all available. The given experimental data is fitted to an arbitrary function in an empirical model. This approach is not based on physical theory, and it may be used to interpolate between experimental data. However, because the models are not founded on physical theory, it is important not to extend them to other physical systems or fluid combinations. Because the correlation and prediction approach based on theoretical models is based on physical theory, its models may be used for interpolation and extrapolation as long as the assumptions made during creation are taken into account. The semi-theoretical technique of prediction and correlation aims to extract as much information as possible from the limited data provided. The construction of these models is based on a strict approach, which involves making simplifying assumptions and approximations in order to 13develop a function with parameters that cannot be measured and are replaced by regression coefficients. The term for this procedure is molecular thermodynamics. [5]

3.7 Redlich and Kister correlation

The algebraic description of the thermodynamic properties of nonelectrolyte solutions is investigated by Redlich and Kister. [10] It is easy to master and has been utilized for a number of liquid combinations in the past. The excess molar volume of a binary mixture is stated in a power series as follows: [11]

$$V^E = x_2(1 - x_2)\sum_{i=0}^{i=n} A_i(1 - 2x_2)^i \tag{3.11}$$

3.8 Previous research in the literature

Many studies have been conducted on the measurement and correlation of solution amine densities for various amine systems with loaded and unloaded CO_2, as well as the use of these data to analyze their thermodynamic properties using correlation and prediction approaches. A review and presentation of some previously published literature on this topic is provided.

- Diego D. D. Pinto et al. [12] developed a model to precisely compute the density of aqueous amine solutions used in CO_2 capture as a function of temperature and composition. The model relies on excess Gibbs energy functions, and the functional form of the non-random two-liquid (NRTL) model was employed in this study. In most situations, the model can properly describe the density of the studied systems with variances of less than 0.2%.
- Karunarathne et al. [13] used Eyring's viscosity model based on absolute rate theory to correlate the viscosity of ternary mixtures of N-methyldiethanol amine (MDEA) + monoethanol amine (MEA) + H_2O, Nmethyldiethanol amine (MDEA) + diethanol amine (DEA) + H_2O and 2-amino-2-methyl-1-propanol (AMP) + diethanol amine (DEA) + H_2O. For the combinations MDEA + MEA + H_2O, MDEA + DEA + H_2O, and AMP + DEA + H_2O, the correlations were capable of reflecting viscosity data within AARD 1.9 percent, 1.4 percent, and 2.1 percent, respectively. To further understand the intermolecular interactions in mixes, the excess characteristics of volume V, viscosity, and free energy of activation for viscous flow G were investigated.
- Karunarathne et al. [14] discussed the densities and viscosities of aqueous AMP (2-amino-2-methyl-1-propanol) + MEA (monoethanol amine) + H_2O solutions with and without CO_2. Temperatures of 293.15 K to 343.15 K were used to test density, while temperatures of 293.15 K to 363.15 K were used to measure viscosity. Experimental density data were used to calculate the excess molar volume. The density of unloaded aqueous mixes was represented by a Redlich-Kister type polynomial of excess molar volume. Setschenow-type correlations and modified Weiland's density and viscosity correlations were used to fit density and viscosity data for CO_2 loaded solutions. The free energy of activation for viscous flow of mixtures was calculated using Eyring's viscosity model and observed density and viscosity data. Molecular structure and interactions were used to investigate the volumetric and viscometric characteristics of aqueous mixes. To depict the viscosity of CO_2 loaded solutions, a correlation was developed for the free energy of activation of viscous flow.

The findings show that the suggested relationships for mixture density and viscosity are accurate.

- Tomasz Spietz and Marcin Stec evaluated the densities of carbonated aqueous amine solutions in varied concentrations and CO_2 loadings at temperatures ranging from 293.15K to 333.15K. Temperature and CO_2 loading were used to connect density experimental results. In the instance of monoethanolamine, the amine concentration was also included into the equation.
  A correlation for density prediction of carbonated monoethanoloamine solutions was also found and compared to the Jouyban–Acree model. The fitted models are capable of accurately predicting the density of carbonated amine solutions. If the density of carbonated amine solutions is known, the presented correlations can be used to forecast density or to quantify CO_2 loading of the examined solution. [15]
- Shokouhi et al. [16] evaluated the density and viscosity of aqueous methyldiethanolamine (MDEA) solution, as well as its aqueous mixes with 2-amino-2-methyl-1-propanol (AMP) and diisopropylamine (DIPA) under CO_2 gas loading. Using the experimental apparatus recently constructed in the laboratory [16], measurements of CO_2 solubility were made concurrently at temperatures ranging from 303.15 to 363.15, and pressures up to 2.0 MPa (Jalili et al., 2015). The density and viscosity of solutions are significantly affected by acid gas addition. When the temperature of a mixture is raised, the density and viscosity of the mixture decrease.

3.9 Problem description

By reviewing previous literatures main problems and challenges have been observed as: [17] [18] [19]

- Accurate depiction of a solvent's physical characteristics, which is required for the design and simulation of processes such as density and viscosity, which play a key part in the modeling and design of absorption and desorption towers.
- The effect of excess volume, viscosity, and free energy of activation for viscous flow signs on intermolecular interactions in mixtures
- Temperature effect on the density and viscosity of mixtures.
- Finding a correlation to proposed for the free energy of activation of viscous flow to represent viscosity of CO_2 loaded solutions,
- and accurately predicting the density of carbonated amine solutions developing correlations that may be utilized to forecast the density of carbonated amine solutions or identify the amount of CO_2 in the solution,

4 Method

This chapter details how to calculate and evaluate equations that look at density, viscosity, and Gibbs free energy. Measurement data applied to the aqueous mixture is also included in this section.

4.1 Evaluation of correlation

Curves adapted from the measured properties were evaluated using the density, viscosity, and activation free energy of the viscous flow in aqueous and CO_2-loaded MEA aqueous solutions. The correlation used to represent the density and viscosity data was evaluated using the mean absolute relative deviations and absolute maximum deviations (AARD and AMD) given in equations (4.1) and (4.2). [3]

$$AARD\ (\%) = \frac{100\%}{N} \sum_{i=1}^{N} \left| \frac{Y_i^E - Y_i^C}{Y_i^E} \right| \tag{4.1}$$

$$AMD = MAX \left| Y_i^E - Y_i^C \right| \tag{4.2}$$

Where N, Y_i^E and Y_i^C denote the number of data points, measured property, and computed property, respectively.

4.2 Measurement data

To perform the calculation, measured data including density and dynamic viscosity of pure water and aqueous mixtures in addition of dynamic viscosity for different Amines in different temperatures from 293.15K to 353.15K gathered from literatures. [6] [20] [21] [22]

4.3 Calculations method

Calculations were performed manually with an Excel sheet and applying the curve fitting tools in MATLAB R2021b. For this purpose, 4 different Amines have been considered as MEA, MDEA, DMEA and DEEA. By having measured data for density and viscosity of pure water, Amines and aqueous mixture, molar volume of Amine and mixture and also Gibb's free energy and excess free energy have been calculated. To evaluate the results, in first stage the excess free energy of activation for viscous flow ΔG^{E*} of each Amine illustrated based on different molar fraction for each temperature. In the next stage by using the Redlich-Kister type correlation, the derived term ΔG is fitted and the estimated parameters are shown in Table 4.1. and in the last stage, estimated parameters were used to find a new correlation which shows the best fitting curves.

4.4 Eyring model

According to the principle of absolute rate, Eyring [23] described the process of fluid friction or viscosity between neighboring fluid layers. In a pure liquid that is at rest, individual molecules are continually in motion. Due to the dense packing of molecules, these movements are limited to vibrations of each molecule within a cage generated by its nearest neighbors [8]. The cage is shown as an energy barrier, and the activation energy is defined as the energy required for an individual molecule in the same plane to slip over this potential barrier to the next equilibrium position. [8] [23]

Eyring model provide an expression for dynamic viscosity according to Eq (4.7) [6]

$$\eta = \left(\frac{\delta}{a}\right)^2 \frac{hN}{V} \exp\left(\frac{\Delta G^*}{RT}\right) \tag{4.7}$$

This model has a wide range of applications and is used to analyze both pure and mixed liquids. To create a viscosity model for pure liquids, Salinas, et al. [24] used Eyring's theory and cubic equations of state. Using Eyring's theory and a modified Gibbs energy model, Atashrouz et al. [25] studied the viscosity of ionic liquids. Based on Eyring's theory [26], McAllister created a model to link kinematic viscosities. The rate of each individual intermolecular contact was related to the energy of activation, just as the rate of a chemical reaction.

The key assumption behind the model's construction is that the free energy of activation for viscous flow is additive, and that the likelihood of interactions is solely dependent on concentration and not on the free energy of activation. [6]

5 Calculation

Equation (5.1) represents the absolute rate theory-based Eyring's viscosity model. In this work, viscous flow is represented as a chemical reaction, with the basic operation being the movement of a single molecule from one equilibrium position to another over a potential energy barrier. [1]

$$\eta = \frac{hN_A}{V} \exp\left(\frac{\Delta G^*}{RT}\right) \tag{5.1}$$

where dynamic viscosity, molar volume, Planck's constant, Avogadro's number, free energy of activation for viscous flow, universal gas constant, and temperature are, respectively η, V, h, N_A, ΔG^*, R, and T. Equations (5.1) and (5.2) were used to generate Equation (5.3) for calculating excess free energy of activation for viscous flow ΔG^{E*} for binary liquid mixtures. [1]

$$\frac{\eta}{\eta_{ideal}} = \frac{V_{ideal}}{V} \exp\left(\frac{\Delta G^{E*}}{RT}\right) \tag{5.2}$$

$$\frac{\Delta G^{E*}}{RT} = ln(\eta V) - \sum_{i=1}^{i=2} x_i \ln\left(\eta_i V_i^0\right) \tag{5.3}$$

The mole fraction of components in the mixture, dynamic viscosity, and molar volume of pure liquids are represented by x_i, η_i and $V^0{}_i$ (i = 1 for MEA and i = 2 for H_2O). [1]

Considering other way of derivation of Eq (5.1), ΔG^* Can be expressed as:

$$\Delta G^* = RT \times (\ln \eta \,/\, \ln \frac{hN_A}{V}) \tag{5.4}$$

And with the same derivation for ΔG^{E*}, the new expression can be written as:

$$\Delta G^{E*} = RT \times ((\ln(\eta V) - (x_1 \ln \eta_1 V_1 + x_2 \ln \eta_2 V_2)) \tag{5.5}$$

5.1 Excess free energy of activation calculation

The ΔG^{E*} was calculated using aqueous MEA, MDEA, DMEA and DEEA viscosity and density data for w_1 ranging from 0.3 to 1 and temperatures ranging from 293.15 K to 353.15 K. For this investigation, the viscosity and density of pure water, pure amines and mixtures were collected from Karunarathne et al. [1]. Table 5.1 and Appendix B show the calculated values. To fit the generated term $\Delta G^{E*}/RT$, a Redlich–Kister type correlation was utilized, and the estimated parameters are listed in Table 5.5.

Table 5.1. MEA free excess energy values

Temperatures K	Measured density ρ/kg.m-3 of aqueousMEA	x MEA	x H2O	Density pure MEA kgm-3	Density pure H2O kgm-3	Viscosity pure MEA Pa.s	Viscosity H2O Pa.s	M mea /kgmol-1	M H_2O /kgmol-1	V mea m3/mol	V H_2O m3/mol	η mixture pa.s	ΔG* J/mol	ΔGE* J/mol	Measured Viscosity η/Ps.s	ΔGE*/RT	Ḡ1	Ḡ2
293.15	1012.6	0.1122	0.8878	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.002836	12377.82	1890.554302	0.023376	66656.88	275847.2	88185.98
303.15	1008.2	0.1122	0.8878	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.002109	12064.5	1852.591452	0.014748	67546.55	287660.2	89166.61
313.15	1003.15	0.1122	0.8878	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.001628	11801.55	1815.121708	0.010108	68363.47	299534.4	90163.91
323.15	997.9	0.1122	0.8878	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.00129	11567.27	1810.643432	0.006935	70372.51	311383.2	91162.3
353.15	979.4	0.1122	0.8878	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.00074	11064.26	1734.467966	0.002974	73670.13	347132.6	94260.27
363.15	972.3	0.1122	0.8878	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.000687	11175.14	1957.61517	0.002364	85502.6	359078.9	95303.83
293.15	1018.4	0.1643	0.8357	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.004285	13598.19	2558.085344	0.023376	90192.59	272951.9	120524.9
303.15	1013.3	0.1643	0.8357	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.00308	13242.46	2488.684677	0.014748	90738.88	282979.3	121448.4
313.15	1007.8	0.1643	0.8357	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.002305	12938.79	2416.118544	0.010108	90999	293068	122388.5
323.15	1001.8	0.1643	0.8357	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.001782	12676.57	2392.526045	0.006935	92987.97	303131.2	123329.8
353.15	981.9	0.1643	0.8357	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.00096	12096.09	2253.289613	0.002974	95706.66	333523.9	126256.3
363.15	974.6	0.1643	0.8357	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.000808	11940.68	2212.679923	0.002364	96643.04	343684.6	127242.7
293.15	1023.6	0.2278	0.7722	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.00661	14894.44	3180.519174	0.023376	112138.3	270098.5	154468.7
303.15	1017.8	0.2278	0.7722	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.00458	14492.11	3077.897757	0.014748	112221.9	277896.3	155118.5
313.15	1011.6	0.2278	0.7722	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.00331	14140.52	2964.281507	0.010108	111644.6	285755.2	155784.9
323.15	1005.2	0.2278	0.7722	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.002454	13805.16	2878.277549	0.006935	111867.2	293588.7	156452.4
353.15	984.1	0.2278	0.7722	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.001243	13151.85	2683.791678	0.002974	113991.9	317292.3	158557.7
363.15	976.4	0.2278	0.7722	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.001029	12977.5	2627.318125	0.002364	114753.2	325223.4	159270.4
293.15	1027.7	0.3067	0.6933	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.010217	16226.93	3675.773028	0.023376	129599.9	266254.4	188775.7
303.15	1021.2	0.3067	0.6933	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.006769	15758.76	3523.943329	0.014748	128485	271449.2	189067.3
313.15	1014.5	0.3067	0.6933	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.004736	15365.8	3377.482611	0.010108	127207.1	276705.3	189375.7
323.15	1007.9	0.3067	0.6933	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.003444	15018.11	3292.497981	0.006935	127966.3	281936	189685.1

353.15	985.4	0.3067	0.6933	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.00162	14264.08	3019.120757	0.002974	128234.7	297831	190716.1
363.15	977.4	0.3067	0.6933	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.001319	14071.96	2948.709838	0.002364	128790.6	303159.2	191070.7
293.15	1029.3	0.4077	0.5923	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.015348	17532.87	3909.975682	0.023376	137857.3	258361.1	221196.5
303.15	1022.4	0.4077	0.5923	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.009823	17023.1	3737.83079	0.014748	136283.5	260863	221459.8
313.15	1015.2	0.4077	0.5923	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.006664	16592.8	3564.940755	0.010108	134267.4	263426.1	221739.7
323.15	1007.9	0.4077	0.5923	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.00472	16215.34	3467.272407	0.006935	134759.1	265963.8	222020.8
353.15	984.8	0.4077	0.5923	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.002029	15309.81	3070.343464	0.002974	130410.4	273779.9	222966.8
363.15	976.4	0.4077	0.5923	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.001616	15082.02	2969.161891	0.002364	129683.8	276415.1	223293.1
293.15	1028.1	0.5412	0.4588	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.020521	18608.84	3569.340124	0.023376	125847.3	237874.2	247561.6
303.15	1020.8	0.5412	0.4588	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.01284	18079.75	3406.009986	0.014748	124185.1	238346.6	249159.8
313.15	1013.3	0.5412	0.4588	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.008534	17631.73	3229.826749	0.010108	121645.9	238880.3	250774.7
323.15	1005.7	0.5412	0.4588	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.005937	17240.08	3140.543223	0.006935	122060.4	239388.6	252390.7
353.15	981.9	0.5412	0.4588	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.002483	16351.27	2797.269437	0.002974	118811.8	241116.3	257341.5
363.15	973.6	0.5412	0.4588	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.001962	16128.83	2707.931071	0.002364	118274.1	241722.1	259002.7
293.15	1023.5	0.7264	0.2736	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.024027	19434.37	2429.664879	0.023376	85664.76	180010.9	263395.8
303.15	1015.8	0.7264	0.2736	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.014963	18922.64	2322.710637	0.014748	84687.37	180344.2	269735.4
313.15	1008.1	0.7264	0.2736	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.009879	18485.68	2177.61222	0.010108	82016.06	180738.7	276091.6
323.15	1000.3	0.7264	0.2736	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.006829	18104.8	2130.426185	0.006935	82801.19	181107.8	282449
353.15	976.1	0.7264	0.2736	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.002832	17273.02	1895.426771	0.002974	80506.73	182418	301623.8
363.15	967.8	0.7264	0.2736	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.002222	17055.49	1819.980228	0.002364	79491.13	182884.6	308026.4
293.15	1015.9	1	0	1015.9	998.2336	0.023376	0.001002	0.06108	0.018015	6.01E-05	1.8E-05	0.023376	19907.95	0	0.023376	0	8645.911	281936.5
303.15	1008.1	1	0	1008.1	995.6783	0.014748	0.000797	0.06108	0.018015	6.06E-05	1.81E-05	0.014748	19445.52	0	0.014748	0	8445.08	296938.1
313.15	1000.1	1	0	1000.1	992.2473	0.010108	0.000653	0.06108	0.018015	6.11E-05	1.82E-05	0.010108	19124.09	0	0.010108	0	8305.488	311956.5
323.15	992.1	1	0	992.1	998.07	0.006935	0.000547	0.06108	0.018015	6.16E-05	1.8E-05	0.006935	18744.12	0	0.006935	0	8140.47	326975.9
353.15	967.6	1	0	967.6	971.6	0.002974	0.000354	0.06108	0.018015	6.31E-05	1.85E-05	0.002974	18071.63	0	0.002974	0	7848.41	372137
363.15	959.3	1	0	959.3	965.06	0.002364	0.000314	0.06108	0.018015	6.37E-05	1.87E-05	0.002364	17916.26	0	0.002364	0	7780.933	387201.6

For each amine, the calculated value for ΔG^{E*} related to each molar fraction of the amine for each temperature showed on the graph. Figures 5.1 to 5.4 illustrates the mentions graphs for each amine.

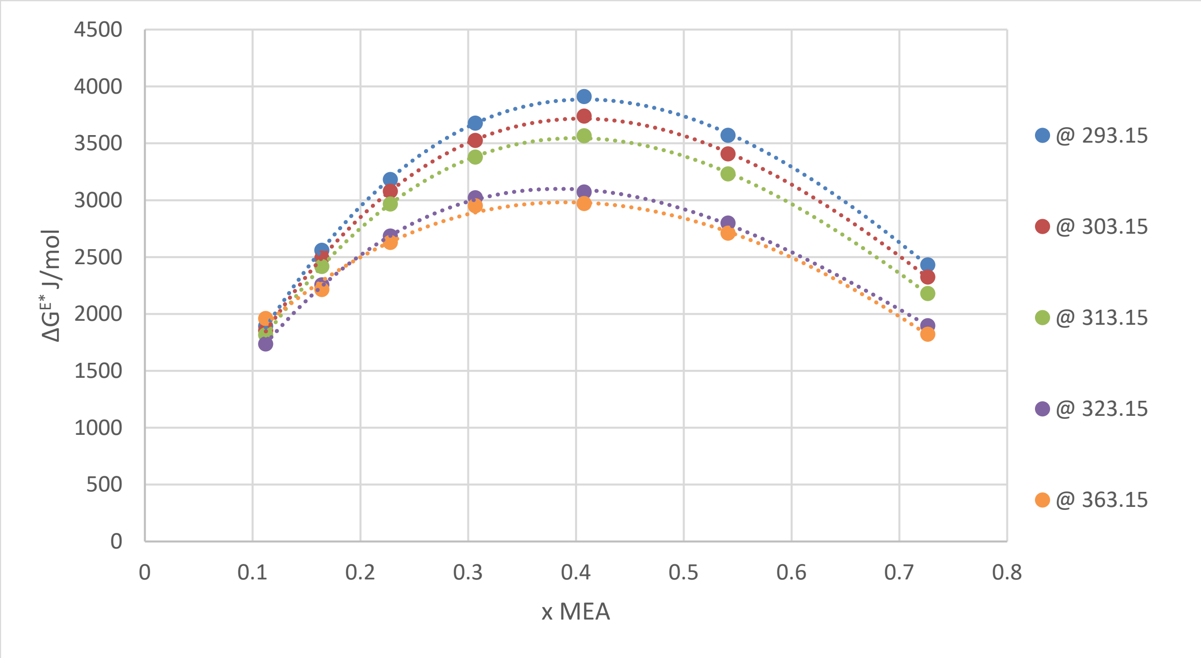

Figure 5.1: Calculated and fitted ΔG^{E*} for aqueous MEA solutions at different concentrations and temperatures.

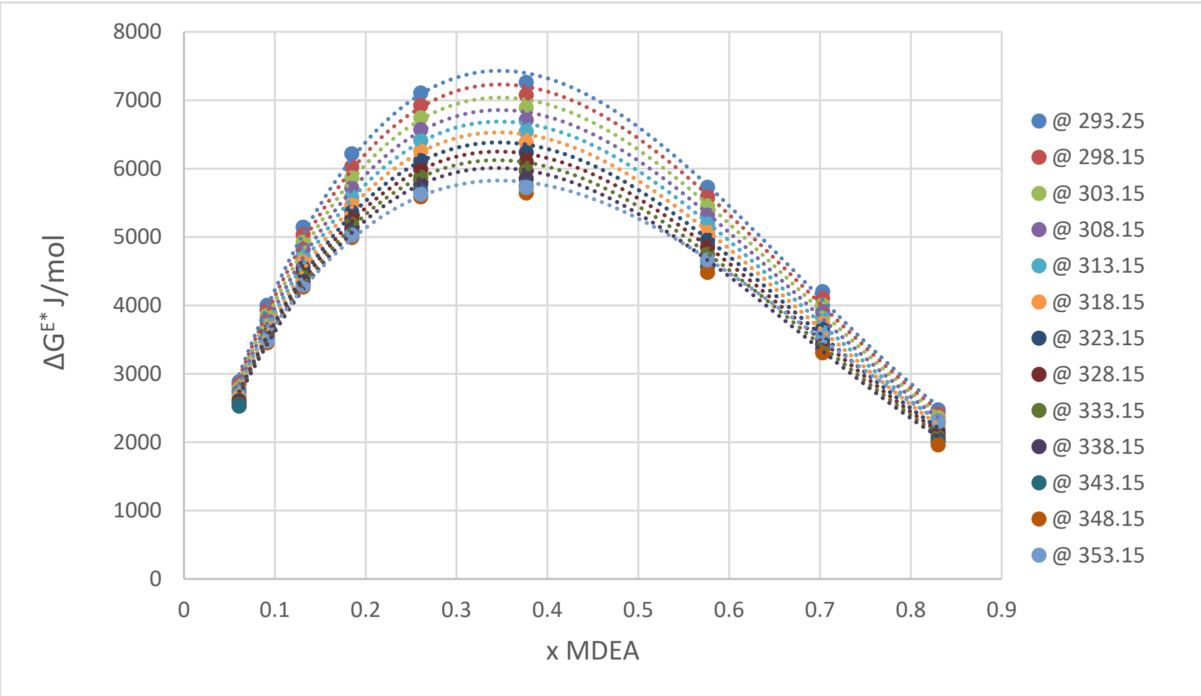

Figure 5.2: Calculated and fitted ΔG^{E*} for aqueous MDEA solutions at different concentrations and temperatures.

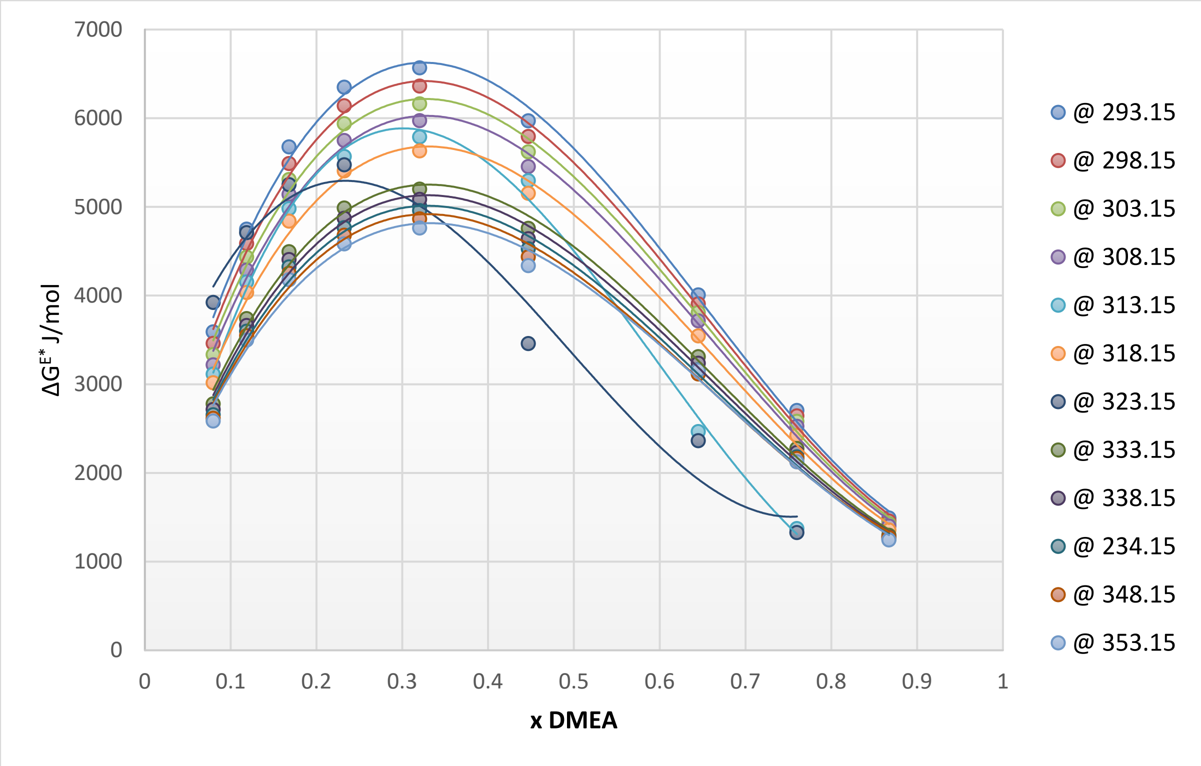

Figure 5.3: Calculated and fitted ΔG^{E*} for aqueous DMEA solutions at different concentrations and temperatures.

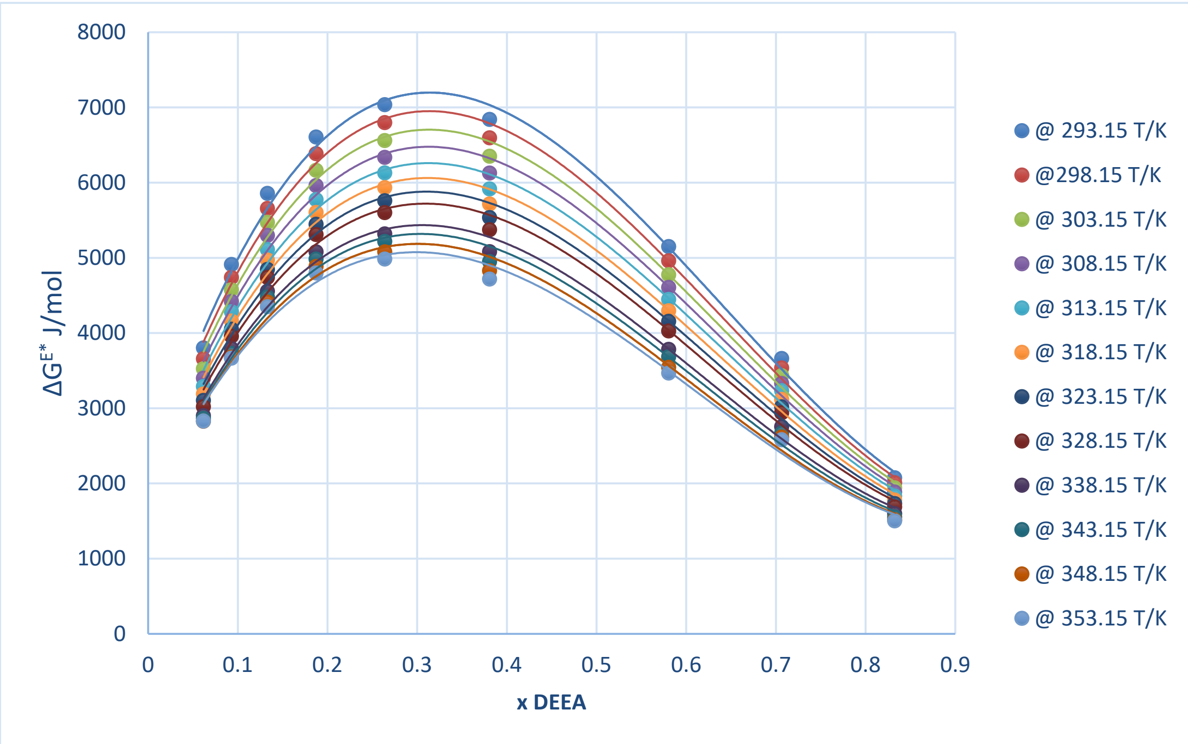

Figure 5.4: Calculated and fitted ΔG^{E*} for aqueous DEEA solutions at different concentrations and temperatures.

5.2 Data fitting to the Redlich–Kister correlation

In order to estimate the Redlich–Kister correlation parameter, the calculated values were imported to MATLAB R2021b. Figures 5.5 to 5.9 show the data fitted graph and the estimated parameter have been shown in table 5.5.

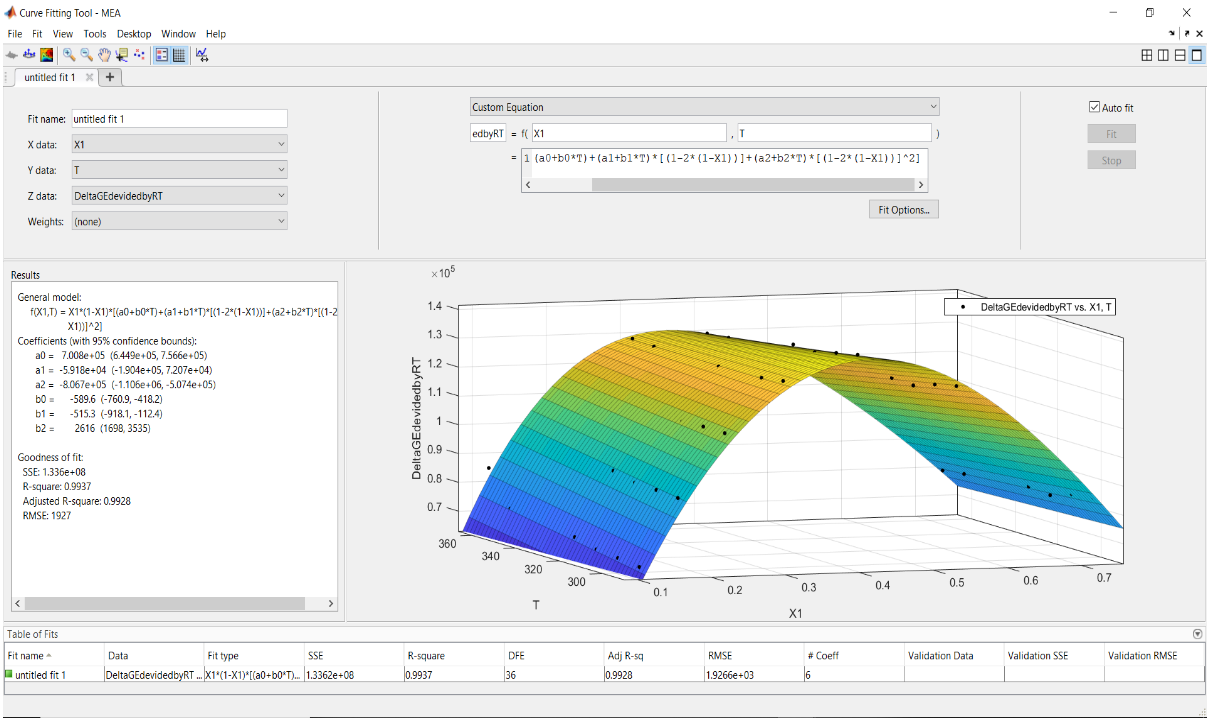

Figure 5.5: Data fitting of the excess free energy of activation for MEA.

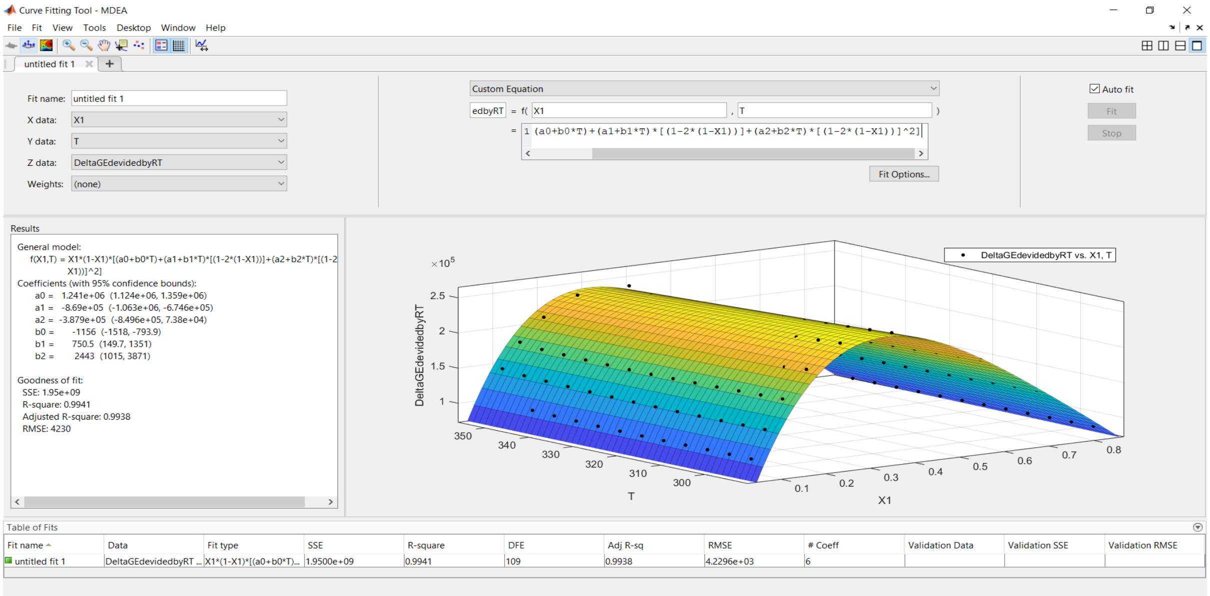

Figure 5.6: Data fitting of the excess free energy of activation for MDEA.

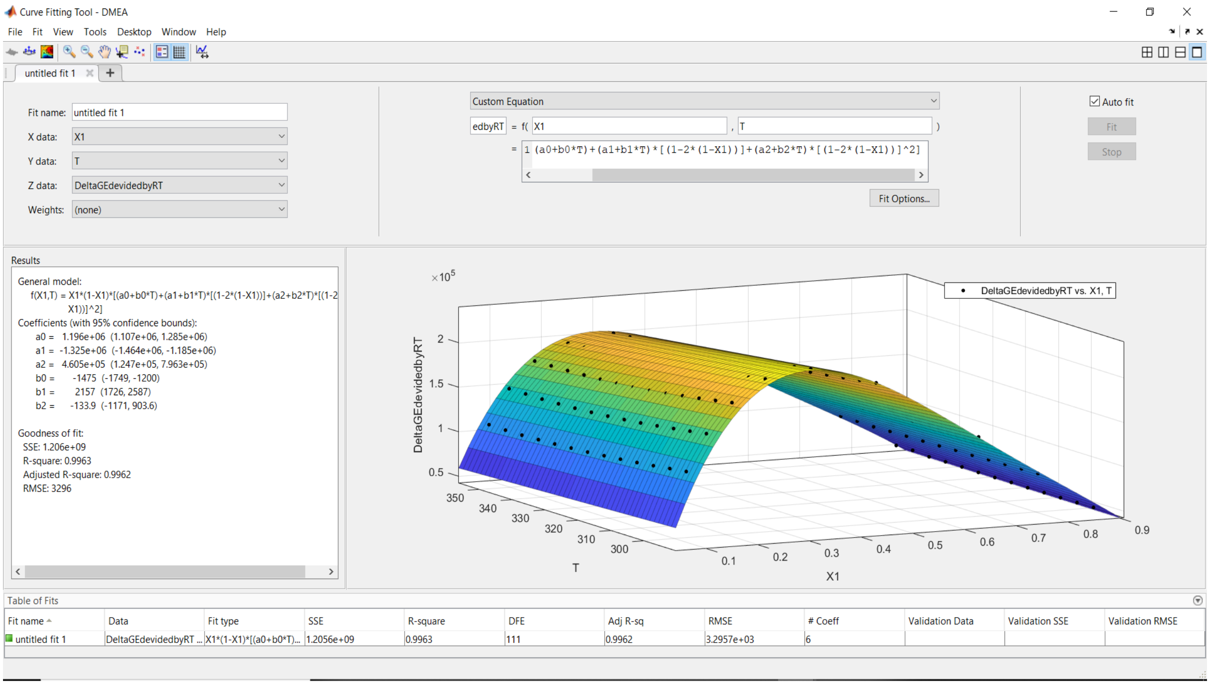

Figure 5.7: Data fitting of the excess free energy of activation for DMEA.

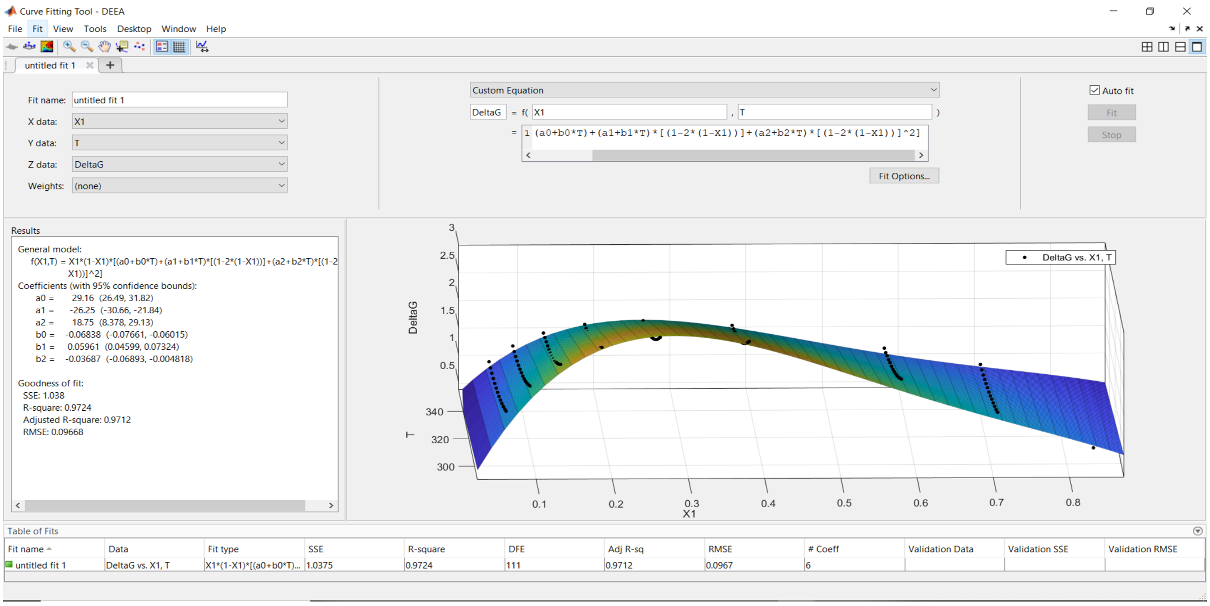

Figure 5.8: Data fitting of the excess free energy of activation for DEEA.

Table 5.5. Excess free energy of activation parameters for viscous flow correlation

Amine	W_1	T/K	Parameter		R^2
MEA	0 - 1	293.15 – 363.15	a_0	700800	0.9928
			b_0	-589.6	
			a_1	-59180	
			b_1	-515.3	
			a_2	-806700	
			b_2	2616	
MDEA	0 - 1	293.15 – 363.15	a_0	1241000	0.9941
			b_0	-1156	
			a_1	-869000	
			b_1	750.5	
			a_2	-387900	
			b_2	2443	

DMEA	0 - 1	293.15 – 363.15	a_0	1196000	0.9962
			b_0	-1475	
			a_1	-1325000	
			b_1	2157	
			a_2	460500	
			b_2	-133.9	
DEEA	0 - 1	293.15 – 363.15	a_0	29.16	0.9724
			b_0	-0.06838	
			a_1	-26.25	
			b_1	0.05961	
			a_2	18.75	
			b_2	-0.03687	

By rewrite the Eq (5.4), $\frac{\Delta G^*}{RT}$ can be expressed as:

$$\log\left(\frac{\eta V}{hN_A}\right) = \frac{\Delta G^*}{RT} \quad and\ for\ pure\ component\ \bar{G}_1^0 = \Delta G^* \tag{5.6}$$

In order to calculate $\overline{M_1}$ in Eq (3.6), first it is needed to have the expression for *M*. From Eq (3.7) it is known that:

$$M \equiv M^E + M^{id}$$

Then,

$$M = x_1 M_1^0 + x_2 M_2^0 + M^E \tag{5.7}$$

By combining the Eq (3.6), Eq (5.7) and Eq (3.11), we have:

$$\overline{G_1} = G_1^{\circ} + x_1[-4a_1 - 4b_1(T) - 2a_0 - 2b_0(T) - 2a_2 - 2b_2(T)] + x_1^2[a_0 + b_0(T) + a_1 + b_1(T) - 3a_2 - 3b_2(T)] + x_1^3[2a_1 + 2b_1(T) + 8a_2 + 8b_2(T)] + x_1^4[-4a_2 - 4b_2(T)] + b_0(T) + a_0 + a_1 + b_1(T) + a_2 + b_2(T) \tag{5.8}$$

By applying estimated data from curve fitting operation, the obtained values are shown in the graphs for each amine.

Figure 5.9 illustrates the $\overline{G_1}$ for MEA amine aqueous mixture.

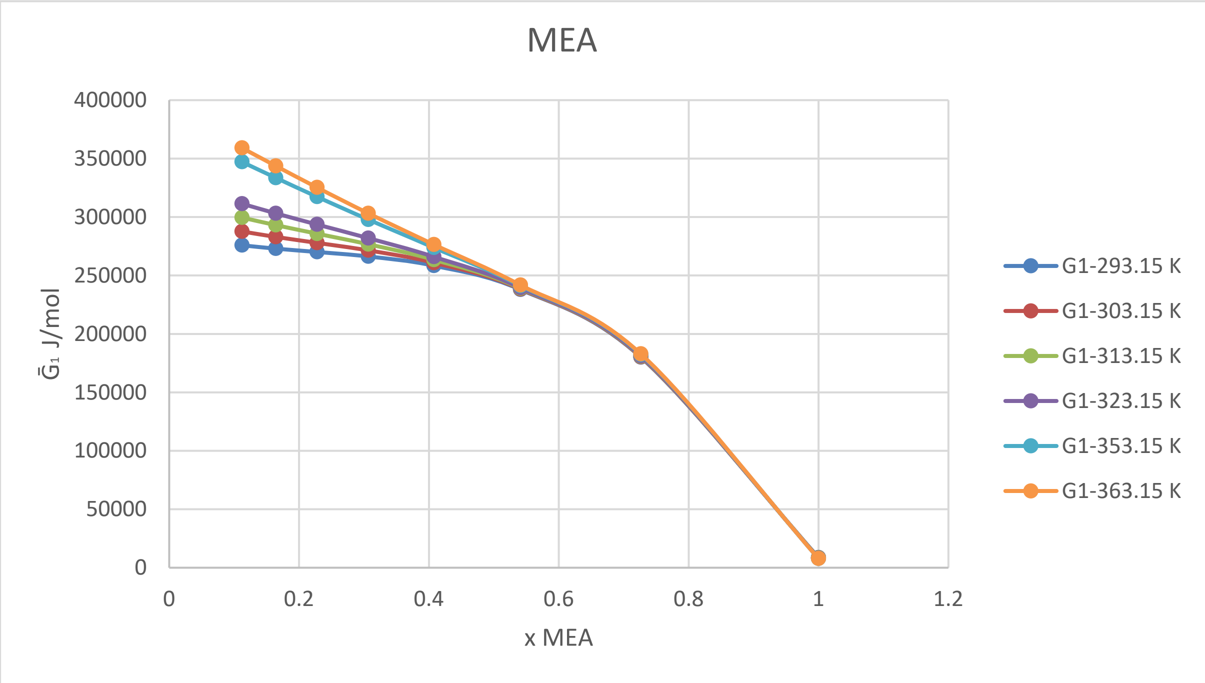

Figure 5.9. $\overline{G_1}$ for MEA amine aqueous mixture.

$\overline{G_1}$ for MDEA, DMEA and DEEA amine aqueous mixture also have been shown in figure 5.10 to 5.12.

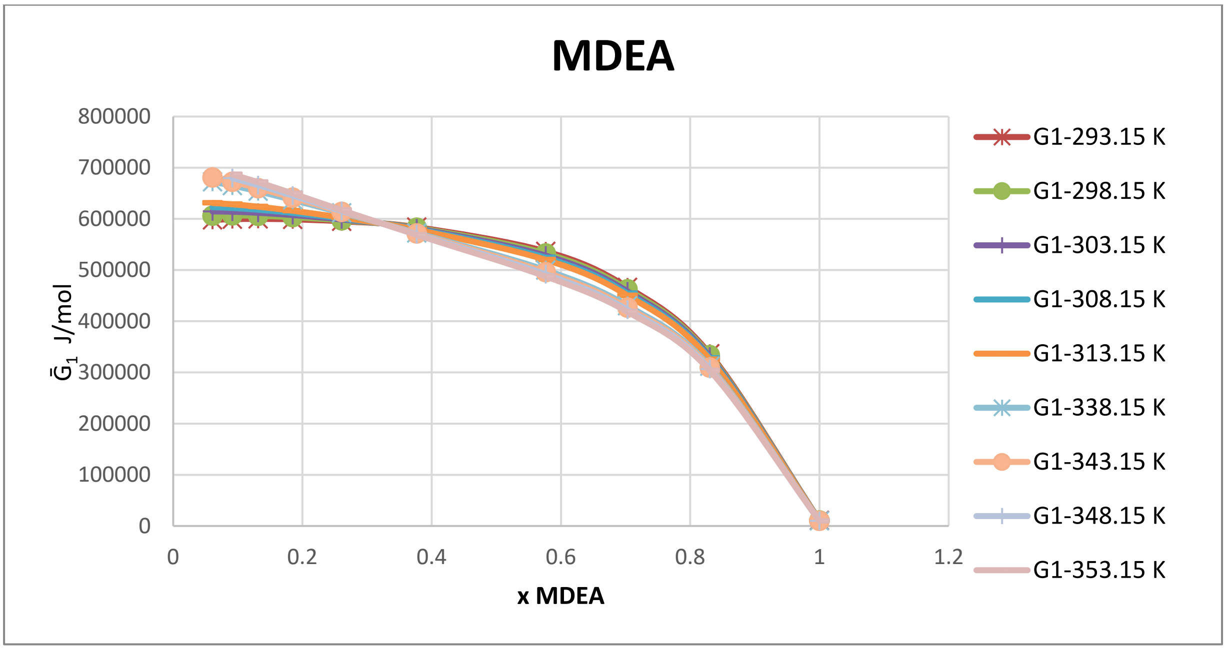

Figure 5.10. $\overline{G_1}$ for MDEA amine aqueous mixture.

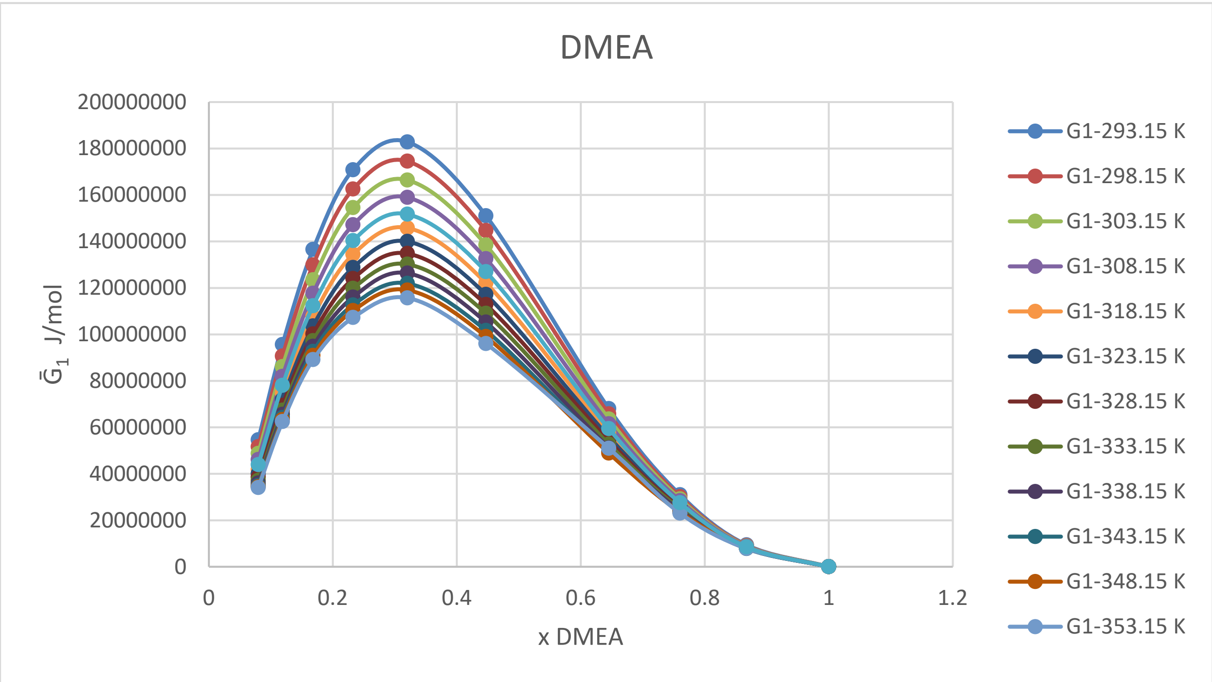

Figure 5.11. $\overline{G_1}$ for DMEA amine aqueous mixture.

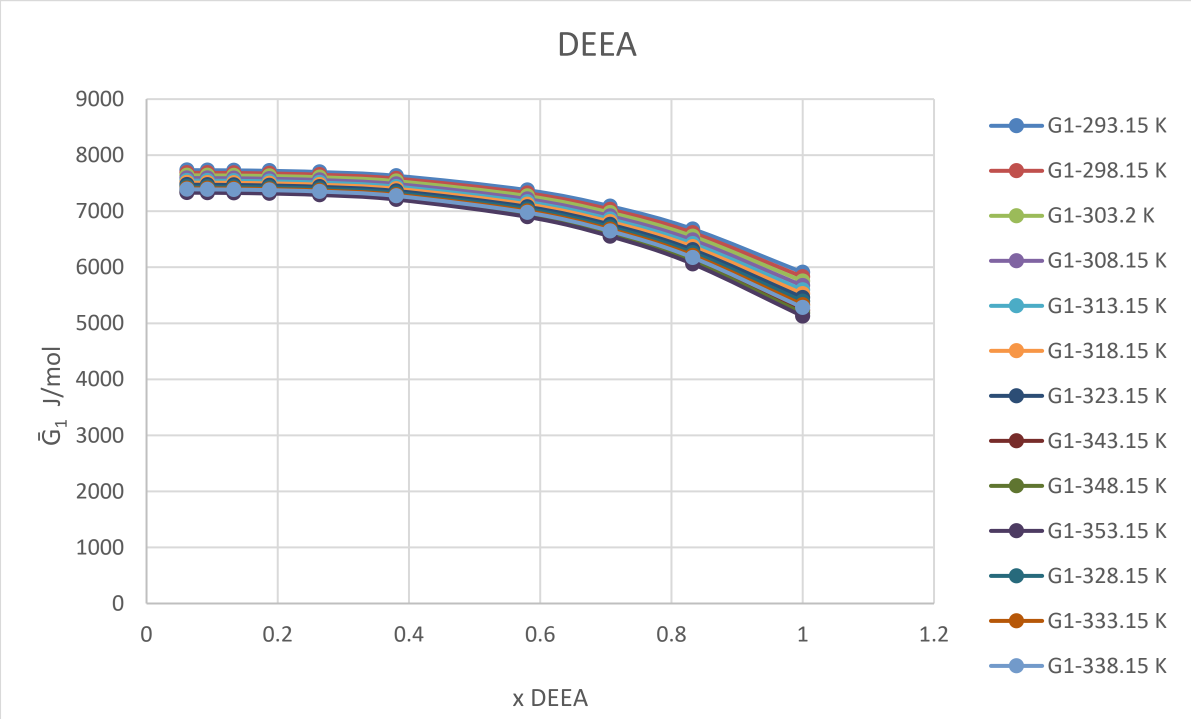

Figure 5.12. $\overline{G_1}$ for DEEA amine aqueous mixture.

The exact values of the calculated terms also have been shown in table (5.1) and appendix B.

6 Result

To introduce new correlation, different equations have been fitted to the calculated data by try and error method in which the result for each amine has been shown in figures (6.1) to (6.4).

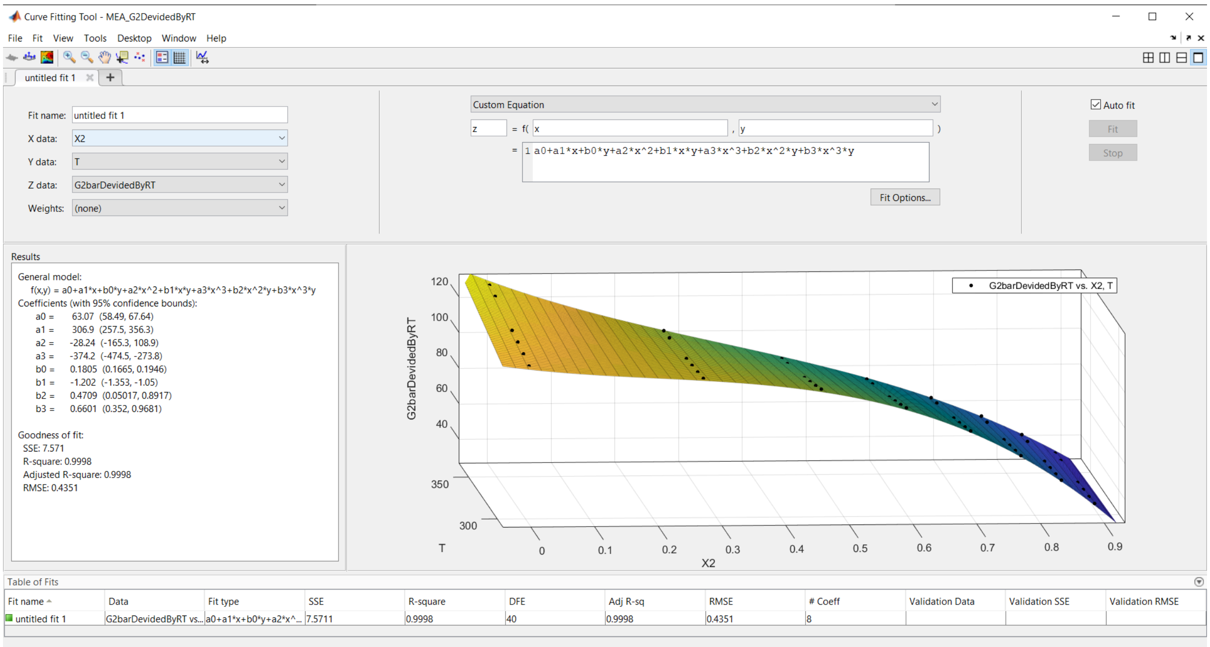

Figure 6.1. New correlation by curve fitting to calculated value of $\overline{G_1}/RT$ for MEA aqueous mixture.

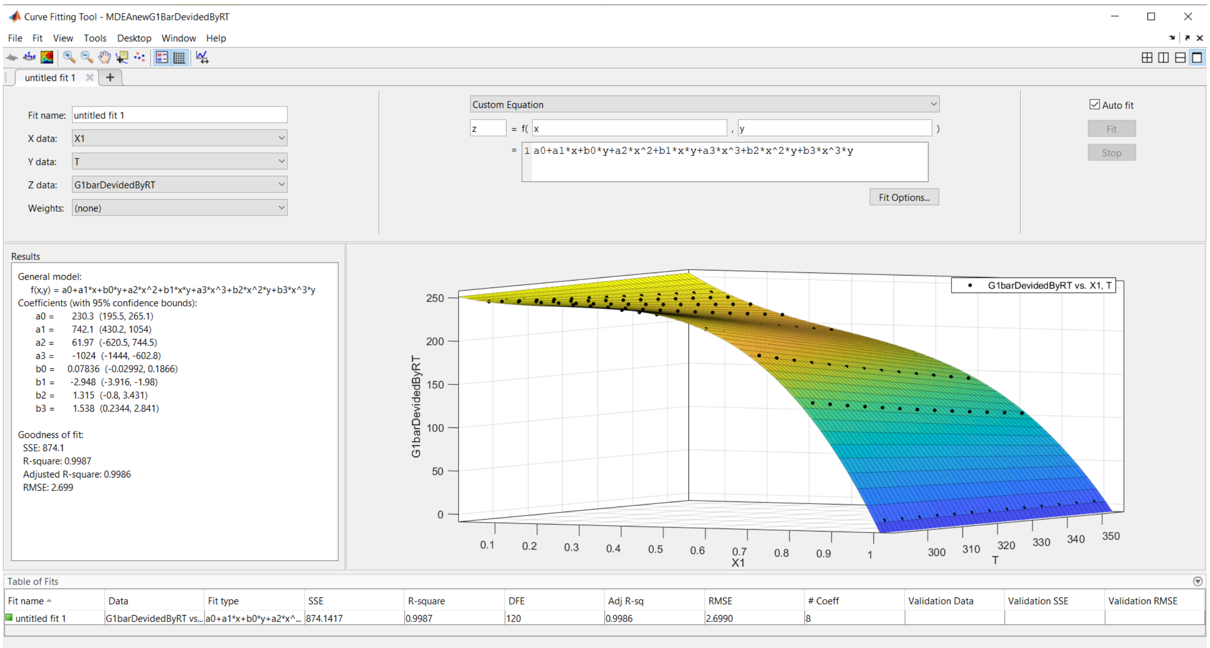

Figure 6.2. New correlation by curve fitting to calculated value of $\overline{G_1}/RT$ for MDEA aqueous mixture.

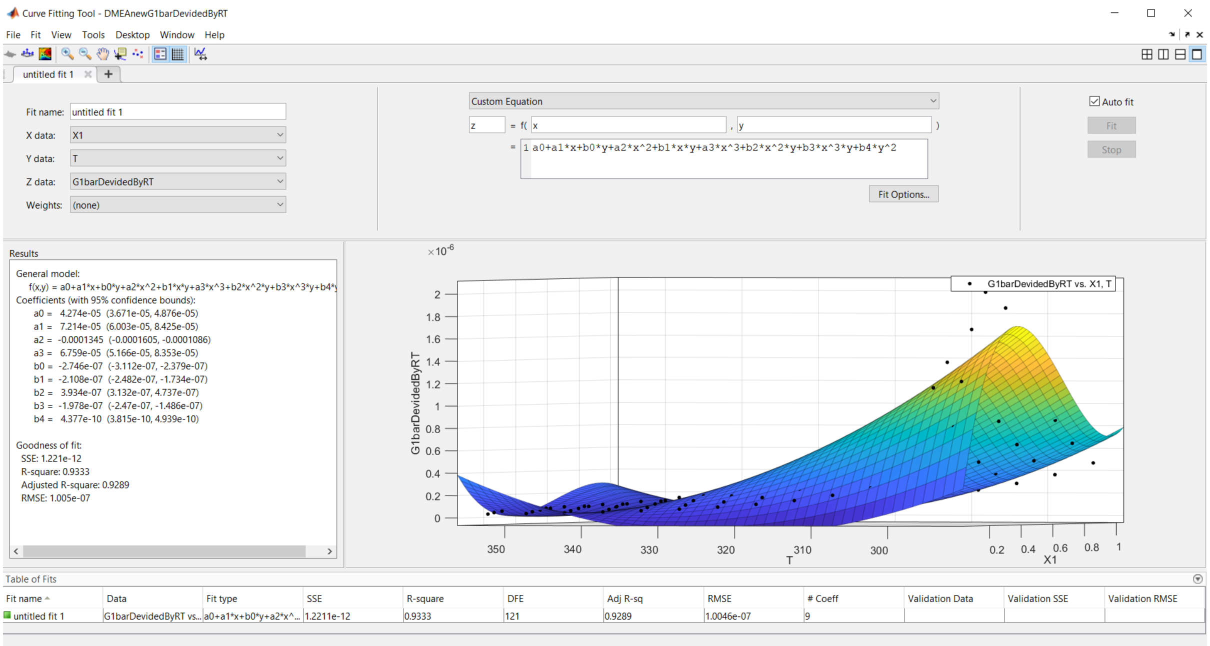

Figure 6.3. New correlation by curve fitting to calculated value of $\overline{G_1}/RT$ for DMEA aqueous mixture.

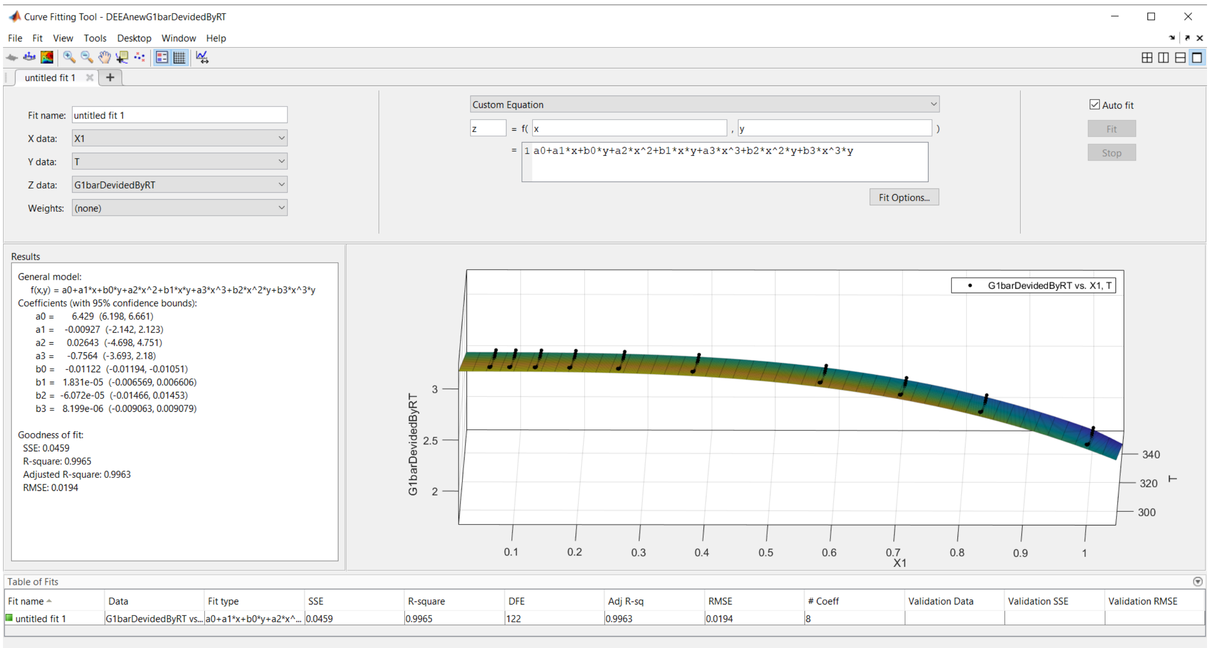

Figure 6.4. New correlation by curve fitting to calculated value of $\overline{G_1}/RT$ for DEEA aqueous mixture.

Table 6.1 shows the new correlation and estimated parameter obtained by curve fitting operation.

Table 6.1. new correlation and estimated parameter

Amine	W_1	T/K	New correlation	Parameter		R^2
MEA	0 - 1	293.15 – 363.15	$a_0 + a_1x_2 + b_0T + a_2x_2^2 + b_1x_2T + a_3x_2^3 + b_2x_2^2T + b_3x_2^3T$	a_0	31.66	0.9999
				a_1	-517.6	
				a_2	-47.92	
				a_3	-1.957	
				b_0	540.5	
				b_1	2.054	
				b_2	-0.3953	
				b_3	0.2878	
MDEA	0 - 1	293.15 – 363.15	$a_0 + a_1x_2 + b_0T + a_2x_2^2 + b_1x_2T + a_3x_2^3 + b_2x_2^2T + b_3x_2^3T$	a_0	230.3	0.9987
				a_1	742.1	
				a_2	61.97	
				a_3	-1024	
				b_0	0.07836	
				b_1	-2.948	
				b_2	1.315	
				b_3	1.538	
DMEA	0 - 1	293.15 – 363.15	$a_0 + a_1x_2 + b_0T + a_2x_2^2 + b_1x_2T + a_3x_2^3 + b_2x_2^2T + b_3x_2^3T + b_4T^2$	a_0	4.274e-05	0.9333
				a_1	7.214e-05	
				a_2	-0.0001345	
				a_3	6.759e-05	
				b_0	-2.746e-07	
				b_1	-2.108e-07	
				b_2	3.934e-07	
				b_3	-1.978e-07	
				b_4	4.377e-10	
DEEA	0 - 1	293.15 – 363.15	$a_0 + a_1x_2 + b_0T + a_2x_2^2 + b_1x_2T + a_3x_2^3 + b_2x_2^2T + b_3x_2^3T$	a_0	6.429	0.9965
				a_1	-0.00927	

				a_2	0.02643	
				a_3	-0.7564	
				b_0	-0.01122	
				b_1	1.831e-05	
				b_2	-6.072e-05	
				b_3	8.199e-06	

7 Discussion

In this chapter the trend of excess free energy of activation change for different amines in various temperature and molar fraction will be discuss. Then the accuracy of model in which used to estimated correlation parameter and the new correlation which was developed will be check and the excess free energy of different amines in same temperature will be compare.

7.1 Free energy of activation and excess free energy of activation

As can be seen in figure 5.1, the maximum of ΔG^{E*} is observed at the lowest temperature which is 293.15K and in the molar fraction of around 0.4 mole. It is obvious from the graph that by increasing the temperature, ΔG^{E*} is supposed to be less and less to become an ideal solution. Figures 5.2, 5.3 and 5.4 also show the same trend as the figure 5.1, which can prove that temperature has a direct effect on the excess molar property of the amins.

Figure 5.9 shows the $\bar{G}_1$ for MEA. The $\bar{G}_1$ has the maximum value on the lowest molar fraction and gradually decrease till the amount of that become almost equal in different temperatures around $x_1 = 0.5$ and then fall to zero by increasing the molar fraction of MEA to 1 which means pure MEA. MDEA follows the same trend except that $\bar{G}_1$ graphs cross each other around $x_1 = 3.7$ and the rate of decrease is a little faster in higher temperatures. DMEA, however, follows a different pattern which is expected due to different viscosity change orientation and rich the maximum around $x_1 = 3.5$ and shows higher values at lower temperatures, while the DEEA follows the same pattern as other 4 amines except that the $\bar{G}_1$ decreases much more smoothly.

Figures 7.1 and 7.2 illustrate ΔG^{E*} for different amines at the same temperature and as can be clearly seen, in both cases the maximum ΔG^{E*} is for MDEA and the minimum ΔG^{E*} is for MEA. DMEA and DEEA however, have a very similar trend in regard of temperature dependency.

The same as Figures 7.1 and 7.2, figures 7.3 and 7.4 show the $\bar{G}_1$ for different amines at the same temperatures. These figures show that MDEA has the maximum value of $\bar{G}_1$ which is much higher than other amins, and the next high value is for MEA. The differences in $\bar{G}_1$ value between these amines is enough big to show the other amines as an almost flat line in the scale of the graph.

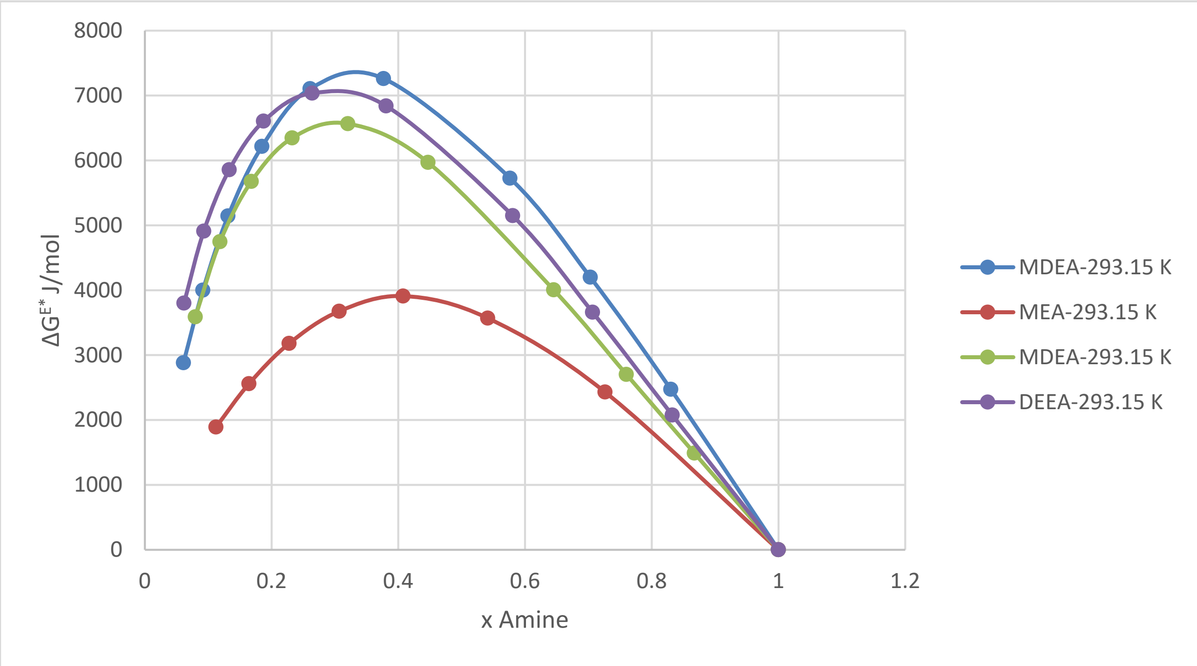

Figure 7.1. ΔG^{E*} for all amine cases at 293.15K temperature.

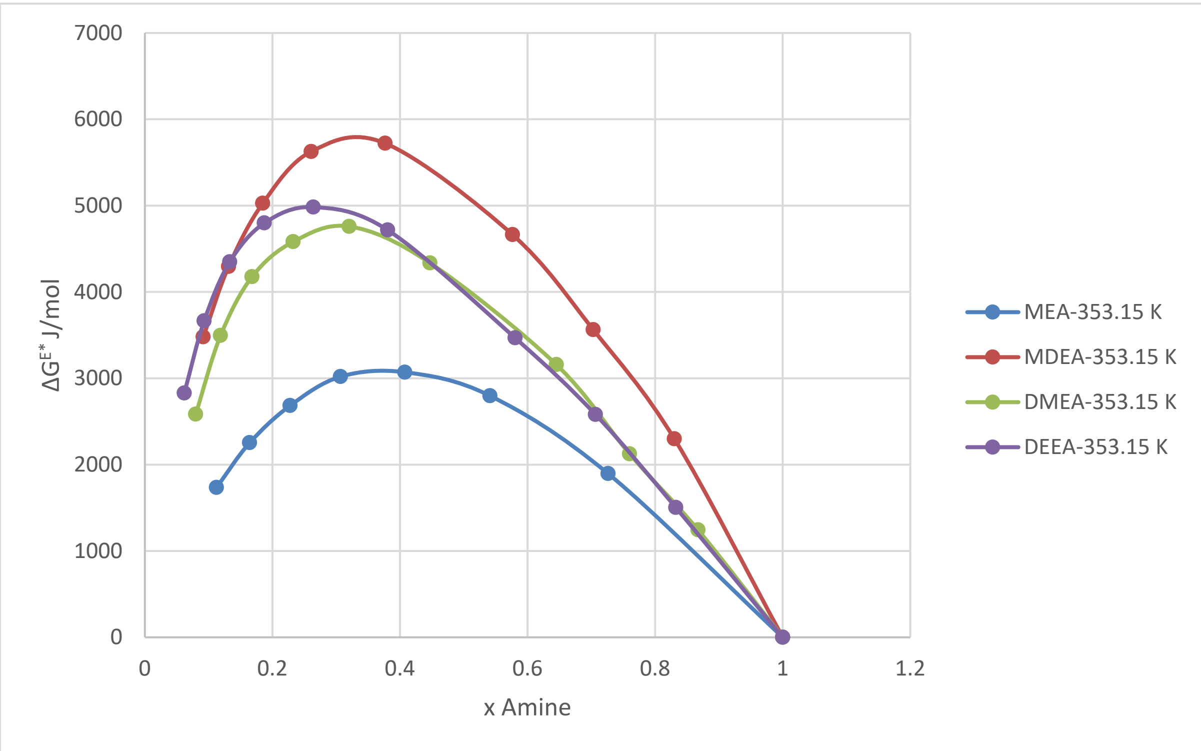

Figure 7.2. ΔG^{E*} for all amine cases at 353.15K temperature.

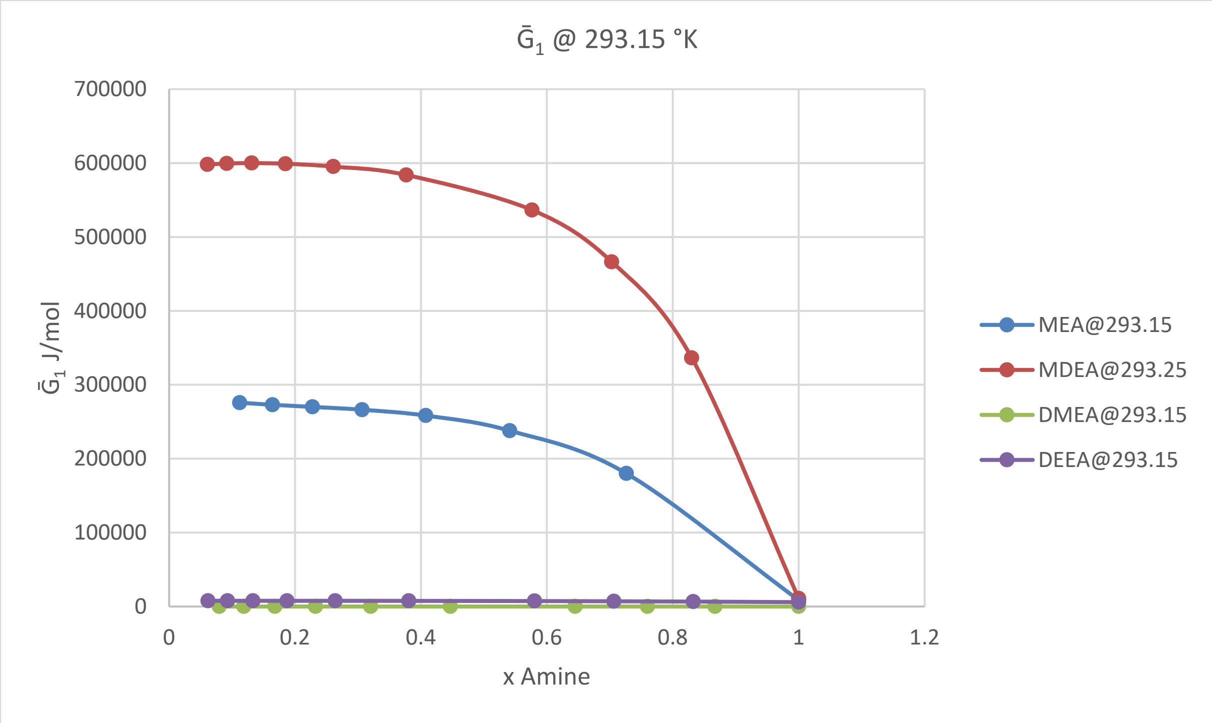

Figure 7.3. $\overline{G_1}$ for all amine cases at 293.15K temperature.

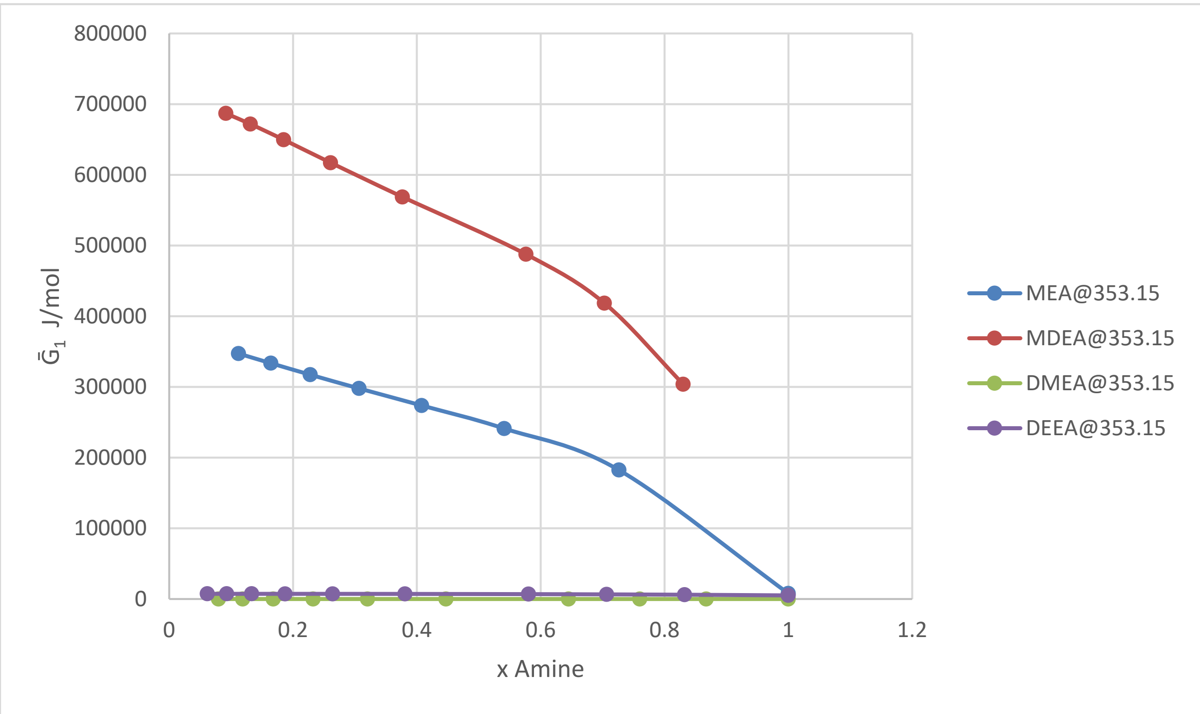

Figure 7.4. $\overline{G_1}$ for all amine cases at 353.15K temperature.

7.2 Model accuracy check

With reference to figures 5.5 to 5.8 and table 5.5, parameter R^2 shows that the selected model is a trustable model with an enough accuracy, however, in order to have a better judgement the term $AARD\%$ was calculated for each model and the values were 0.034% for MEA, 2.6% for MDEA, 3% for DMEA and 15.6% for DEEA which is not ideal but still acceptable for industry. However, the new correlation developed for $\overline{G_1}/RT$ came with very satisfactory parameter R^2 in the range of 0.9333 to 0.9999 which have been mentioned in table 6.1 and the new values for $AARD\%$ term calculated for new correlation to model the $\overline{G_1}$ and $\overline{G_2}$ were 2.8% for MEA, 0.9% for MDEA, 1% for DMEA and 0.9% for DEEA that shows a very accurate model for this property.

8 Conclusion and suggestions

8.1 Aim

The main goal of this research was to evaluate the molar property and excess molar property, particularly the free energy of activation and excess free energy of activation effect on aqueous amine mixtures, and to develop empirical correlations to fit measured data and propose a new correlation for $\overline{G_1}/RT$ and $\overline{G_2}/RT$, compare the results, and evaluate the accuracy of the model chosen.

8.2 Conclusion

Free energy of activation and excess free energy of activation were calculated based on measured density and viscosity from literatures for viscous flow for the MEA + H_2O + CO_2, MDEA + H_2O + CO_2, DMEA + H_2O + CO_2 and DEEA + H_2O + CO_2 and was reported at different CO_2 loadings and temperatures. Redlich – Kister type polynomial for excess molar volume were used to fit the calculated values. In virtually all situations, the proposed correlations were able to match the data with less than 3% AARD. To fit computed values with AARD less than 1%, partial free energy of activation correlations based on Redlich – Kister type polynomials for viscosity deviation and excess free energy of activation for viscous flow from Eyring's viscosity model were constructed. It is advised that engineering calculations be performed using the derived partial energy of activation correlation.

8.3 Suggestions for future work

New correlations were provided to match the free energy of activation and excess free energy of activation data with acceptable accuracies in this master's study. This project might be expanded in the following ways.

- The density and viscosity of amines, pure water, and aqueous mixed solutions in particular temperatures are unknown.
- This job has been done with measured data in atmospheric condition, the effect of the pressure on the trend changes of the free energy of activation and excess free energy of activation can be interesting.

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Appendices

Appendix A: Mater thesis signed task description

University of
South-Eastern Norway

Faculty of Technology, Natural Sciences and Maritime Sciences, Campus Porsgrunn

FMH606 Master's Thesis

Title: Density and viscosity correlations and thermodynamic properties in post-combustion CO_2 capture processes.

USN supervisor: Sumudu Karunarathne, Lars Erik Øi

External partner:

Task background:
Physicochemical properties like density and viscosity are vital in the design of process equipment in the post-combustion amine-based CO_2 capture process as they appear in most of the mass transfer and interfacial area correlations of the random and structured packing in the absorption column. The density and viscosity of potential absorbents have been measured and reported in the literature under conditions like different amine concentrations and temperatures. Measured properties can be fitted to empirical correlations to represent the data and are useful to determine other physical properties.

Task description:

- Perform a literature search on available density and viscosity correlations for pure liquids and liquid mixtures based on measured data.
- Calculate different molar properties such as molar volume, free energy of activation for viscous flow from density and viscosity data for binary aqueous amine mixtures.
- Investigate the partial molar properties and excess molar properties of different amine mixtures.
- Develop correlations to represent partial molar properties and excess molar properties of different amine mixtures.

Student category: Pt and EET students

Is the task suitable for online students (not present at the campus)? Yes

Practical arrangements:

Supervision:
As a general rule, the student is entitled to 15-20 hours of supervision. This includes necessary time for the supervisor to prepare for supervision meetings (reading material to be discussed, etc).

Signatures:

Supervisor (date and signature): 16/05/2022

Student (write clearly in all capitalized letters):

Student (date and signature): 31.01.2022

Appendix B: Calculated values

Table B.1. MDEA free excess energy values.

Temperatures K	x MDEA	x H_2O	Measured density ρ/kg.m-3 of aqueous MDEA	η mixture (Pa.s)	molar volume V of mixture	molar volume V of MDEA m3/mol	molar volume V of water m3/mol	Density pure H_2O kgm-3	Dynamic viscosity of water Pa.s	ΔG* J/mol	ΔGE* J/mol	η MDEA (Pa.s)	ΔGE*/RT	Ḡ1/RT	Ḡ2/RT	Ḡ1	Ḡ2
293.15	0.0609	0.9391	1026.9	0.003712	2.35416E-05	0.000115	1.8E-05	998.2336	0.001002	1241.567	2881.169728	0.10072	101583.8558	245.3733	59.83663	598068.9	145844.8
298.15	0.0609	0.9391	1024.7	0.003136	2.35922E-05	0.000115	1.81E-05	997.0751	0.00089	1300.538	2832.23308	0.0759	101561.652	244.588	58.42515	606323	144833.4
303.15	0.0609	0.9391	1022.4	0.002673	2.36453E-05	0.000115	1.81E-05	995.6783	0.000798	1358.713	2781.199787	0.05782	101404.146	243.8293	57.06218	614578.8	143826.9
308.15	0.0609	0.9391	1019.9	0.002301	2.37032E-05	0.000116	1.81E-05	994.0635	0.00072	1415.743	2732.994828	0.04462	101290.0845	243.0971	55.74511	622839.4	142824.6
313.15	0.0609	0.9391	1017.3	0.001995	2.37638E-05	0.000116	1.82E-05	992.2473	0.000653	1472.171	2682.764822	0.03489	101041.7759	242.3905	54.47151	631105.6	141826
318.15	0.0609	0.9391	1014.5	0.001748	2.38294E-05	0.000117	1.82E-05	990.24	0.000596	1527.091	2641.389732	0.02767	101071.8848	241.7089	53.23912	639379.4	140830.5
323.15	0.0609	0.9391	1011.7	0.001544	2.38953E-05	0.000117	1.82E-05	988.07	0.000547	1581.009	2603.929656	0.02222	101204.3919	241.0508	52.04593	647659.5	139837.9
328.15	0.0609	0.9391	1008.7	0.001376	2.39664E-05	0.000118	1.83E-05	985.73	0.000504	1633.6	2574.614282	0.0181	101613.295	240.4161	50.89001	655948.9	138847.8
333.15	0.0609	0.9391	1005.5	0.001236	2.40427E-05	0.000118	1.83E-05	983.24	0.000467	1685.014	2552.746695	0.01489	102285.3633	239.8021	49.76962	664242.8	137860
338.15	0.0609	0.9391	1002.2	0.001117	2.41218E-05	0.000118	1.84E-05	980.59	0.000433	1735.643	2534.384767	0.01238	103073.7064	239.2085	48.68308	672542.9	136874.2
343.15	0.0609	0.9391	998.6	0.001017	2.42088E-05	0.000119	1.84E-05	977.81	0.000404	1785.027	2525.746792	0.01038	104241.2871	238.6335	47.6288	680846.9	135890.1
293.15	0.0916	0.9084	1036.8	0.00641	2.63119E-05	0.000115	1.8E-05	998.2336	0.001002	1415.743	4000.600194	0.10072	141052.5695	245.9359	84.49232	599440.3	205940.2
298.15	0.0916	0.9084	1034.2	0.00529	2.6378E-05	0.000115	1.81E-05	997.0751	0.00089	1170.687	3925.958275	0.0759	140781.7777	244.7449	82.46959	606711.8	204438.5
303.15	0.0916	0.9084	1031.5	0.00441	2.64471E-05	0.000115	1.81E-05	995.6783	0.000798	1231.345	3850.61194	0.05782	140395.5289	243.5937	80.51554	613984.9	202941.7
308.15	0.0916	0.9084	1028.6	0.003721	2.65216E-05	0.000116	1.81E-05	994.0635	0.00072	1290.53	3781.807085	0.04462	140161.0993	242.4818	78.62657	621262.9	201449.2
313.15	0.0916	0.9084	1025.6	0.00317	2.65992E-05	0.000116	1.82E-05	992.2473	0.000653	1348.689	3715.615782	0.03489	139942.3513	241.4076	76.79932	628546.5	199960.3
318.15	0.0916	0.9084	1022.5	0.002732	2.66799E-05	0.000117	1.82E-05	990.24	0.000596	1405.25	3659.023986	0.02767	140011.3154	240.37	75.0307	635837.7	198474.6
323.15	0.0916	0.9084	1019.4	0.002376	2.6761E-05	0.000117	1.82E-05	988.07	0.000547	1460.696	3607.454916	0.02222	140207.4285	239.3669	73.31787	643135.2	196991.8

328.15	0.0916	0.9084	1016.1	0.002088	2.68479E-05	0.000118	1.83E-05	985.73	0.000504	1514.574	3566.384851	0.0181	140755.8866	238.3977	71.65814	650441.9	195511.4
333.15	0.0916	0.9084	1012.7	0.001849	2.6938E-05	0.000118	1.83E-05	983.24	0.000467	1567.466	3530.514808	0.01489	141463.3071	237.4593	70.04907	657753.2	194033.3
338.15	0.0916	0.9084	1009.2	0.001649	2.70315E-05	0.000118	1.84E-05	980.59	0.000433	1619.428	3499.550601	0.01238	142327.1067	236.5508	68.48829	665070.6	192557.2
343.15	0.0916	0.9084	1005.4	0.001478	2.71336E-05	0.000119	1.84E-05	977.81	0.000404	1670.886	3470.082845	0.01038	143215.4257	235.6701	66.9736	672392	191082.8
348.15	0.0916	0.9084	1001.5	0.001335	2.72393E-05	0.000119	1.85E-05	974.68	0.000378	1721.1	3450.008044	0.00878	144461.6127	234.8164	65.50299	679718.2	189610.1
353.15	0.0916	0.9084	996.9	0.001213	2.7365E-05	0.00012	1.85E-05	971.6	0.000354	1770.364	3478.909744	0.00643	147763.8928	233.9223	64.07441	686854.8	188138.6
293.15	0.1313	0.8687	1045.6	0.011633	2.99309E-05	0.000115	1.8E-05	998.2336	0.001002	967.0068	5142.445405	0.10072	181311.5789	246.1741	112.2663	600020.7	273636
298.15	0.1313	0.8687	1042.6	0.009323	3.0017E-05	0.000115	1.81E-05	997.0751	0.00089	1032.116	5031.459739	0.0759	180424.1912	244.4534	109.5297	605989.3	271519.2
303.15	0.1313	0.8687	1039.5	0.007561	3.01065E-05	0.000115	1.81E-05	995.6783	0.000798	1096.155	4922.153977	0.05782	179464.5687	242.7902	106.8853	611959.7	269407.4
308.15	0.1313	0.8687	1036.3	0.0062	3.01995E-05	0.000116	1.81E-05	994.0635	0.00072	1159.185	4814.18543	0.04462	178423.0413	241.1829	104.3284	617934.8	267299.8
313.15	0.1313	0.8687	1033	0.005152	3.0296E-05	0.000116	1.82E-05	992.2473	0.000653	1220.557	4715.844521	0.03489	177614.2662	239.629	101.8545	623915.6	265195.8
318.15	0.1313	0.8687	1029.6	0.004335	3.0396E-05	0.000117	1.82E-05	990.24	0.000596	1280.311	4627.140964	0.02767	177055.9841	238.1268	99.45958	629903.9	263095
323.15	0.1313	0.8687	1026.1	0.003683	3.04997E-05	0.000117	1.82E-05	988.07	0.000547	1338.983	4543.01314	0.02222	176568.8567	236.6735	97.13984	635898.6	260997
328.15	0.1313	0.8687	1022.5	0.003168	3.06071E-05	0.000118	1.83E-05	985.73	0.000504	1395.811	4471.941318	0.0181	176495.833	235.2679	94.89169	641902.6	258901.6
333.15	0.1313	0.8687	1018.9	0.002749	3.07152E-05	0.000118	1.83E-05	983.24	0.000467	1451.557	4406.930899	0.01489	176580.2023	233.9061	92.71187	647911	256808.4
338.15	0.1313	0.8687	1015.1	0.002408	3.08302E-05	0.000118	1.84E-05	980.59	0.000433	1505.935	4351.619386	0.01238	176980.8377	232.5867	90.59722	653925.6	254717.2
343.15	0.1313	0.8687	1011.3	0.002128	3.0946E-05	0.000119	1.84E-05	977.81	0.000404	1559.016	4306.215089	0.01038	177723.8339	231.3072	88.5448	659944.1	252627.8
348.15	0.1313	0.8687	1007.4	0.001894	3.10658E-05	0.000119	1.85E-05	974.68	0.000378	1611.128	4267.000517	0.00878	178671.4026	230.0661	86.5519	665967.5	250540
353.15	0.1313	0.8687	1003.4	0.001698	3.11897E-05	0.00012	1.85E-05	971.6	0.000354	1662.156	4295.104794	0.00643	182431.1209	228.7955	84.61583	671801.3	248453.3
293.15	0.1849	0.8151	1052.5	0.021915	3.48858E-05	0.000115	1.8E-05	998.2336	0.001002	818.3363	6215.774029	0.10072	219154.8407	245.801	143.2528	599111.5	349162
298.15	0.1849	0.8151	1049.2	0.016721	3.49955E-05	0.000115	1.81E-05	997.0751	0.00089	890.9763	6023.48666	0.0759	215997.4969	243.3745	139.692	603314.7	346290.3
303.15	0.1849	0.8151	1045.7	0.013075	3.51126E-05	0.000115	1.81E-05	995.6783	0.000798	960.1016	5861.372406	0.05782	213709.0135	241.0287	136.2506	607519.6	343423.6
308.15	0.1849	0.8151	1042.2	0.010404	3.52305E-05	0.000116	1.81E-05	994.0635	0.00072	1027.055	5713.746307	0.04462	211762.5107	238.7608	132.9226	611729.3	340561.1
313.15	0.1849	0.8151	1038.6	0.008418	3.53527E-05	0.000116	1.82E-05	992.2473	0.000653	1091.811	5581.884814	0.03489	210232.2014	236.5676	129.7022	615944.8	337702.2
318.15	0.1849	0.8151	1035	0.006916	3.54756E-05	0.000117	1.82E-05	990.24	0.000596	1154.525	5464.039268	0.02767	209079.6147	234.4462	126.5843	620167.7	334846.5
323.15	0.1849	0.8151	1031.2	0.005759	3.56063E-05	0.000117	1.82E-05	988.07	0.000547	1215.439	5358.815322	0.02222	208275.8437	232.3927	123.5639	624396.9	331993.7
328.15	0.1849	0.8151	1027.4	0.004863	3.5738E-05	0.000118	1.83E-05	985.73	0.000504	1274.306	5268.260765	0.0181	207924.4798	230.4053	120.6365	628635.5	329143.3

333.15	0.1849	0.8151	1023.6	0.004147	3.58707E-05	0.000118	1.83E-05	983.24	0.000467	1331.977	5184.957508	0.01489	207754.7542	228.4791	117.7977	632878.5	326295.2
338.15	0.1849	0.8151	1019.6	0.003572	3.60114E-05	0.000118	1.84E-05	980.59	0.000433	1388.278	5111.059794	0.01238	207867.3623	226.6121	115.0436	637127.7	323449.2
343.15	0.1849	0.8151	1015.6	0.003104	3.61533E-05	0.000119	1.84E-05	977.81	0.000404	1443.421	5045.415603	0.01038	208231.7269	224.8008	112.3704	641380.8	320604.8
348.15	0.1849	0.8151	1011.5	0.002723	3.62998E-05	0.000119	1.85E-05	974.68	0.000378	1497.131	4991.001069	0.00878	208987.3572	223.0433	109.7746	645638.8	317762.2
353.15	0.1849	0.8151	1007.3	0.002407	3.64512E-05	0.00012	1.85E-05	971.6	0.000354	1549.786	5027.301706	0.00643	213530.5958	221.2709	107.2526	649707.1	314920.6
293.15	0.2608	0.7392	1056.5	0.042784	4.20203E-05	0.000115	1.8E-05	998.2336	0.001002	664.1833	7105.171553	0.10072	250513.0869	244.2149	176.4107	595245.5	429980.6
298.15	0.2608	0.7392	1052.9	0.032161	4.21639E-05	0.000115	1.81E-05	997.0751	0.00089	736.469	6922.309925	0.0759	248228.5926	240.8501	171.9612	597056.9	426284.2
303.15	0.2608	0.7392	1049.3	0.024522	4.23086E-05	0.000115	1.81E-05	995.6783	0.000798	807.6634	6742.487856	0.05782	245834.9903	237.597	167.6603	598869.9	422592.6
308.15	0.2608	0.7392	1045.6	0.018988	4.24583E-05	0.000116	1.81E-05	994.0635	0.00072	877.3423	6570.012564	0.04462	243497.3975	234.4513	163.5007	600687.8	418905.4
313.15	0.2608	0.7392	1041.8	0.014936	4.26132E-05	0.000116	1.82E-05	992.2473	0.000653	945.2692	6408.18996	0.03489	241353.5799	231.4082	159.4754	602511.3	415221.8
318.15	0.2608	0.7392	1038	0.01193	4.27692E-05	0.000117	1.82E-05	990.24	0.000596	1011.378	6257.379586	0.02767	239436.5136	228.4636	155.5778	604342.4	411541.3
323.15	0.2608	0.7392	1034.1	0.009659	4.29305E-05	0.000117	1.82E-05	988.07	0.000547	1075.904	6116.235526	0.02222	237713.7553	225.6125	151.8018	606179.8	407863.7
328.15	0.2608	0.7392	1030.2	0.007938	4.3093E-05	0.000118	1.83E-05	985.73	0.000504	1138.386	5988.896588	0.0181	236366.0918	222.8517	148.1418	608026.5	404188.6
333.15	0.2608	0.7392	1026.2	0.0066	4.3261E-05	0.000118	1.83E-05	983.24	0.000467	1199.443	5871.438416	0.01489	235261.1845	220.1754	144.5925	609877.6	400515.8
338.15	0.2608	0.7392	1022.1	0.005554	4.34345E-05	0.000118	1.84E-05	980.59	0.000433	1258.851	5765.99907	0.01238	234503.8145	217.5804	141.1489	611735	396845
343.15	0.2608	0.7392	1018	0.004722	4.36094E-05	0.000119	1.84E-05	977.81	0.000404	1316.929	5670.611001	0.01038	234034.4611	215.0625	137.8062	613596.2	393175.9
348.15	0.2608	0.7392	1013.8	0.004055	4.37901E-05	0.000119	1.85E-05	974.68	0.000378	1373.62	5585.613096	0.00878	233885.4477	212.6185	134.5601	615462.3	389508.4
353.15	0.2608	0.7392	1009.5	0.003513	4.39766E-05	0.00012	1.85E-05	971.6	0.000354	1429.121	5626.422597	0.00643	238977.7737	210.1791	131.4064	617138.8	385842.2
293.15	0.3768	0.6232	1056	0.076266	5.31511E-05	0.000115	1.8E-05	998.2336	0.001002	531.559	7260.955062	0.10072	256005.6788	239.5649	208.7982	583911.5	508921.5
298.15	0.3768	0.6232	1052.4	0.056123	5.33329E-05	0.000115	1.81E-05	997.0751	0.00089	604.8754	7074.674833	0.0759	253692.2784	235.0313	203.6163	582632.3	504755.9
303.15	0.3768	0.6232	1048.6	0.041834	5.35262E-05	0.000115	1.81E-05	995.6783	0.000798	677.5553	6887.528544	0.05782	251123.2573	230.648	198.6073	581354.9	500595.3
308.15	0.3768	0.6232	1044.9	0.031721	5.37157E-05	0.000116	1.81E-05	994.0635	0.00072	748.5537	6709.550442	0.04462	248668.9417	226.4088	193.7624	580082.2	496438.9
313.15	0.3768	0.6232	1041	0.024435	5.3917E-05	0.000116	1.82E-05	992.2473	0.000653	817.968	6540.284964	0.03489	246328.7137	222.3072	189.0737	578815.2	492286.2
318.15	0.3768	0.6232	1037.1	0.019137	5.41197E-05	0.000117	1.82E-05	990.24	0.000596	885.4646	6382.461231	0.02767	244222.7205	218.3373	184.5336	577555.7	488136.7
323.15	0.3768	0.6232	1033.2	0.015206	5.4324E-05	0.000117	1.82E-05	988.07	0.000547	951.3498	6233.917623	0.02222	242287.5905	214.4926	180.135	576302.6	483990
328.15	0.3768	0.6232	1029.2	0.012272	5.45351E-05	0.000118	1.83E-05	985.73	0.000504	1015.209	6097.775493	0.0181	240663.2575	210.7685	175.8714	575058.8	479845.7
333.15	0.3768	0.6232	1025.1	0.010019	5.47533E-05	0.000118	1.83E-05	983.24	0.000467	1077.823	5969.150359	0.01489	239176.3797	207.1578	171.7366	573819.4	475703.8

338.15	0.3768	0.6232	1021	0.008281	5.49731E-05	0.000118	1.84E-05	980.59	0.000433	1138.892	5850.424655	0.01238	237937.4123	203.6561	167.7247	572586.2	471563.9
343.15	0.3768	0.6232	1016.9	0.006923	5.51948E-05	0.000119	1.84E-05	977.81	0.000404	1198.507	5742.923062	0.01038	237018.8862	200.2578	163.8304	571356.9	467425.7
348.15	0.3768	0.6232	1012.7	0.005844	5.54237E-05	0.000119	1.85E-05	974.68	0.000378	1256.961	5642.62369	0.00878	236272.6428	196.9588	160.0485	570132.5	463289.2
353.15	0.3768	0.6232	1008.4	0.004984	5.566E-05	0.00012	1.85E-05	971.6	0.000354	1314.009	5721.919134	0.00643	243033.9122	193.6886	156.3741	568718.5	459153.8
293.15	0.5764	0.4236	1050.7	0.107892	7.26342E-05	0.000115	1.8E-05	998.2336	0.001002	448.0491	5725.816087	0.10072	201879.9761	220.1171	233.8923	536509.9	570085.4
298.15	0.5764	0.4236	1047	0.079249	7.28908E-05	0.000115	1.81E-05	997.0751	0.00089	518.6836	5589.309048	0.0759	200428.229	214.7764	229.0849	532421.3	567891.5
303.15	0.5764	0.4236	1043.3	0.058937	7.31493E-05	0.000115	1.81E-05	995.6783	0.000798	588.8121	5451.69917	0.05782	198772.0914	209.6125	224.438	528334.3	565702.4
308.15	0.5764	0.4236	1039.5	0.044492	7.34167E-05	0.000116	1.81E-05	994.0635	0.00072	657.7617	5317.823175	0.04462	197088.8322	204.6181	219.9436	524252.2	563517.7
313.15	0.5764	0.4236	1035.7	0.034108	7.36861E-05	0.000116	1.82E-05	992.2473	0.000653	725.2942	5189.861132	0.03489	195467.296	199.7853	215.5941	520175.7	561336.6
318.15	0.5764	0.4236	1031.8	0.026566	7.39646E-05	0.000117	1.82E-05	990.24	0.000596	791.1381	5069.363127	0.02767	193977.4656	195.1073	211.3825	516106.7	559158.7
323.15	0.5764	0.4236	1027.9	0.020977	7.42453E-05	0.000117	1.82E-05	988.07	0.000547	855.6202	4954.018569	0.02222	192543.0035	190.5764	207.3023	512044.1	556983.6
328.15	0.5764	0.4236	1024	0.016823	7.4528E-05	0.000118	1.83E-05	985.73	0.000504	918.1891	4847.060508	0.0181	191300.8067	186.187	203.3474	507990.8	554810.9
333.15	0.5764	0.4236	1020	0.013644	7.48203E-05	0.000118	1.83E-05	983.24	0.000467	979.6585	4745.261936	0.01489	190136.7033	181.931	199.512	503941.9	552640.6
338.15	0.5764	0.4236	1015.8	0.011201	7.51297E-05	0.000118	1.84E-05	980.59	0.000433	1039.691	4650.967301	0.01238	189155.3502	177.803	195.7907	499899.3	550472.3
343.15	0.5764	0.4236	1011.9	0.009291	7.54192E-05	0.000119	1.84E-05	977.81	0.000404	1098.631	4562.453841	0.01038	188299.1842	173.7967	192.1785	495860.5	548305.7
348.15	0.5764	0.4236	1007.8	0.007788	7.5726E-05	0.000119	1.85E-05	974.68	0.000378	1156.292	4481.647945	0.00878	187659.2986	169.9071	188.6706	491826.6	546140.8
353.15	0.5764	0.4236	1003.7	0.006587	7.60354E-05	0.00012	1.85E-05	971.6	0.000354	1212.952	4663.489446	0.00643	198077.9627	166.0631	185.2624	487603.1	543977
293.15	0.7031	0.2969	1046.8	0.111511	8.51473E-05	0.000115	1.8E-05	998.2336	0.001002	435.693	4199.288046	0.10072	148057.8764	191.3391	240.2703	466366.8	585631
298.15	0.7031	0.2969	1043.2	0.082357	8.54411E-05	0.000115	1.81E-05	997.0751	0.00089	504.2022	4101.070098	0.0759	147061.1501	186.5109	236.571	462352.3	586449.1
303.15	0.7031	0.2969	1039.4	0.061546	8.57535E-05	0.000115	1.81E-05	995.6783	0.000798	572.2972	4002.037236	0.05782	145916.5825	181.8426	232.9956	458339.5	587272.1
308.15	0.7031	0.2969	1035.7	0.046689	8.60598E-05	0.000116	1.81E-05	994.0635	0.00072	639.1984	3906.595668	0.04462	144786.006	177.3277	229.5379	454331.5	588099.4
313.15	0.7031	0.2969	1031.8	0.035949	8.63851E-05	0.000116	1.82E-05	992.2473	0.000653	704.7675	3816.038881	0.03489	143724.6166	172.9592	226.1921	450329.1	588930.3
318.15	0.7031	0.2969	1028	0.028108	8.67044E-05	0.000117	1.82E-05	990.24	0.000596	768.7639	3730.171675	0.02767	142733.7576	168.7308	222.9526	446334.3	589764.4
323.15	0.7031	0.2969	1024.1	0.022277	8.70346E-05	0.000117	1.82E-05	988.07	0.000547	831.4176	3648.613074	0.02222	141807.0825	164.6356	219.8144	442345.8	590601.3
328.15	0.7031	0.2969	1020.2	0.017927	8.73673E-05	0.000118	1.83E-05	985.73	0.000504	892.2195	3573.01956	0.0181	141017.7412	160.6686	216.7728	438366.6	591440.7
333.15	0.7031	0.2969	1016.3	0.01458	8.77026E-05	0.000118	1.83E-05	983.24	0.000467	952.0663	3500.189133	0.01489	140248.1953	156.8223	213.8233	434391.9	592282.4
338.15	0.7031	0.2969	1012.3	0.011996	8.80492E-05	0.000118	1.84E-05	980.59	0.000433	1010.617	3431.986165	0.01238	139579.2537	153.092	210.9617	430423.4	593126.2

343.15	0.7031	0.2969	1008.3	0.009962	8.83985E-05	0.000119	1.84E-05	977.81	0.000404	1068.295	3366.917878	0.01038	138957.6557	149.4717	208.1841	426458.7	593971.6
348.15	0.7031	0.2969	1004.3	0.008353	8.87505E-05	0.000119	1.85E-05	974.68	0.000378	1124.924	3305.679891	0.00878	138418.184	145.9571	205.4869	422499	594818.7
353.15	0.7031	0.2969	1000.3	0.007065	8.91054E-05	0.00012	1.85E-05	971.6	0.000354	572.2972	3561.920574	0.00643	151289.711	142.4774	202.8665	418349.6	595666.9
293.15	0.8302	0.1698	1043.7	0.108675	9.77178E-05	0.000115	1.8E-05	998.2336	0.001002	435.9182	2471.474022	0.10072	87138.86526	138.026	243.1715	336422.4	592702.4
298.15	0.8302	0.1698	1040.1	0.080921	9.8056E-05	0.000115	1.81E-05	997.0751	0.00089	502.1213	2415.184649	0.0759	86606.62306	134.6106	241.012	333693.7	597458.3
303.15	0.8302	0.1698	1036.3	0.06095	9.84156E-05	0.000115	1.81E-05	995.6783	0.000798	567.9247	2358.919536	0.05782	86007.5648	131.3085	238.9257	330966.7	602219.1
308.15	0.8302	0.1698	1032.6	0.046555	9.87682E-05	0.000116	1.81E-05	994.0635	0.00072	632.7029	2304.175353	0.04462	85397.20379	128.1154	236.9088	328244.6	606984.1
313.15	0.8302	0.1698	1028.8	0.036084	9.9133E-05	0.000116	1.82E-05	992.2473	0.000653	696.1736	2253.428575	0.03489	84871.55609	125.0265	234.9576	325528.1	611752.9
318.15	0.8302	0.1698	1024.9	0.028378	9.95103E-05	0.000117	1.82E-05	990.24	0.000596	758.2076	2205.012982	0.02767	84374.07604	122.0375	233.069	322819.1	616524.7
323.15	0.8302	0.1698	1021.1	0.022607	9.98806E-05	0.000117	1.82E-05	988.07	0.000547	819.032	2158.055029	0.02222	83875.01807	119.1433	231.2399	320116.4	621299.5
328.15	0.8302	0.1698	1017.2	0.018264	0.000100264	0.000118	1.83E-05	985.73	0.000504	878.2547	2112.413293	0.0181	83371.43026	116.3408	229.4674	317423	626076.6
333.15	0.8302	0.1698	1013.3	0.014924	0.000100649	0.000118	1.83E-05	983.24	0.000467	936.3346	2071.380606	0.01489	82997.62688	113.624	227.749	314734.1	630856.1
338.15	0.8302	0.1698	1009.4	0.012326	0.000101038	0.000118	1.84E-05	980.59	0.000433	993.309	2031.396335	0.01238	82617.11171	110.9897	226.0821	312051.4	635637.7
343.15	0.8302	0.1698	1005.5	0.010278	0.00010143	0.000119	1.84E-05	977.81	0.000404	1049.334	1994.991244	0.01038	82336.22452	108.4336	224.4644	309372.6	640420.9
348.15	0.8302	0.1698	1001.5	0.008642	0.000101835	0.000119	1.85E-05	974.68	0.000378	1104.59	1958.324153	0.00878	82000.58137	105.9526	222.8937	306698.7	645205.8
353.15	0.8302	0.1698	997.5	0.007337	0.000102244	0.00012	1.85E-05	971.6	0.000354	1158.688	2298.073465	0.00643	97608.82177	103.4772	221.3679	303835.1	649991.8
293.15	1	0	1040.6	0.10072	0.000114514	0.000115	1.8E-05	998.2336	0.001002	445.1592	0	0.10072	0	4.461364	240.1883	10874.06	585431
298.15	1	0	1036.8	0.0759	0.000114933	0.000115	1.81E-05	997.0751	0.00089	508.4092	0	0.0759	0	4.340079	240.2468	10758.87	595561.4
303.15	1	0	1033.1	0.05782	0.000115345	0.000115	1.81E-05	995.6783	0.000798	571.3229	0	0.05782	0	4.223468	240.3054	10645.37	605696.7
308.15	1	0	1029.3	0.04462	0.000115771	0.000116	1.81E-05	994.0635	0.00072	633.3603	0	0.04462	0	4.11252	240.3638	10536.69	615836.3
313.15	1	0	1025.5	0.03489	0.0001162	0.000116	1.82E-05	992.2473	0.000653	694.3477	0	0.03489	0	4.007298	240.4217	10433.69	625979.5
318.15	1	0	1021.7	0.02767	0.000116632	0.000117	1.82E-05	990.24	0.000596	753.9536	0	0.02767	0	3.908218	240.479	10338.2	636125.9
323.15	1	0	1017.9	0.02222	0.000117067	0.000117	1.82E-05	988.07	0.000547	812.388	0	0.02222	0	3.814571	240.5355	10249.06	646275.1
328.15	1	0	1014	0.0181	0.000117518	0.000118	1.83E-05	985.73	0.000504	869.1356	0	0.0181	0	3.727173	240.5913	10169.18	656426.8
333.15	1	0	1010.2	0.01489	0.00011796	0.000118	1.83E-05	983.24	0.000467	925.0406	0	0.01489	0	3.64402	240.6462	10093.8	666580.8
338.15	1	0	1006.3	0.01238	0.000118417	0.000118	1.84E-05	980.59	0.000433	979.8233	0	0.01238	0	3.565526	240.7002	10024.6	676736.8
343.15	1	0	1002.4	0.01038	0.000118878	0.000119	1.84E-05	977.81	0.000404	1033.886	0	0.01038	0	3.490689	240.7532	9959.309	686894.6

348.15	1	0	998.5	0.00878	0.000119342	0.000119	1.85E-05	974.68	0.000378	1087.057	0	0.00878	0	3.419679	240.8052	9898.874	697053.9
353.15	1	0	994.6	0.00643	0.00011981	0.00012	1.85E-05	971.6	0.000354	1174.841	0	0.00643	0	3.286095	240.8562	9648.802	707214.5

Table B.2. DMEA free excess energy values

Temperatures K	x DMEA	x H_2O	Measured density ρ/kg.m-3 of aqueous DMEA	η mixture (Pa.s)	molar volume V of mixture	molar volume V of DMEA m3/mol	ΔG* J/mol	ΔGE* J/mol	molar volume V of water m3/mol	Density pure H_2O kgm-3	Dynamic viscosity of water Pa.s	η DMEA (Pa.s)	molar volume V of pure DMEA m3/mol	ΔGE*/RT	Ḡ1/RT	Ḡ2/RT	Ḡ1	Ḡ2
293.15	0.0797	0.9203	991	0.004214	2.39E-05	0.0001	1211.765	3588.770385	1.8E-05	998.2336	0.001002	0.00389	0.0001	126532.3	5.08E-07	79.27591	0.001238	193225.8
298.15	0.0797	0.9203	988.2	0.003457	2.4E-05	0.000101	1276.724	3459.377487	1.81E-05	997.0751	0.00089	0.00339	0.000101	124050.6	3.7E-07	76.71066	0.000918	190162.4
303.15	0.0797	0.9203	985.4	0.002869	2.4E-05	0.000101	1340.493	3332.977122	1.81E-05	995.6783	0.000798	0.00296	0.000101	121522.3	2.75E-07	74.23199	0.000694	187103.9
308.15	0.0797	0.9203	982.4	0.002413	2.41E-05	0.000102	1402.505	3217.407203	1.81E-05	994.0635	0.00072	0.00259	0.000102	119243.3	2.09E-07	71.83543	0.000535	184049.6
313.15	0.0797	0.9203	979.2	0.002055	2.42E-05	0.000102	1462.807	3112.665114	1.82E-05	992.2473	0.000653	0.00228	0.000102	117233.2	1.61E-07	69.5168	0.00042	180999
318.15	0.0797	0.9203	976	0.001768	2.43E-05	0.000103	1521.842	3015.553704	1.82E-05	990.24	0.000596	0.00201	0.000103	115389.1	1.27E-07	67.27224	0.000335	177951.6
323.15	0.0797	0.9203	972.7	0.001536	2.43E-05	0.000103	1579.581	2925.334194	1.82E-05	988.07	0.000547	0.00179	0.000103	113696.1	1.01E-07	65.09819	0.000272	174907
328.15	0.0797	0.9203	969.3	0.001349	2.44E-05	0.000104	1635.643	2848.330275	1.83E-05	985.73	0.000504	0.0016	0.000104	112416.1	8.18E-08	62.9913	0.000223	171864.8
333.15	0.0797	0.9203	965.8	0.001193	2.45E-05	0.000104	1690.891	2776.096572	1.83E-05	983.24	0.000467	0.00143	0.000104	111234.7	6.7E-08	60.94849	0.000185	168825
338.15	0.0797	0.9203	962.1	0.001064	2.46E-05	0.000105	1744.838	2712.715174	1.84E-05	980.59	0.000433	0.00129	0.000105	110326.4	5.55E-08	58.96681	0.000156	165787.2
343.15	0.0797	0.9203	958.3	0.000955	2.47E-05	0.000106	1797.948	2654.309966	1.84E-05	977.81	0.000404	0.00117	0.000106	109547.3	4.64E-08	57.04348	0.000132	162751.1
348.15	0.0797	0.9203	954.3	0.000865	2.48E-05	0.000106	1849.41	2613.921929	1.85E-05	974.68	0.000378	0.00105	0.000106	109452.3	3.93E-08	55.17596	0.000114	159716.7
353.15	0.0797	0.9203	950.4	0.00079	2.49E-05	0.000107	1899.39	2583.436601	1.85E-05	971.6	0.000354	0.00096	0.000107	109729.4	3.36E-08	53.36172	9.87E-05	156683.4
293.15	0.1187	0.8813	987.1	0.006814	2.68E-05	0.0001	1093.888	4747.592029	1.8E-05	998.2336	0.001002	0.00389	0.0001	167389.9	8.21E-07	108.7949	0.002002	265174.9
298.15	0.1187	0.8813	983.8	0.005464	2.69E-05	0.000101	1161.436	4584.291301	1.81E-05	997.0751	0.00089	0.00339	0.000101	164389.1	5.85E-07	105.2623	0.00145	260940.6
303.15	0.1187	0.8813	980.3	0.004446	2.7E-05	0.000101	1227.256	4431.006409	1.81E-05	995.6783	0.000798	0.00296	0.000101	161557	4.26E-07	101.8482	0.001075	256711.3
308.15	0.1187	0.8813	976.8	0.003664	2.71E-05	0.000102	1291.643	4285.473575	1.81E-05	994.0635	0.00072	0.00259	0.000102	158828	3.17E-07	98.54657	0.000812	252486.2
313.15	0.1187	0.8813	973.1	0.00306	2.72E-05	0.000102	1354.293	4151.371696	1.82E-05	992.2473	0.000653	0.00228	0.000102	156354.4	2.4E-07	95.35177	0.000626	248264.8
318.15	0.1187	0.8813	969.5	0.00259	2.73E-05	0.000103	1415.078	4032.080242	1.82E-05	990.24	0.000596	0.00201	0.000103	154286.2	1.86E-07	92.25858	0.000491	244046.6
323.15	0.1187	0.8813	965.7	0.002216	2.74E-05	0.000103	1474.432	3921.035114	1.82E-05	988.07	0.000547	0.00179	0.000103	152395	1.46E-07	89.26217	0.000392	239831.2
328.15	0.1187	0.8813	961.9	0.001918	2.75E-05	0.000104	1532.081	3823.757995	1.83E-05	985.73	0.000504	0.0016	0.000104	150913.7	1.16E-07	86.35797	0.000317	235618.2

333.15	0.1187	0.8813	958	0.001676	2.76E-05	0.000104	1588.377	3737.902085	1.83E-05	983.24	0.000467	0.00143	0.000104	149773.1	9.41E-08	83.54179	0.000261	231407.6
338.15	0.1187	0.8813	954	0.001478	2.77E-05	0.000105	1643.311	3661.121254	1.84E-05	980.59	0.000433	0.00129	0.000105	148898.2	7.7E-08	80.8096	0.000217	227199
343.15	0.1187	0.8813	950	0.001315	2.79E-05	0.000106	1696.871	3595.108632	1.84E-05	977.81	0.000404	0.00117	0.000106	148375.4	6.39E-08	78.15764	0.000182	222992.1
348.15	0.1187	0.8813	945.7	0.001179	2.8E-05	0.000106	1749.216	3544.345356	1.85E-05	974.68	0.000378	0.00105	0.000106	148411.8	5.35E-08	75.58242	0.000155	218786.9
353.15	0.1187	0.8813	941.5	0.001064	2.81E-05	0.000107	1800.625	3495.753321	1.85E-05	971.6	0.000354	0.00096	0.000107	148479.3	4.53E-08	73.08051	0.000133	214582.8
293.15	0.1681	0.8319	979.9	0.010169	3.06E-05	0.0001	994.2918	5675.247399	1.8E-05	998.2336	0.001002	0.00389	0.0001	200097	1.23E-06	139.4485	0.002987	339889.6
298.15	0.1681	0.8319	976.2	0.008011	3.07E-05	0.000101	1063.463	5486.828802	1.81E-05	997.0751	0.00089	0.00339	0.000101	196753.4	8.58E-07	134.9102	0.002126	334436.5
303.15	0.1681	0.8319	972.3	0.006398	3.08E-05	0.000101	1131.259	5305.519043	1.81E-05	995.6783	0.000798	0.00296	0.000101	193442.3	6.14E-07	130.5236	0.001547	328988.4
308.15	0.1681	0.8319	968.4	0.005189	3.09E-05	0.000102	1197.165	5138.021365	1.81E-05	994.0635	0.00072	0.00259	0.000102	190425	4.49E-07	126.2809	0.00115	323544.5
313.15	0.1681	0.8319	964.5	0.004262	3.11E-05	0.000102	1261.646	4978.560671	1.82E-05	992.2473	0.000653	0.00228	0.000102	187509	3.35E-07	122.1752	0.000872	318104.3
318.15	0.1681	0.8319	960.5	0.003552	3.12E-05	0.000103	1324.098	4836.905415	1.82E-05	990.24	0.000596	0.00201	0.000103	185082.5	2.55E-07	118.1997	0.000674	312667.3
323.15	0.1681	0.8319	956.4	0.002999	3.13E-05	0.000103	1384.734	4707.347075	1.82E-05	988.07	0.000547	0.00179	0.000103	182955.9	1.97E-07	114.3483	0.00053	307233
328.15	0.1681	0.8319	952.3	0.002564	3.15E-05	0.000104	1443.541	4593.417669	1.83E-05	985.73	0.000504	0.0016	0.000104	181290.2	1.55E-07	110.6152	0.000424	301801.3
333.15	0.1681	0.8319	948.1	0.002215	3.16E-05	0.000104	1500.889	4492.973902	1.83E-05	983.24	0.000467	0.00143	0.000104	180027.8	1.24E-07	106.9949	0.000344	296371.9
338.15	0.1681	0.8319	943.8	0.001934	3.18E-05	0.000105	1556.598	4404.288994	1.84E-05	980.59	0.000433	0.00129	0.000105	179122.9	1.01E-07	103.4824	0.000283	290944.5
343.15	0.1681	0.8319	939.5	0.001701	3.19E-05	0.000106	1611.417	4320.861926	1.84E-05	977.81	0.000404	0.00117	0.000106	178328.3	8.26E-08	100.0729	0.000236	285518.8
348.15	0.1681	0.8319	935.1	0.001505	3.21E-05	0.000106	1665.593	4248.318925	1.85E-05	974.68	0.000378	0.00105	0.000106	177889.2	6.83E-08	96.76192	0.000198	280094.7
353.15	0.1681	0.8319	930.7	0.001341	3.22E-05	0.000107	1718.79	4176.394314	1.85E-05	971.6	0.000354	0.00096	0.000107	177389	5.71E-08	93.54505	0.000168	274671.8
293.15	0.2326	0.7674	969.3	0.01401	3.57E-05	0.0001	912.4207	6346.867186	1.8E-05	998.2336	0.001002	0.00389	0.0001	223776.9	1.69E-06	169.8645	0.004115	414025.1
298.15	0.2326	0.7674	965.4	0.010886	3.58E-05	0.000101	982.4916	6138.92292	1.81E-05	997.0751	0.00089	0.00339	0.000101	220137	1.17E-06	164.342	0.00289	407396.7
303.15	0.2326	0.7674	961.4	0.008571	3.59E-05	0.000101	1051.424	5936.564771	1.81E-05	995.6783	0.000798	0.00296	0.000101	216450.6	8.22E-07	159.0037	0.002072	400773.3
308.15	0.2326	0.7674	957.3	0.006848	3.61E-05	0.000102	1118.744	5746.254659	1.81E-05	994.0635	0.00072	0.00259	0.000102	212967.3	5.93E-07	153.8402	0.001518	394154.2
313.15	0.2326	0.7674	953.2	0.005548	3.63E-05	0.000102	1184.475	5566.271566	1.82E-05	992.2473	0.000653	0.00228	0.000102	209644.2	4.36E-07	148.8431	0.001135	387538.7
318.15	0.2326	0.7674	949	0.004562	3.64E-05	0.000103	1248.237	5404.549163	1.82E-05	990.24	0.000596	0.00201	0.000103	206803.2	3.27E-07	144.0041	0.000865	380926.3
323.15	0.2326	0.7674	944.7	0.003794	3.66E-05	0.000103	1310.695	5248.690204	1.82E-05	988.07	0.000547	0.00179	0.000103	203995.7	2.5E-07	139.316	0.000671	374316.8
328.15	0.2326	0.7674	940.4	0.003199	3.67E-05	0.000104	1371.157	5110.907115	1.83E-05	985.73	0.000504	0.0016	0.000104	201714.1	1.94E-07	134.7717	0.000529	367709.8
333.15	0.2326	0.7674	936	0.002725	3.69E-05	0.000104	1430.321	4985.901666	1.83E-05	983.24	0.000467	0.00143	0.000104	199778.8	1.53E-07	130.3646	0.000424	361105.1

338.15	0.2326	0.7674	931.5	0.002346	3.71E-05	0.000105	1487.978	4870.585635	1.84E-05	980.59	0.000433	0.00129	0.000105	198087.3	1.22E-07	126.0886	0.000344	354502.3
343.15	0.2326	0.7674	927	0.002038	3.73E-05	0.000106	1544.424	4764.025897	1.84E-05	977.81	0.000404	0.00117	0.000106	196618.4	9.9E-08	121.9377	0.000282	347901.3
348.15	0.2326	0.7674	922.4	0.001786	3.75E-05	0.000106	1599.613	4678.30833	1.85E-05	974.68	0.000378	0.00105	0.000106	195894	8.11E-08	117.9067	0.000235	341302
353.15	0.2326	0.7674	917.8	0.001572	3.77E-05	0.000107	1654.591	4581.596241	1.85E-05	971.6	0.000354	0.00096	0.000107	194599.6	6.69E-08	113.9902	0.000196	334703.8
293.15	0.3204	0.6796	954.9	0.01675	4.27E-05	0.0001	860.5658	6566.068957	1.8E-05	998.2336	0.001002	0.00389	0.0001	231505.5	2.02E-06	197.4771	0.00492	481327.5
298.15	0.3204	0.6796	950.9	0.012989	4.29E-05	0.000101	929.3336	6360.753035	1.81E-05	997.0751	0.00089	0.00339	0.000101	228091.6	1.39E-06	191.1248	0.003448	473790
303.15	0.3204	0.6796	946.8	0.010197	4.31E-05	0.000101	997.1935	6160.079054	1.81E-05	995.6783	0.000798	0.00296	0.000101	224600	9.78E-07	184.984	0.002465	466257.5
308.15	0.3204	0.6796	942.7	0.00812	4.33E-05	0.000102	1063.589	5971.225854	1.81E-05	994.0635	0.00072	0.00259	0.000102	221305.2	7.03E-07	179.0442	0.0018	458729.2
313.15	0.3204	0.6796	938.4	0.00654	4.35E-05	0.000102	1128.992	5786.662898	1.82E-05	992.2473	0.000653	0.00228	0.000102	217944.8	5.14E-07	173.2954	0.001338	451204.6
318.15	0.3204	0.6796	934.1	0.005362	4.37E-05	0.000103	1191.836	5628.592944	1.82E-05	990.24	0.000596	0.00201	0.000103	215376.2	3.85E-07	167.7285	0.001017	443683.2
323.15	0.3204	0.6796	929.8	0.004442	4.39E-05	0.000103	1253.65	5472.340791	1.82E-05	988.07	0.000547	0.00179	0.000103	212688.1	2.92E-07	162.335	0.000785	436164.6
328.15	0.3204	0.6796	925.4	0.003723	4.41E-05	0.000104	1314.01	5328.824776	1.83E-05	985.73	0.000504	0.0016	0.000104	210314.8	2.26E-07	157.1067	0.000616	428648.4
333.15	0.3204	0.6796	920.9	0.003151	4.43E-05	0.000104	1373.241	5197.618752	1.83E-05	983.24	0.000467	0.00143	0.000104	208262.1	1.77E-07	152.0362	0.00049	421134.6
338.15	0.3204	0.6796	916.4	0.002703	4.45E-05	0.000105	1430.358	5082.152755	1.84E-05	980.59	0.000433	0.00129	0.000105	206691.7	1.41E-07	147.1164	0.000396	413622.8
343.15	0.3204	0.6796	911.8	0.002324	4.48E-05	0.000106	1487.946	4955.881	1.84E-05	977.81	0.000404	0.00117	0.000106	204536.5	1.13E-07	142.3405	0.000322	406112.7
348.15	0.3204	0.6796	907.1	0.002022	4.5E-05	0.000106	1543.593	4862.511028	1.85E-05	974.68	0.000378	0.00105	0.000106	203607.1	9.18E-08	137.7024	0.000266	398604.2
353.15	0.3204	0.6796	902.3	0.00177	4.52E-05	0.000107	1598.628	4758.952852	1.85E-05	971.6	0.000354	0.00096	0.000107	202132.7	7.53E-08	133.196	0.000221	391096.9
293.15	0.447	0.553	936.6	0.015539	5.32E-05	0.0001	860.1132	5968.245979	1.8E-05	998.2336	0.001002	0.00389	0.0001	210427.5	1.87E-06	217.9548	0.004564	531239.5
298.15	0.447	0.553	932.6	0.012214	5.34E-05	0.000101	925.0246	5791.425707	1.81E-05	997.0751	0.00089	0.00339	0.000101	207676	1.31E-06	211.2232	0.003242	523613.2
303.15	0.447	0.553	928.4	0.009704	5.36E-05	0.000101	989.2754	5618.895186	1.81E-05	995.6783	0.000798	0.00296	0.000101	204868.2	9.31E-07	204.7157	0.002346	515991.7
308.15	0.447	0.553	924.3	0.007796	5.39E-05	0.000102	1052.693	5452.839603	1.81E-05	994.0635	0.00072	0.00259	0.000102	202092.8	6.75E-07	198.421	0.001728	508374.6
313.15	0.447	0.553	920	0.00634	5.41E-05	0.000102	1114.894	5294.391538	1.82E-05	992.2473	0.000653	0.00228	0.000102	199404.3	4.98E-07	192.3287	0.001297	500761
318.15	0.447	0.553	915.7	0.00522	5.44E-05	0.000103	1175.735	5150.534549	1.82E-05	990.24	0.000596	0.00201	0.000103	197083.5	3.74E-07	186.4291	0.00099	493150.7
323.15	0.447	0.553	911.3	0.00434	5.47E-05	0.000103	1235.663	5006.164418	1.82E-05	988.07	0.000547	0.00179	0.000103	194569.7	2.86E-07	180.7131	0.000767	485543.2
328.15	0.447	0.553	906.9	0.003652	5.49E-05	0.000104	1294.065	4876.150531	1.83E-05	985.73	0.000504	0.0016	0.000104	192448.9	2.21E-07	175.1722	0.000604	477938.1
333.15	0.447	0.553	902.4	0.003099	5.52E-05	0.000104	1351.649	4756.820791	1.83E-05	983.24	0.000467	0.00143	0.000104	190599.9	1.74E-07	169.7985	0.000482	470335.4
338.15	0.447	0.553	897.9	0.002653	5.55E-05	0.000105	1408.245	4638.791569	1.84E-05	980.59	0.000433	0.00129	0.000105	188660.2	1.38E-07	164.5844	0.000389	462734.6

343.15	0.447	0.553	893.2	0.002289	5.58E-05	0.000106	1463.971	4525.337031	1.84E-05	977.81	0.000404	0.00117	0.000106	186767.3	1.11E-07	159.5228	0.000317	455135.6
348.15	0.447	0.553	888.6	0.001988	5.61E-05	0.000106	1519.084	4434.749405	1.85E-05	974.68	0.000378	0.00105	0.000106	185695.5	9.03E-08	154.6072	0.000261	447538.3
353.15	0.447	0.553	882.5	0.001739	5.64E-05	0.000107	1573.134	4335.816426	1.85E-05	971.6	0.000354	0.00096	0.000107	184160.3	7.4E-08	149.8312	0.000217	439942
293.15	0.6452	0.3548	914.2	0.009712	6.99E-05	0.0001	935.5092	4004.836564	1.8E-05	998.2336	0.001002	0.00389	0.0001	141201.9	1.17E-06	225.7633	0.002853	550272
298.15	0.6452	0.3548	910.1	0.007955	7.02E-05	0.000101	992.0671	3904.980391	1.81E-05	997.0751	0.00089	0.00339	0.000101	140029.5	8.52E-07	219.7725	0.002112	544806.3
303.15	0.6452	0.3548	906	0.006565	7.05E-05	0.000101	1048.387	3807.623537	1.81E-05	995.6783	0.000798	0.00296	0.000101	138828.1	6.3E-07	213.9812	0.001587	539345.7
308.15	0.6452	0.3548	901.8	0.005458	7.09E-05	0.000102	1104.41	3713.906681	1.81E-05	994.0635	0.00072	0.00259	0.000102	137644.6	4.72E-07	208.3795	0.00121	533889.2
313.15	0.6452	0.3548	897.5	0.004577	7.12E-05	0.000102	1159.789	3621.762828	1.82E-05	992.2473	0.000653	0.00228	0.000102	136407.5	3.6E-07	202.9581	0.000936	528436.5
318.15	0.6452	0.3548	893.3	0.003877	7.15E-05	0.000103	1214.143	3543.041789	1.82E-05	990.24	0.000596	0.00201	0.000103	135573.3	2.78E-07	197.7083	0.000736	522986.9
323.15	0.6452	0.3548	888.9	0.003307	7.19E-05	0.000103	1268.025	3456.853852	1.82E-05	988.07	0.000547	0.00179	0.000103	134354.2	2.18E-07	192.622	0.000585	517540.1
328.15	0.6452	0.3548	884.5	0.002845	7.22E-05	0.000104	1321.026	3378.593425	1.83E-05	985.73	0.000504	0.0016	0.000104	133344.2	1.73E-07	187.6916	0.000471	512095.8
333.15	0.6452	0.3548	880	0.002462	7.26E-05	0.000104	1373.655	3308.725783	1.83E-05	983.24	0.000467	0.00143	0.000104	132576.5	1.38E-07	182.91	0.000383	506653.8
338.15	0.6452	0.3548	875.5	0.002146	7.3E-05	0.000105	1425.553	3234.825764	1.84E-05	980.59	0.000433	0.00129	0.000105	131560.7	1.12E-07	178.2706	0.000315	501213.8
343.15	0.6452	0.3548	870.9	0.001882	7.34E-05	0.000106	1476.898	3160.937078	1.84E-05	977.81	0.000404	0.00117	0.000106	130456.5	9.14E-08	173.7669	0.000261	495775.6
348.15	0.6452	0.3548	866.3	0.001658	7.38E-05	0.000106	1528.008	3114.418844	1.85E-05	974.68	0.000378	0.00105	0.000106	130409.5	7.53E-08	169.3932	0.000218	490339
353.15	0.6452	0.3548	861.6	0.001468	7.42E-05	0.000107	1578.711	3157.728615	1.85E-05	971.6	0.000354	0.00096	0.0001	134122	6.25E-08	165.1437	0.000183	484903.5
293.15	0.76	0.24	904.2	0.007129	7.97E-05	0.0001	987.1932	2702.5879	1.8E-05	998.2336	0.001002	0.00389	0.000101	95287.44	8.59E-07	223.8435	0.002094	545592.4
298.15	0.76	0.24	900.2	0.005976	8.01E-05	0.000101	1039.484	2641.977503	1.81E-05	997.0751	0.00089	0.00339	0.000101	94739.24	6.4E-07	218.773	0.001586	542328.7
303.15	0.76	0.24	896	0.005031	8.04E-05	0.000101	1092.031	2580.389795	1.81E-05	995.6783	0.000798	0.00296	0.000102	94082.5	4.83E-07	213.8718	0.001216	539069.9
308.15	0.76	0.24	891.8	0.004264	8.08E-05	0.000102	1144.297	2523.899065	1.81E-05	994.0635	0.00072	0.00259	0.000102	93540.59	3.69E-07	209.1313	0.000945	535815.4
313.15	0.76	0.24	887.6	0.003637	8.12E-05	0.000102	1196.292	2464.536187	1.82E-05	992.2473	0.000653	0.00228	0.000103	92822.57	2.86E-07	204.5435	0.000744	532564.5
318.15	0.76	0.24	883.3	0.003131	8.16E-05	0.000103	1247.314	2420.187388	1.82E-05	990.24	0.000596	0.00201	0.000103	92607.65	2.25E-07	200.1012	0.000594	529316.8
323.15	0.76	0.24	878.9	0.002708	8.2E-05	0.000103	1298.275	2362.038271	1.82E-05	988.07	0.000547	0.00179	0.000104	91803.04	1.78E-07	195.7974	0.000479	526071.9
328.15	0.76	0.24	874.5	0.002363	8.24E-05	0.000104	1348.202	2314.147745	1.83E-05	985.73	0.000504	0.0016	0.000104	91333.36	1.43E-07	191.6256	0.000391	522829.4
333.15	0.76	0.24	870	0.002071	8.28E-05	0.000104	1398.007	2273.518128	1.83E-05	983.24	0.000467	0.00143	0.000105	91097.02	1.16E-07	187.5799	0.000322	519589.4
338.15	0.76	0.24	865.6	0.001828	8.33E-05	0.000105	1447.048	2227.009428	1.84E-05	980.59	0.000433	0.00129	0.000106	90572.72	9.53E-08	183.6546	0.000268	516351.3
343.15	0.76	0.24	861	0.001621	8.37E-05	0.000106	1495.786	2179.478866	1.84E-05	977.81	0.000404	0.00117	0.000106	89950.3	7.87E-08	179.8443	0.000225	513114.9

348.15	0.76	0.24	856.4	0.001444	8.42E-05	0.000106	1544.218	2161.963655	1.85E-05	974.68	0.000378	0.00105	0.000107	90527.54	6.56E-08	176.1439	0.00019	509880.2
353.15	0.76	0.24	851.7	0.001291	8.46E-05	0.000107	1592.505	2123.747445	1.85E-05	971.6	0.000354	0.00096	0.000107	90204.46	5.49E-08	172.5488	0.000161	506646.6
293.15	0.8673	0.1327	896.5	0.005383	8.89E-05	0.0001	1034.04	1489.258273	1.8E-05	998.2336	0.001002	0.00389	0.0001	52508.05	6.49E-07	218.487	0.001581	532536.6
298.15	0.8673	0.1327	892.4	0.004591	8.93E-05	0.000101	1083.309	1455.601552	1.81E-05	997.0751	0.00089	0.00339	0.000101	52196.73	4.92E-07	214.5114	0.001219	531764.4
303.15	0.8673	0.1327	888.3	0.003937	8.97E-05	0.000101	1132.495	1426.470704	1.81E-05	995.6783	0.000798	0.00296	0.000101	52009.94	3.78E-07	210.669	0.000952	530997.2
308.15	0.8673	0.1327	884	0.003391	9.02E-05	0.000102	1181.746	1400.19517	1.81E-05	994.0635	0.00072	0.00259	0.000102	51893.95	2.93E-07	206.9529	0.000752	530234.3
313.15	0.8673	0.1327	879.7	0.002937	9.06E-05	0.000102	1230.789	1370.890829	1.82E-05	992.2473	0.000653	0.00228	0.000102	51632.27	2.31E-07	203.3569	0.000601	529474.9
318.15	0.8673	0.1327	875.4	0.002564	9.1E-05	0.000103	1279.062	1355.288703	1.82E-05	990.24	0.000596	0.00201	0.000103	51859.66	1.84E-07	199.8751	0.000486	528718.8
323.15	0.8673	0.1327	871	0.002249	9.15E-05	0.000103	1327.165	1326.110744	1.82E-05	988.07	0.000547	0.00179	0.000103	51540.65	1.48E-07	196.5022	0.000398	527965.5
328.15	0.8673	0.1327	866.6	0.001987	9.2E-05	0.000104	1374.513	1304.637362	1.83E-05	985.73	0.000504	0.0016	0.000104	51490.63	1.2E-07	193.2329	0.000329	527214.6
333.15	0.8673	0.1327	862.2	0.001765	9.24E-05	0.000104	1421.446	1295.220645	1.83E-05	983.24	0.000467	0.00143	0.000104	51897.87	9.91E-08	190.0625	0.000274	526466.1
338.15	0.8673	0.1327	857.6	0.001575	9.29E-05	0.000105	1468.064	1274.352122	1.84E-05	980.59	0.000433	0.00129	0.000105	51828.04	8.21E-08	186.9867	0.000231	525719.6
343.15	0.8673	0.1327	853.1	0.001413	9.34E-05	0.000106	1514.183	1251.713149	1.84E-05	977.81	0.000404	0.00117	0.000106	51660.04	6.86E-08	184.0011	0.000196	524974.8
348.15	0.8673	0.1327	848.5	0.001274	9.39E-05	0.000106	1559.807	1269.730756	1.85E-05	974.68	0.000378	0.00105	0.000106	53167.22	5.78E-08	181.1018	0.000167	524231.6
353.15	0.8673	0.1327	843.9	0.001151	9.44E-05	0.000107	1605.603	1243.141043	1.85E-05	971.6	0.000354	0.00096	0.000107	52801.42	4.9E-08	178.285	0.000144	523489.6
293.15	1	0	887.9	0.00389	0.0001	0.0001	1087.597	0	1.8E-05	998.2336	0.001002	0.00389	0.0001	0	4.69E-07	203.5844	0.001143	496213.4
298.15	1	0	883.7	0.00339	0.000101	0.000101	1133.138	0	1.81E-05	997.0751	0.00089	0.00339	0.000101	0	3.63E-07	201.2528	0.0009	498896.8
303.15	1	0	879.4	0.00296	0.000101	0.000101	1179.159	0	1.81E-05	995.6783	0.000798	0.00296	0.000101	0	2.84E-07	199	0.000716	501585.1
308.15	1	0	875.1	0.00259	0.000102	0.000102	1225.613	0	1.81E-05	994.0635	0.00072	0.00259	0.000102	0	2.24E-07	196.8219	0.000574	504277.7
313.15	1	0	870.8	0.00228	0.000102	0.000102	1271.655	0	1.82E-05	992.2473	0.000653	0.00228	0.000102	0	1.79E-07	194.7149	0.000466	506973.9
318.15	1	0	866.4	0.00201	0.000103	0.000103	1318.19	0	1.82E-05	990.24	0.000596	0.00201	0.000103	0	1.44E-07	192.6752	0.000381	509673.3
323.15	1	0	862	0.00179	0.000103	0.000103	1363.344	0	1.82E-05	988.07	0.000547	0.00179	0.000103	0	1.18E-07	190.6998	0.000316	512375.5
328.15	1	0	857.6	0.0016	0.000104	0.000104	1408.419	0	1.83E-05	985.73	0.000504	0.0016	0.000104	0	9.7E-08	188.7854	0.000265	515080.2
333.15	1	0	853.1	0.00143	0.000104	0.000104	1454.215	0	1.83E-05	983.24	0.000467	0.00143	0.000104	0	8.03E-08	186.9293	0.000222	517787.2
338.15	1	0	848.6	0.00129	0.000105	0.000105	1498.623	0	1.84E-05	980.59	0.000433	0.00129	0.000105	0	6.72E-08	185.1289	0.000189	520496.2
343.15	1	0	843.8	0.00117	0.000106	0.000106	1542.4	0	1.84E-05	977.81	0.000404	0.00117	0.000106	0	5.68E-08	183.3815	0.000162	523206.9
348.15	1	0	839.6	0.00105	0.000106	0.000106	1589.323	0	1.85E-05	974.68	0.000378	0.00105	0.000106	0	4.77E-08	181.6848	0.000138	525919.3

353.15	1	0	834.7	0.00096	0.000107	0.000107	1632.447	0	1.85E-05	971.6	0.000354	0.00096	0.000107	0	4.09E-08	180.0366	0.00012	528632.9

Table B.3. DEEA free excess energy values

Temperatures K	x DEEA	x H_2O	Measured density ρ/kg.m-3 of aqueous DEEA	η mixture (Pa.s)	molar volume V of mixture	molar volume V of DEEA m3/mol	ΔG* J/mol	ΔGE* J/mol	molar volume V of water m3/mol	Density pure H_2O kgm-3	Dynamic viscosity of water Pa.s	η DEEA (Pa.s)	ΔGE*/RT	Ḡ1/RT	Ḡ2/RT	Ḡ1	Ḡ2
293.15	0.0618	0.9382	989.6	0.004511	2.36452E-05	0.000118896	1197.837076	3801.053631	1.80469E-05	998.2336	0.001002	0.00495	1.559481	3.172379	1.041715	7732.305	2539.058
298.15	0.0618	0.9382	986.6	0.003666	2.37171E-05	0.000119518	1264.701929	3656.893826	1.80678E-05	997.0751	0.0008903	0.00417	1.475175	3.100023	0.99055	7684.821	2455.53
303.15	0.0618	0.9382	983.4	0.003025	2.37943E-05	0.000120146	1329.582104	3523.674553	1.80932E-05	995.6783	0.0007975	0.00354	1.39799	3.03102	0.943026	7639.773	2376.925
308.15	0.0618	0.9382	980.2	0.002529	2.3872E-05	0.000120795	1392.823403	3399.637695	1.81226E-05	994.0635	0.0007195	0.00301	1.326895	2.96278	0.898715	7590.941	2302.6
313.15	0.0618	0.9382	976.8	0.002143	2.39551E-05	0.000121437	1454.164692	3288.267666	1.81558E-05	992.2473	0.0006532	0.00258	1.262934	2.897997	0.857219	7545.437	2231.918
318.15	0.0618	0.9382	973.4	0.001839	2.40388E-05	0.0001221	1513.680744	3188.68499	1.81926E-05	990.24	0.0005963	0.00224	1.20544	2.838856	0.818221	7509.472	2164.395
323.15	0.0618	0.9382	969.8	0.001597	2.4128E-05	0.000122784	1571.381824	3103.289317	1.82325E-05	988.07	0.0005471	0.00195	1.155006	2.780941	0.781488	7471.883	2099.717
328.15	0.0618	0.9382	966.2	0.001397	2.42179E-05	0.000123462	1628.300013	3020.569849	1.82758E-05	985.73	0.0005042	0.00171	1.107089	2.726168	0.746776	7438.05	2037.496
333.15	0.0618	0.9382	962.4	0.001238	2.43135E-05	0.000124162	1682.894975	2957.974312	1.83221E-05	983.24	0.0004666	0.00151	1.067875	2.674483	0.713946	7408.216	1977.604
338.15	0.0618	0.9382	958.5	0.001105	2.44124E-05	0.000124884	1736.512511	2900.280796	1.83716E-05	980.59	0.0004334	0.00135	1.031565	2.628242	0.6828	7389.393	1919.717
343.15	0.0618	0.9382	954.6	0.000998	2.45122E-05	0.0001256	1787.890449	2863.609985	1.84238E-05	977.81	0.0004039	0.00121	1.003681	2.583062	0.653164	7369.753	1863.547
348.15	0.0618	0.9382	950.5	0.000905	2.46179E-05	0.000126325	1838.902937	2827.168363	1.8483E-05	974.68	0.0003775	0.00109	0.976678	2.54009	0.624952	7352.746	1809.037
353.15	0.0618	0.9382	946.3	0.000834	2.47272E-05	0.000127073	1886.303022	2829.008785	1.85416E-05	971.6	0.0003538	0.00098	0.963476	2.496346	0.597928	7329.9	1755.666
293.15	0.093	0.907	983.2	0.007057	2.65639E-05	0.000118896	1087.081985	4910.632152	1.80469E-05	998.2336	0.001002	0.00495	2.014714	3.171931	1.101439	7731.213	2684.63
298.15	0.093	0.907	979.7	0.005616	2.66588E-05	0.000119518	1156.228786	4738.503304	1.80678E-05	997.0751	0.0008903	0.00417	1.911491	3.099574	1.050287	7683.709	2603.615
303.15	0.093	0.907	976	0.004536	2.67599E-05	0.000120146	1223.653509	4574.794251	1.80932E-05	995.6783	0.0007975	0.00354	1.815014	3.030571	1.002775	7638.64	2527.524
308.15	0.093	0.907	972.3	0.003713	2.68617E-05	0.000120795	1289.547102	4419.803985	1.81226E-05	994.0635	0.0007195	0.00301	1.72507	2.96233	0.958476	7589.789	2455.713
313.15	0.093	0.907	968.5	0.00309	2.69671E-05	0.000121437	1353.006848	4283.52198	1.81558E-05	992.2473	0.0006532	0.00258	1.645184	2.897547	0.916991	7544.264	2387.545
318.15	0.093	0.907	964.6	0.002607	2.70761E-05	0.0001221	1414.522552	4160.206515	1.81926E-05	990.24	0.0005963	0.00224	1.572711	2.838405	0.878004	7508.278	2322.536
323.15	0.093	0.907	960.6	0.002226	2.71889E-05	0.000122784	1474.356143	4050.003878	1.82325E-05	988.07	0.0005471	0.00195	1.507361	2.78049	0.841282	7470.669	2260.372
328.15	0.093	0.907	956.5	0.001926	2.73054E-05	0.000123462	1532.065471	3957.511712	1.82758E-05	985.73	0.0005042	0.00171	1.450493	2.725716	0.80658	7436.816	2200.664
333.15	0.093	0.907	952.4	0.001678	2.7423E-05	0.000124162	1589.088004	3866.832638	1.83221E-05	983.24	0.0004666	0.00151	1.395987	2.674029	0.77376	7406.961	2143.287
338.15	0.093	0.907	948.2	0.00148	2.75444E-05	0.000124884	1643.977852	3793.385375	1.83716E-05	980.59	0.0004334	0.00135	1.349222	2.627788	0.742624	7388.118	2087.913

343.15	0.093	0.907	943.8	0.001314	2.76728E-05	0.0001256	1698.037655	3725.930741	1.84238E-05	977.81	0.0004039	0.00121	1.30592	2.582608	0.712997	7368.457	2034.257
348.15	0.093	0.907	939.5	0.00118	2.77995E-05	0.000126325	1749.992443	3677.707547	1.8483E-05	974.68	0.0003775	0.00109	1.270506	2.539635	0.684795	7351.429	1982.261
353.15	0.093	0.907	935	0.001076	2.79333E-05	0.000127073	1798.642478	3665.398363	1.85416E-05	971.6	0.0003538	0.00098	1.248326	2.495891	0.657779	7328.563	1931.404
293.15	0.1332	0.8668	974.6	0.010454	3.0392E-05	0.000118896	988.8611737	5855.332734	1.80469E-05	998.2336	0.001002	0.00495	2.402302	3.170724	1.172524	7728.271	2857.89
298.15	0.1332	0.8668	970.7	0.008157	3.05141E-05	0.000119518	1060.061272	5656.466558	1.80678E-05	997.0751	0.0008903	0.00417	2.281794	3.098366	1.121388	7680.714	2779.871
303.15	0.1332	0.8668	966.7	0.006477	3.06404E-05	0.000120146	1129.113806	5471.113582	1.80932E-05	995.6783	0.0007975	0.00354	2.170622	3.029362	1.073892	7635.594	2706.776
308.15	0.1332	0.8668	962.6	0.005222	3.07709E-05	0.000120795	1196.336569	5298.910084	1.81226E-05	994.0635	0.0007195	0.00301	2.06819	2.961121	1.029608	7586.69	2637.96
313.15	0.1332	0.8668	958.5	0.004223	3.09025E-05	0.000121437	1264.393565	5108.827012	1.81558E-05	992.2473	0.0006532	0.00258	1.962161	2.896337	0.988138	7541.114	2572.789
318.15	0.1332	0.8668	954.3	0.003517	3.10385E-05	0.0001221	1327.047419	4970.304521	1.81926E-05	990.24	0.0005963	0.00224	1.878958	2.837195	0.949165	7505.076	2510.775
323.15	0.1332	0.8668	950	0.002964	0.000031179	0.000122784	1388.156741	4843.980267	1.82325E-05	988.07	0.0005471	0.00195	1.802869	2.779279	0.912457	7467.415	2451.607
328.15	0.1332	0.8668	945.6	0.002535	3.13241E-05	0.000123462	1446.899053	4738.265335	1.82758E-05	985.73	0.0005042	0.00171	1.736652	2.724504	0.877769	7433.51	2394.895
333.15	0.1332	0.8668	941.1	0.002189	3.14739E-05	0.000124162	1504.371235	4641.000267	1.83221E-05	983.24	0.0004666	0.00151	1.675474	2.672817	0.844962	7403.603	2340.513
338.15	0.1332	0.8668	936.6	0.001911	3.16251E-05	0.000124884	1560.149062	4555.348089	1.83716E-05	980.59	0.0004334	0.00135	1.620235	2.626575	0.813839	7384.708	2288.136
343.15	0.1332	0.8668	932	0.001682	3.17812E-05	0.0001256	1614.794794	4479.322639	1.84238E-05	977.81	0.0004039	0.00121	1.569981	2.581395	0.784224	7364.996	2237.475
348.15	0.1332	0.8668	927.3	0.001491	3.19423E-05	0.000126325	1668.49137	4409.926098	1.8483E-05	974.68	0.0003775	0.00109	1.523459	2.538421	0.756033	7347.916	2188.474
353.15	0.1332	0.8668	922.6	0.00133	3.2105E-05	0.000127073	1721.393807	4348.925593	1.85416E-05	971.6	0.0003538	0.00098	1.481115	2.494676	0.729029	7324.997	2140.613
293.15	0.1874	0.8126	963.9	0.014648	3.56284E-05	0.000118896	902.9555863	6604.882447	1.80469E-05	998.2336	0.001002	0.00495	2.709824	3.167501	1.2584	7720.416	3067.205
298.15	0.1874	0.8126	959.8	0.011239	3.57806E-05	0.000119518	975.5951918	6384.380638	1.80678E-05	997.0751	0.0008903	0.00417	2.575431	3.095143	1.207287	7672.723	2992.811
303.15	0.1874	0.8126	955.6	0.008731	3.59379E-05	0.000120146	1047.359494	6163.517113	1.80932E-05	995.6783	0.0007975	0.00354	2.445327	3.026138	1.159812	7627.466	2923.34
308.15	0.1874	0.8126	951.2	0.006903	3.61041E-05	0.000120795	1116.937932	5961.294425	1.81226E-05	994.0635	0.0007195	0.00301	2.326721	2.957895	1.115549	7578.427	2858.149
313.15	0.1874	0.8126	946.8	0.005546	3.62719E-05	0.000121437	1184.509965	5773.499283	1.81558E-05	992.2473	0.0006532	0.00258	2.217444	2.89311	1.074099	7532.714	2796.602
318.15	0.1874	0.8126	942.4	0.004533	3.64412E-05	0.0001221	1249.638116	5603.385116	1.81926E-05	990.24	0.0005963	0.00224	2.118286	2.833967	1.035145	7496.54	2738.214
323.15	0.1874	0.8126	937.8	0.00375	3.662E-05	0.000122784	1313.317007	5445.313016	1.82325E-05	988.07	0.0005471	0.00195	2.026677	2.776051	0.998456	7458.742	2682.67
328.15	0.1874	0.8126	933.2	0.003151	3.68005E-05	0.000123462	1374.596573	5308.270155	1.82758E-05	985.73	0.0005042	0.00171	1.945569	2.721275	0.963786	7424.701	2629.583
333.15	0.1874	0.8126	928.5	0.002675	3.69868E-05	0.000124162	1434.585956	5179.883195	1.83221E-05	983.24	0.0004666	0.00151	1.870019	2.669588	0.930997	7394.658	2578.826
338.15	0.1874	0.8126	923.8	0.002311	3.7175E-05	0.000124884	1491.408926	5079.074683	1.83716E-05	980.59	0.0004334	0.00135	1.806513	2.623345	0.89989	7375.627	2530.073
343.15	0.1874	0.8126	919	0.00201	3.73691E-05	0.0001256	1547.550002	4983.234354	1.84238E-05	977.81	0.0004039	0.00121	1.746599	2.578164	0.870292	7355.778	2483.037

348.15	0.1874	0.8126	914.1	0.001756	3.75694E-05	0.000126325	1603.509372	4885.257025	1.8483E-05	974.68	0.0003775	0.00109	1.687668	2.53519	0.842118	7338.562	2437.662
353.15	0.1874	0.8126	909.1	0.001545	3.77761E-05	0.000127073	1658.562079	4798.079819	1.85416E-05	971.6	0.0003538	0.00098	1.634083	2.491444	0.81513	7315.507	2393.426
293.15	0.264	0.736	950.8	0.018849	4.31384E-05	0.000118896	835.0360455	7035.456191	1.80469E-05	998.2336	0.001002	0.00495	2.886478	3.158563	1.361576	7698.63	3318.684
298.15	0.264	0.736	946.5	0.014255	4.33344E-05	0.000119518	908.6638497	6796.523055	1.80678E-05	997.0751	0.0008903	0.00417	2.741687	3.086202	1.310493	7650.56	3248.654
303.15	0.264	0.736	942	0.010922	4.35414E-05	0.000120146	981.3869279	6558.327998	1.80932E-05	995.6783	0.0007975	0.00354	2.601965	3.017195	1.263047	7604.925	3183.547
308.15	0.264	0.736	937.6	0.00851	4.37457E-05	0.000120795	1052.258998	6336.23945	1.81226E-05	994.0635	0.0007195	0.00301	2.473064	2.94895	1.218812	7555.508	3122.72
313.15	0.264	0.736	933	0.00674	4.39614E-05	0.000121437	1121.170387	6128.793002	1.81558E-05	992.2473	0.0006532	0.00258	2.353903	2.884163	1.177389	7509.417	3065.537
318.15	0.264	0.736	928.4	0.005425	4.41792E-05	0.0001221	1188.014462	5933.976134	1.81926E-05	990.24	0.0005963	0.00224	2.243261	2.825018	1.138462	7472.865	3011.512
323.15	0.264	0.736	923.6	0.004432	4.44088E-05	0.000122784	1252.889313	5758.303663	1.82325E-05	988.07	0.0005471	0.00195	2.143169	2.767099	1.101798	7434.69	2960.332
328.15	0.264	0.736	918.8	0.003676	4.46408E-05	0.000123462	1315.595739	5601.190654	1.82758E-05	985.73	0.0005042	0.00171	2.052929	2.712322	1.067153	7400.271	2911.609
333.15	0.264	0.736	914	0.003086	4.48753E-05	0.000124162	1376.703733	5456.109326	1.83221E-05	983.24	0.0004666	0.00151	1.969741	2.660632	1.034388	7369.85	2865.215
338.15	0.264	0.736	909.1	0.002619	4.51171E-05	0.000124884	1436.364341	5317.763772	1.83716E-05	980.59	0.0004334	0.00135	1.89141	2.614388	1.003305	7350.442	2820.826
343.15	0.264	0.736	904.1	0.002265	4.53667E-05	0.0001256	1492.500463	5218.033611	1.84238E-05	977.81	0.0004039	0.00121	1.828895	2.569204	0.973729	7330.215	2778.154
348.15	0.264	0.736	899.1	0.001943	4.5619E-05	0.000126325	1551.634878	5078.84647	1.8483E-05	974.68	0.0003775	0.00109	1.754546	2.526228	0.945577	7312.621	2737.142
353.15	0.264	0.736	893.8	0.001697	4.58895E-05	0.000127073	1607.228561	4982.830716	1.85416E-05	971.6	0.0003538	0.00098	1.697004	2.482481	0.91861	7289.189	2697.27
293.15	0.3808	0.6192	934.4	0.020569	5.47862E-05	0.000118896	800.1746719	6839.426181	1.80469E-05	998.2336	0.001002	0.00495	2.806052	3.130916	1.48217	7631.244	3612.617
298.15	0.3808	0.6192	930	0.015446	5.50454E-05	0.000119518	873.4918361	6594.307597	1.80678E-05	997.0751	0.0008903	0.00417	2.660115	3.058546	1.431126	7582.002	3547.7
303.15	0.3808	0.6192	925.4	0.011757	5.5319E-05	0.000120146	945.8618608	6351.322961	1.80932E-05	995.6783	0.0007975	0.00354	2.519838	2.98953	1.38372	7535.194	3487.706
308.15	0.3808	0.6192	920.8	0.009104	5.55954E-05	0.000120795	1016.371729	6127.321308	1.81226E-05	994.0635	0.0007195	0.00301	2.391522	2.921276	1.339522	7484.604	3431.992
313.15	0.3808	0.6192	916.1	0.007161	5.58806E-05	0.000121437	1085.161274	5915.508444	1.81558E-05	992.2473	0.0006532	0.00258	2.271986	2.85648	1.298136	7437.341	3379.922
318.15	0.3808	0.6192	911.4	0.005729	5.61688E-05	0.0001221	1151.789328	5716.216335	1.81926E-05	990.24	0.0005963	0.00224	2.16094	2.797327	1.259244	7399.617	3331.009
323.15	0.3808	0.6192	906.6	0.00465	5.64661E-05	0.000122784	1216.639645	5535.319939	1.82325E-05	988.07	0.0005471	0.00195	2.060177	2.7394	1.222614	7360.269	3284.942
328.15	0.3808	0.6192	901.7	0.003832	5.6773E-05	0.000123462	1279.386014	5372.548576	1.82758E-05	985.73	0.0005042	0.00171	1.969128	2.684615	1.188002	7324.677	3241.332
333.15	0.3808	0.6192	896.8	0.003196	5.70832E-05	0.000124162	1340.628453	5220.617595	1.83221E-05	983.24	0.0004666	0.00151	1.884725	2.632918	1.155269	7293.084	3200.052
338.15	0.3808	0.6192	891.7	0.002703	5.74097E-05	0.000124884	1399.753266	5081.469139	1.83716E-05	980.59	0.0004334	0.00135	1.807365	2.586666	1.124217	7272.502	3160.776
343.15	0.3808	0.6192	886.6	0.002304	5.77399E-05	0.0001256	1458.111464	4949.545209	1.84238E-05	977.81	0.0004039	0.00121	1.734791	2.541476	1.094672	7251.103	3123.216
348.15	0.3808	0.6192	881.5	0.001983	5.8074E-05	0.000126325	1515.169348	4828.258284	1.8483E-05	974.68	0.0003775	0.00109	1.667977	2.498493	1.066549	7232.337	3087.317

353.15	0.3808	0.6192	876.3	0.001717	5.84186E-05	0.000127073	1571.719132	4716.532401	1.85416E-05	971.6	0.0003538	0.00098	1.606311	2.454739	1.039611	7207.732	3052.558
293.15	0.5805	0.4195	912.9	0.015023	7.51354E-05	0.000118896	842.4162487	5148.275822	1.80469E-05	998.2336	0.001002	0.00495	2.112214	3.025911	1.60448	7375.307	3910.733
298.15	0.5805	0.4195	908.5	0.011561	7.54992E-05	0.000119518	909.8817567	4959.666209	1.80678E-05	997.0751	0.0008903	0.00417	2.000707	2.953501	1.553482	7321.601	3851.013
303.15	0.5805	0.4195	903.9	0.009009	7.58835E-05	0.000120146	976.4672247	4773.870068	1.80932E-05	995.6783	0.0007975	0.00354	1.893996	2.884447	1.506119	7270.331	3796.216
308.15	0.5805	0.4195	899.2	0.007122	7.62801E-05	0.000120795	1041.661534	4605.870382	1.81226E-05	994.0635	0.0007195	0.00301	1.797693	2.816157	1.461964	7215.278	3745.699
313.15	0.5805	0.4195	894.6	0.005711	7.66723E-05	0.000121437	1105.366284	4447.654032	1.81558E-05	992.2473	0.0006532	0.00258	1.708223	2.751326	1.420619	7163.552	3698.827
318.15	0.5805	0.4195	889.8	0.004649	7.70859E-05	0.0001221	1167.230245	4296.18818	1.81926E-05	990.24	0.0005963	0.00224	1.624117	2.692138	1.381767	7121.365	3655.112
323.15	0.5805	0.4195	884.9	0.003822	7.75128E-05	0.000122784	1228.253666	4154.368335	1.82325E-05	988.07	0.0005471	0.00195	1.546204	2.634177	1.345176	7077.555	3614.242
328.15	0.5805	0.4195	880.2	0.003187	7.79267E-05	0.000123462	1287.402772	4027.492112	1.82758E-05	985.73	0.0005042	0.00171	1.476142	2.57936	1.310601	7037.5	3575.829
333.15	0.5805	0.4195	875.3	0.002697	7.83629E-05	0.000124162	1344.358319	3919.936803	1.83221E-05	983.24	0.0004666	0.00151	1.415159	2.527631	1.277904	7001.444	3539.746
338.15	0.5805	0.4195	870.3	0.002282	7.88131E-05	0.000124884	1402.417227	3782.305796	1.83716E-05	980.59	0.0004334	0.00135	1.345282	2.481349	1.246887	6976.4	3505.667
343.15	0.5805	0.4195	865.3	0.001967	7.92685E-05	0.0001256	1457.219468	3683.698335	1.84238E-05	977.81	0.0004039	0.00121	1.291118	2.436129	1.217376	6950.538	3473.305
348.15	0.5805	0.4195	860.2	0.001681	7.97385E-05	0.000126325	1514.997528	3543.699553	1.8483E-05	974.68	0.0003775	0.00109	1.224211	2.393118	1.189287	6927.308	3442.604
353.15	0.5805	0.4195	855	0.001471	8.02235E-05	0.000127073	1568.077647	3467.791793	1.85416E-05	971.6	0.0003538	0.00098	1.181027	2.349336	1.162381	6898.241	3413.042
293.15	0.7066	0.2934	902.4	0.010786	8.81843E-05	0.000118896	897.0756999	3660.594293	1.80469E-05	998.2336	0.001002	0.00495	1.501854	2.908405	1.640896	7088.9	3999.495
298.15	0.7066	0.2934	897.9	0.008548	8.86263E-05	0.000119518	958.8296094	3535.277963	1.80678E-05	997.0751	0.0008903	0.00417	1.426116	2.835955	1.589911	7030.208	3941.32
303.15	0.7066	0.2934	893.3	0.006905	8.90826E-05	0.000120146	1018.183228	3432.239905	1.80932E-05	995.6783	0.0007975	0.00354	1.361714	2.766861	1.542561	6973.953	3888.07
308.15	0.7066	0.2934	888.7	0.005607	8.95437E-05	0.000120795	1077.839623	3328.591839	1.81226E-05	994.0635	0.0007195	0.00301	1.299165	2.698533	1.498418	6913.914	3839.099
313.15	0.7066	0.2934	884	0.004609	9.00198E-05	0.000121437	1136.25553	3232.378951	1.81558E-05	992.2473	0.0006532	0.00258	1.241469	2.633665	1.457085	6857.203	3793.772
318.15	0.7066	0.2934	879.3	0.00381	9.0501E-05	0.0001221	1194.733773	3117.607132	1.81926E-05	990.24	0.0005963	0.00224	1.17857	2.574442	1.418244	6810.03	3751.603
323.15	0.7066	0.2934	874.5	0.003184	9.09977E-05	0.000122784	1252.058286	3017.813554	1.82325E-05	988.07	0.0005471	0.00195	1.123193	2.516447	1.381664	6761.234	3712.28
328.15	0.7066	0.2934	869.7	0.002704	9.15E-05	0.000123462	1306.982473	2939.748392	1.82758E-05	985.73	0.0005042	0.00171	1.077466	2.461596	1.3471	6716.194	3675.413
333.15	0.7066	0.2934	864.8	0.002302	9.20184E-05	0.000124162	1362.391714	2847.672812	1.83221E-05	983.24	0.0004666	0.00151	1.028055	2.409835	1.314413	6675.152	3640.876
338.15	0.7066	0.2934	859.9	0.001981	9.25428E-05	0.000124884	1416.377248	2753.805074	1.83716E-05	980.59	0.0004334	0.00135	0.979467	2.363521	1.283407	6645.122	3608.343
343.15	0.7066	0.2934	854.9	0.001717	9.3084E-05	0.0001256	1469.654406	2668.929244	1.84238E-05	977.81	0.0004039	0.00121	0.935447	2.318271	1.253906	6614.275	3577.527
348.15	0.7066	0.2934	849.9	0.001513	9.36316E-05	0.000126325	1519.967401	2615.216201	1.8483E-05	974.68	0.0003775	0.00109	0.903456	2.27523	1.225825	6586.06	3548.372
353.15	0.7066	0.2934	844.8	0.001342	9.41969E-05	0.000127073	1569.508649	2579.887222	1.85416E-05	971.6	0.0003538	0.00098	0.878633	2.231419	1.198928	6552.007	3520.355

293.15	0.8325	0.1675	893.6	0.007593	0.000101328	0.000118896	955.8060594	2074.934545	1.80469E-05	998.2336	0.001002	0.00495	0.851296	2.740664	1.65643	6680.05	4037.357
298.15	0.8325	0.1675	889.1	0.006191	0.000101841	0.000119518	1012.356582	2008.513443	1.80678E-05	997.0751	0.0008903	0.00417	0.810225	2.668165	1.60545	6614.264	3979.839
303.15	0.8325	0.1675	884.5	0.005092	0.00010237	0.000120146	1068.45061	1941.259976	1.80932E-05	995.6783	0.0007975	0.00354	0.77018	2.599024	1.558104	6550.914	3927.246
308.15	0.8325	0.1675	879.9	0.004223	0.000102906	0.000120795	1124.092687	1885.127991	1.81226E-05	994.0635	0.0007195	0.00301	0.735774	2.53065	1.513965	6483.78	3878.932
313.15	0.8325	0.1675	875.2	0.003536	0.000103458	0.000121437	1178.923012	1831.387325	1.81558E-05	992.2473	0.0006532	0.00258	0.703386	2.465737	1.472636	6419.974	3834.262
318.15	0.8325	0.1675	870.5	0.002999	0.000104017	0.0001221	1232.165339	1777.848573	1.81926E-05	990.24	0.0005963	0.00224	0.672092	2.406471	1.433799	6365.706	3792.75
323.15	0.8325	0.1675	865.7	0.00256	0.000104593	0.000122784	1285.056461	1730.78294	1.82325E-05	988.07	0.0005471	0.00195	0.644176	2.348435	1.397223	6309.816	3754.083
328.15	0.8325	0.1675	861	0.002205	0.000105164	0.000123462	1336.998718	1687.170624	1.82758E-05	985.73	0.0005042	0.00171	0.618376	2.293543	1.362662	6257.681	3717.873
333.15	0.8325	0.1675	856.1	0.001919	0.000105766	0.000124162	1387.563196	1652.452758	1.83221E-05	983.24	0.0004666	0.00151	0.596561	2.241743	1.329979	6209.544	3683.993
338.15	0.8325	0.1675	851.3	0.001678	0.000106363	0.000124884	1437.95321	1597.814104	1.83716E-05	980.59	0.0004334	0.00135	0.568307	2.195392	1.298976	6172.42	3652.117
343.15	0.8325	0.1675	846.4	0.001477	0.000106978	0.0001256	1487.663512	1552.682117	1.84238E-05	977.81	0.0004039	0.00121	0.544207	2.150104	1.269478	6134.477	3621.958
348.15	0.8325	0.1675	841.4	0.00131	0.000107614	0.000126325	1536.397466	1514.186665	1.8483E-05	974.68	0.0003775	0.00109	0.523093	2.107027	1.241401	6099.168	3593.459
353.15	0.8325	0.1675	836.4	0.001172	0.000108257	0.000127073	1583.843382	1502.521648	1.85416E-05	971.6	0.0003538	0.00098	0.511714	2.063181	1.214508	6058.02	3566.1
293.15	1	0	884.3	0.00495	0.000118896	0.000118896	1026.408123	0	1.80469E-05	998.2336	0.001002	0.00495	0	2.423574	1.660058	5907.181	4046.199
298.15	1	0	879.7	0.00417	0.000119518	0.000119518	1077.189642	0	1.80678E-05	997.0751	0.0008903	0.00417	0	2.351009	1.609082	5828.048	3988.844
303.15	1	0	875.1	0.00354	0.000120146	0.000120146	1127.521981	0	1.80932E-05	995.6783	0.0007975	0.00354	0	2.281804	1.561741	5751.352	3936.413
308.15	1	0	870.4	0.00301	0.000120795	0.000120795	1178.552844	0	1.81226E-05	994.0635	0.0007195	0.00301	0	2.213368	1.517607	5670.872	3888.262
313.15	1	0	865.8	0.00258	0.000121437	0.000121437	1228.959513	0	1.81558E-05	992.2473	0.0006532	0.00258	0	2.148395	1.476281	5593.719	3843.754
318.15	1	0	861.1	0.00224	0.0001221	0.0001221	1277.635728	0	1.81926E-05	990.24	0.0005963	0.00224	0	2.089071	1.437449	5526.105	3802.405
323.15	1	0	856.3	0.00195	0.000122784	0.000122784	1326.61732	0	1.82325E-05	988.07	0.0005471	0.00195	0	2.030978	1.400877	5456.867	3763.9
328.15	1	0	851.6	0.00171	0.000123462	0.000123462	1374.899139	0	1.82758E-05	985.73	0.0005042	0.00171	0	1.976032	1.36632	5391.386	3727.853
333.15	1	0	846.8	0.00151	0.000124162	0.000124162	1422.463069	0	1.83221E-05	983.24	0.0004666	0.00151	0	1.924179	1.333641	5329.903	3694.135
338.15	1	0	841.9	0.00135	0.000124884	0.000124884	1468.034017	0	1.83716E-05	980.59	0.0004334	0.00135	0	1.877776	1.302642	5279.431	3662.422
343.15	1	0	837.1	0.00121	0.0001256	0.0001256	1513.740905	0	1.84238E-05	977.81	0.0004039	0.00121	0	1.832438	1.273147	5228.142	3632.425
348.15	1	0	832.3	0.00109	0.000126325	0.000126325	1558.968988	0	1.8483E-05	974.68	0.0003775	0.00109	0	1.789313	1.245074	5179.486	3604.089
353.15	1	0	827.4	0.00098	0.000127073	0.000127073	1605.270774	0	1.85416E-05	971.6	0.0003538	0.00098	0	1.74542	1.218183	5124.992	3576.892