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Benchmark values for the Soret, thermodiffusion and molecular diffusion coefficients of the ternary mixture tetralin+isobutylbenzene+n-dodecane with 0.8-0.1-0.1 mass fraction*

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Abstract. With the aim of providing reliable benchmark values, we have measured the Soret, thermodiffusion and molecular diffusion coefficients for the ternary mixture formed by 1,2,3,4-tetrahydronaphthalene, isobutylbenzene and *n*-dodecane for a mass fraction of 0.8-0.1-0.1 and at a temperature of 25 °C. The experimental techniques used by the six participating laboratories are Optical Digital Interferometry, Taylor Dispersion technique, Open Ended Capillary, Optical Beam Deflection, Thermogravitational technique and Sliding Symmetric Tubes technique in ground conditions and Selectable Optical Diagnostic Instrument (SODI) in microgravity conditions. The measurements obtained in the SODI installation have been analyzed independently by four laboratories. Benchmark values are proposed for the thermodiffusion and Soret coefficients and for the eigenvalues of the diffusion matrix in ground conditions, and for Soret coefficients in microgravity conditions.

1 Introduction

Transport properties play an important role in many natural and technological processes and for the fundamental understanding of the behaviour of liquids. Even today the Soret effect, a cross effect between temperature and concentration gradients, is poorly understood in multicomponent mixtures. The mass diffusion flux, $\mathbf{J}_i$, can be induced by both a temperature and a concentration gradient. Considering the linear laws of irreversible thermodynamics, the mass flux equations for components 1 and 2 in a ternary mixture may be written as [1]

$$\mathbf{J}_1 = -\rho D_{11}\boldsymbol{\nabla} c_1 - \rho D_{12}\boldsymbol{\nabla} c_2 - \rho D'_{T,1}\boldsymbol{\nabla} T, \quad (1)$$

$$\mathbf{J}_2 = -\rho D_{21}\boldsymbol{\nabla} c_1 - \rho D_{22}\boldsymbol{\nabla} c_2 - \rho D'_{T,2}\boldsymbol{\nabla} T, \quad (2)$$

where ρ is the density of the mixture, D_{11}, D_{12}, D_{21} and D_{22} are the molecular diffusion coefficients and $D'_{T,1}$ and $D'_{T,2}$ are the thermodiffusion coefficients. The third mass diffusion flux, $\mathbf{J}_3$, is defined from the condition that the fluxes of all the components must sum to zero. In stationary state, we can define the Soret coefficient for components 1 and 2, $S'_{T,1}$, $S'_{T,2}$, as [2]

$$S'_{T,1} = \frac{D'_{T,1}D_{22} - D'_{T,2}D_{12}}{D_{11}D_{22} - D_{12}D_{21}},$$
$$S'_{T,2} = \frac{D'_{T,2}D_{11} - D'_{T,1}D_{21}}{D_{11}D_{22} - D_{12}D_{21}}. \quad (3)$$

The Soret effect appears in many different processes, both natural and technological, of many different fields, such as biology [3] or food industry [4]. In particular, it is of high interest for the oil industry [5], where these data can be used to predict the initial state of oil reservoirs [6,7].

Binary mixtures have been widely studied and there are several works that show both numerical and experi-

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mental analysis [8–13] that enable the determination of the transport coefficients. The performance of the known Benchmark of Fontainebleau [14–19] came as a great progress. In that work, five groups determined independently the transport coefficients for the three binary mixtures of 1,2,3,4-tetrahydronaphthalene (tetralin), isobutylbenzene and *n*-dodecane for the mass concentration of 50% at the temperature of 25 °C, validating therefore the techniques and establishing reference values for future works.

But the liquids appearing in nature and in industrial applications usually contain more than just two components and the research focus has shifted to multicomponent systems. Fundamental research in ternary mixtures is needed before going to more complex mixtures. We have to point out that, due to the complexity of the problem, up to now there is no unified theory, as it can be seen, for example, in the differences between the theoretical models proposed by Firoozabadi [20], Kempers [21] and Larre [22]. Moreover, there are some tentative efforts to develop prediction models based on non-equilibrium thermodynamics or on molecular dynamics [23], but they cannot yet be validated. All this necessitates the establishment of a database of reliable experimental results that enables a test of the prediction models and, therefore, the theory.

By the time, some works that provide experimental data in ternary mixtures have been published, but they are very limited and the values given are not always comparable [24–30], so the dispersion in the results is quite high. Thus, it was necessary to coordinate all the experimental teams in order to analyse the same system using different techniques with the aim of comparing and evaluating the obtained results. With this purpose, this benchmark has been promoted in the framework of the project DCMIX jointly sponsored by the European Space Agency (ESA) and the Russian space agency Roscosmos, for comparing not only the results obtained in ground laboratories, but also the results obtained by the SODI installation, on board the International Space Station (ISS) under microgravity conditions.

During the workshop held at Mondragon Unibertsitatea, Mondragon (Spain), in October of 2013, the teams participating in the project DCMIX agreed to carry out the first benchmark for ternary mixtures. The chosen mixture is formed by tetrahydronaphtalene (THN), isobutylbenzene (IBB) and *n*-dodecane ($n\mathrm{C}_{12}$) at mass fractions of 0.8-0.1-0.1 and at 25 °C. After individual investigations, the results obtained by each team were compared and discussed during the 11th International Meeting on Thermodiffusion (IMT11) held in Bayonne, in June of 2014. The participating teams in this Benchmark are:

- Team headed by W. Köhler (WK), from Universität Bayreuth, Germany.
- Team headed by V. Shevtsova (VS), from Université Libre de Bruxelles (ULB), Belgium.
- Team headed by S. Van Vaerenbergh (SVV), from Université Libre de Bruxelles (ULB), Belgium.
- Team headed by Z. Saghir (ZS), from Ryerson University, Canada.
- Team headed by T. Lyubimova (RAS), from Russian Academy of Science (RAS), Russia.
- Team headed by M.M. Bou-Ali (MBA), from Mondragon Goi Eskola Politeknikoa (MGEP), Spain.

In this work, the obtained results and conclusions are shown, in order to be the reference for future techniques and measurements, as well as for the setting and the development of new prediction models based on the molecular dynamics or on the non-equilibrium thermodynamics.

2 Experimental techniques

The investigated mixture is formed by THN (purity 98+%), IBB (purity 99%) and $n\mathrm{C}_{12}$ (purity 99%), at the mass fraction of 80% of THN, 10% of IBB and 10% of $n\mathrm{C}_{12}$, at the temperature of 25 °C.

The thermodiffusion and Soret coefficients are related through the four isothermal diffusion coefficients that constitute the diffusion matrix, so the determination of the former allows one to find the latter and vice versa. On the one hand, eq. (3) is used to determine Soret coefficients from the independent experimental measurements of thermodiffusion and molecular diffusion coefficients. On the other hand, in order to determine the thermodiffusion coefficients from the independent experimental measurements of the molecular diffusion and Soret coefficients, the following expressions have been used:

$$\begin{aligned} D'_{T,1} &= D_{11}S'_{T,1} + D_{12}S'_{T,2},\\ D'_{T,2} &= D_{21}S'_{T,1} + D_{22}S'_{T,2}. \end{aligned} \tag{4}$$

The eigenvalues of the diffusion matrix are given by the following formulas [28]:

$$\widehat{D_1} = \frac{D_{11} + D_{22} - \sqrt{(D_{11} - D_{22})^2 + 4D_{12}D_{21}}}{2}, \tag{5}$$

$$\widehat{D_2} = \frac{D_{11} + D_{22} + \sqrt{(D_{11} - D_{22})^2 + 4D_{12}D_{21}}}{2}. \tag{6}$$

In the case of the thermodiffusion and Soret coefficients, the results shown are for components 1 and 3, that is, for THN and $n\mathrm{C}_{12}$. As these two components have the highest difference in density and refractive index, the accuracy reached in the analysis of their coefficients is expected to be higher. In order to compare the coefficients corresponding to these two components, the relationships shown in eq. (7) and eq. (8) have been used. These relationships can be easily deduced from the requirement that the sum of the concentrations of the three components in a ternary mixture must be unity:

$$S'_{T,1} + S'_{T,2} + S'_{T,3} = 0, \tag{7}$$

$$D'_{T,1} + D'_{T,2} + D'_{T,3} = 0. \tag{8}$$

In the case of molecular diffusion, the values of coefficients depend on the order of the components. In this work, the components are ordered in decreasing density, that is, THN-IBB-$n\mathrm{C}_{12}$. In order to compare the results of the different teams, the following equations can be used. They enable the transformation of the coefficients from one order of components to another one, as can be seen for the case where components 2 and 3 are permuted [26]:

$$D^*_{11} = D_{11} - D_{12}, \tag{9}$$

$$D^*_{12} = -D_{12}, \tag{10}$$

$$D^*_{21} = D_{22} + D_{12} - D_{21} - D_{11}, \tag{11}$$

$$D^*_{22} = D_{22} + D_{12}. \tag{12}$$

The detailed descriptions of the different techniques and analysis methods used can be found in the six papers that are accompanied by this summary paper and are written by the participating teams. In the present work, the techniques used by each team to measure the coefficients in ground conditions and the analysis carried out to obtain the results measured in microgravity conditions are briefly described. Finally, the results proposed as benchmark values are shown.

2.1 Ground conditions

– The team of WK (Universität Bayreuth) has employed two-colour Optical Beam Deflection (OBD) to measure the Soret and thermodiffusion coefficients of the three compounds. Similar to the ODI method employed in Brussels and on board the ISS, this method relies on the different refractive index dispersions of the individual components of the mixture. The concentration changes of the two independent components in the mixture are determined from the refractive index gradients in a Soret cell measured at two different wavelengths. In order to take advantage of the strong dispersion near the UV absorption of aromatic π-electron systems, a blue wavelength of 405 nm has been employed in addition to the red laser at 635 nm. By this, it has been possible to obtain a contrast factor matrix with a condition number of 50, which greatly facilitates its necessary inversion. The Soret coefficients are determined from the asymptotic stationary amplitudes of the measured transient beam deflections.

– The team of VS (Université Libre de Bruxelles) used the Optical Digital Interferometry (ODI) technique to determine the Soret coefficients and the Taylor Dispersion Technique (TDT) to determine the molecular diffusion coefficients. A Mach-Zehnder interferometer was used to examine the separation in a Soret cell with a diffusion path of the same order of magnitude as for the space experiment. Laser diodes of 670 and 925 nm wavelength were used as sources of coherent light. Although the choice of wavelengths was not optimal (the condition number of matrix of contrast factors is around 240 [31]), it was intentionally made to be as close as possible to the space instrument. Experiments with different laser light sources have been carried out individually and were repeated 3 times for each laser. The ODI technique enables tracing of the concentration along the entire diffusion path, thus providing an extended amount of data to be fitted to the full analytical model of the separation process. To characterize the diffusion matrix by Taylor Dispersion Technique (see description of instrument in [27]), small injections of three different concentrations have been made into the laminar flow of the carrier solution created in a thin long capillary. The concentration of diffused injected samples as a function of time was monitored at the end of the capillary by a high-sensitivity differential refractometer operating at near infra-red. The injection of each particular concentration was also repeated 3-4 times.

– The team of SVV (Université Libre de Bruxelles) used the Open Ended Capillary (OEC) technique to determine the molecular diffusion coefficients. In the OEC, a concentration difference is created between a solution contained in capillary tubes and a solution contained in a bath. The liquid of different tubes is sampled over time and their composition is measured *ex situ*. Concentration measurements have been performed by ^{1}H-NMR. The diffusion coefficients are determined by fitting the measured composition evolution. For the results presented here, the precision on the estimated coefficients was improved by fitting simultaneously the data collected in two independent experiments.

– The team of MBA (Mondragon Goi Eskola Politeknikoa) used the thermogravitational technique (TG) [24] to determine the thermodiffusion coefficients from the variation of the concentration with the height of the column and the Sliding Symmetric Tubes (SST) [25] to determine the molecular diffusion coefficients from the variation of the concentration with time. Soret coefficients have been determined by eq. (3), from the measurements of thermodiffusion and molecular diffusion coefficients.

2.2 Microgravity conditions

The Selectable Optical Diagnostic Instrument known (SODI) has successfully been in operation on board the International Space Station since 2009 [32]. The current SODI configuration represents two optical modules accommodating Mach-Zehnder interferometers, suitable for accurate monitoring of refractive index inside transparent test objects [29,33]. One module holds a single-wavelength interferometer, another one features a two-wavelength interferometer with 670 and 935 nm lasers light sources. The latter module is equipped with a lateral translational stage that allows for monitoring of spatially separated cells combined in the so-called cell array. While most parts of the apparatus are fixed for each particular experiment, the cell array with the liquid samples can be changed from one experiment to another. The experiment DCMIX comprises a cell array consisting of 5 cells with ternary solutions (to be monitored by 2-wavelength moving optical module) and one reference binary cell (to be monitored by fixed 1-wavelength module). The cell array filled with the mixtures under investigation is the only part that needs to be uploaded to the ISS prior to the start of the experiments. The first experiment in the series, DCMIX-1, was targeting the THN-IBB-$n\mathrm{C}_{12}$ system.

In all DCMIX experiments the mixtures are contained in a 10 mm × 10 mm × 5 mm cell. The mixture chosen for the benchmark was contained in cell #3 of the cell array.

Four teams have independently determined the Soret coefficients from the experiments carried out in the SODI installation. In all cases, the same contrast factors measured in ref. [31] have been used. The teams that have determined the Soret coefficients in microgravity conditions are

- Team of VS (Université Libre de Bruxelles)
- Team of SVV (Université Libre de Bruxelles)
- Team of RAS (Russian Academy of Sciences)
- Team of ZS (Ryerson University).

3 Results

In this section, the results obtained by the participating teams for the transport coefficients are shown. In ground conditions, results obtained for thermodiffusion, molecular diffusion and Soret coefficients and for the eigenvalues of the diffusion matrix are shown, while in microgravity conditions, results for Soret coefficients are provided. Together with the results, the experimental error of each technique is given. In addition, the weighted averages for each coefficient are given. For that, the statistical weights used are directly related to the experimental error of each technique.

3.1 Thermodiffusion coefficient

Here we show the thermodiffusion coefficients determined by the team of VS applying eq. (4) to the results obtained by the ODI and TDT techniques, the thermodiffusion coefficients extracted by the team of WK from OBD measurements, and the thermodiffusion coefficients measured directly by the team of MBA by the TG technique, in all three cases under ground conditions:

Table 1. Thermodiffusion coefficients determined in ground conditions for the mixture THN-IBB-$n\mathrm{C}_{12}$ at the mass fraction of 0.8-0.1-0.1 and at 25 °C.

	Technique	$D'_{T,1} \times 10^{-12}$ (m^2/s K)	$D'_{T,3} \times 10^{-12}$ (m^2/s K)
Ground conditions	ODI+TDT	0.69 ± 0.13	-0.48 ± 0.06
	OBD	0.72 ± 0.26	-0.50 ± 0.16
	TG	0.67 ± 0.05	-0.49 ± 0.06
	Average	0.68 ± 0.05	-0.48 ± 0.04

As can be observed, the agreement between the values independently obtained in the three laboratories, both directly (TG, OBD) and by the combination of two techniques (ODI+TDT), is very good. As reference, we will take the weighted average of the results, with its corresponding weighted deviation (table 1, row 5).

3.2 Molecular diffusion coefficient and eigenvalue of the diffusion matrix

In this section, we present results obtained for the eigenvalues of the diffusion matrix (table 2) and for the corresponding molecular diffusion coefficients (table 3). In ground conditions, they have been directly measured by the team of VS using the TDT technique, by the team of SVV using the OEC technique and by the team of MBA using the SST technique.

Table 2. Eigenvalues of the diffusion matrix measured in ground conditions for the mixture THN-IBB-$n\mathrm{C}_{12}$ at the mass fraction of 0.8-0.1-0.1 and at 25 °C.

	Technique	$\widehat{D_1} \times 10^{-10}$ (m^2/s)	$\widehat{D_2} \times 10^{-10}$ (m^2/s)
Ground conditions	TDT	5.29 ± 0.09	7.30 ± 0.26
	OEC	5.50 ± 0.03	6.60 ± 0.03
	SST	5.43 ± 0.68	8.08 ± 1.02
	Average	5.48 ± 0.03	6.61 ± 0.03

There is a reasonable agreement of the eigenvalues of the diffusion matrix, and the weighted averages with the corresponding weighted deviations have been determined (table 2, row 5). However, the agreement is not good in case of the molecular diffusion coefficients, being the worst in case of the cross-diffusion coefficients, where we can observe even changes in the sign in the results for the coefficient D_{21} (table 3, column 5). It seems that there can be more than one combination of diffusion coefficients in the matrix. Therefore, we propose the eigenvalues of the diffusion matrix as comparable reference parameters, instead of giving reference values for molecular diffusion coefficients.

3.3 Soret coefficients

Here, results for the Soret coefficients are shown. In ground conditions (table 4) they have been directly measured by the team of VS using the ODI technique and by the team of WK using the OBD technique, and they have been determined by applying eq. (3) to the results obtained by the TG and SST techniques. In addition, in microgravity conditions (table 5) Soret coefficients have been determined by teams of RAS, ZS, VS and SVV.

As commented in sect. 2, values are given for THN and $n\mathrm{C}_{12}$ (components 1 and 3, respectively), because they are the components chosen to determine the coefficients in most of the techniques. Therefore, experimental errors accumulate in the results for component 2 and the dispersion is higher. However, results for component 2 can be easily calculated by eq. (8).

As can be observed, the values measured in ground conditions are in good agreement. The weighted average of the three independent results has been proposed as the reference. It is interesting to note that consistent results have been obtained by three different methods: by two direct techniques and by the combination of other two independent techniques.

Table 3. Molecular diffusion coefficients for the mixture THN-IBB-$n\mathrm{C}_{12}$ at the mass fraction of 0.8-0.1-0.1 and at 25 °C.

	Technique	$D_{11} \times 10^{-10}$ (m^2/s)	$D_{12} \times 10^{-10}$ (m^2/s)	$D_{21} \times 10^{-10}$ (m^2/s)	$D_{22} \times 10^{-10}$ (m^2/s)
Ground conditions	TDT	6.61 ± 0.10	-0.59 ± 0.54	-1.55 ± 0.10	5.98 ± 0.44
	OEC	5.50 ± 0.51	-0.99 ± 0.63	0.002 ± 0.03	6.60 ± 0.37
	SST	5.23 ± 0.66	-1.80 ± 0.23	0.39 ± 0.05	8.28 ± 1.00

Table 4. Soret coefficients measured in ground conditions for the mixture THN-IBB-$n\mathrm{C}_{12}$ at the mass fraction of 0.8-0.1-0.1 and at 25°.

	Technique	$S'_{T,1} \times 10^{-3}$ (K^{-1})	$S'_{T,3} \times 10^{-3}$ (K^{-1})
Ground conditions	ODI	1.04 ± 0.15	-0.94 ± 0.10
	OBD	1.20 ± 0.09	-0.86 ± 0.06
	TG+SST	1.19 ± 0.09	-0.91 ± 0.15
	Average	1.17 ± 0.06	-0.88 ± 0.05

As may be observed from the data in table 5, the Soret coefficients determined in microgravity conditions show acceptable agreement. The differences are larger if we compare them to the coefficients measured in ground conditions. The difference between the results measured in different gravity conditions arises from the fact that the design of the cells for the space instrument was subjected to a set of extra conditions (safety, feasibility, etc.) and from the condition number used. This finally resulted in certain deviations of the visible separation developing in the cell from its analytical model. These deviations can, in principle, be accounted for and a better agreement between all measurements may be achieved. This requires, however, a much more detailed and elaborated processing of the data from the space experiments, which appears not yet feasible at the present time. Simplified processing based on a straightforward fit to the analytical model results in a systematic error of 10–15% (overvalued separation for THN and undervalued separation for $n\mathrm{C}_{12}$). It should be noted that the variations of experimental data for the Soret coefficients given in table 5 are not independent. Moreover, they show a linear correlation due to the specific properties of the contrast factor matrix. Further details can be found in the individual contributions of the teams of RAS, VS and WK that accompany this summary paper.

3.4 Benchmark values

In the following table 6 we show the benchmark values of thermodiffusion and Soret coefficients as well as the eigenvalues of diffusion matrix for the mixture THN-IBB-$n\mathrm{C}_{12}$ at a mass fraction of 0.8-0.1-0.1 and at 25 °C. Because of the very different experimental boundary conditions, we give separate values for Soret coefficients measured in ground and in microgravity conditions. However, we also present the Soret coefficients for the combined gravity conditions.

Table 5. Soret coefficients measured in microgravity conditions for the mixture THN-IBB-$n\mathrm{C}_{12}$ at the mass fraction of 0.8-0.1-0.1 and at 25 °C.

	Technique	$S'_{T,1} \times 10^{-3}$ (K^{-1})	$S'_{T,3} \times 10^{-3}$ (K^{-1})
Microgravity conditions	RAS	1.40 ± 0.16	-0.83 ± 0.10
	ZS	1.37 ± 0.06	-0.57 ± 0.05
	VS	1.43 ± 0.21	-0.66 ± 0.07
	SVV	1.39 ± 0.25	-0.49 ± 0.08
	Average	1.38 ± 0.05	-0.61 ± 0.03

Table 6. Benchmark values for the mixture THN-IBB-$n\mathrm{C}_{12}$ at a mass fraction of 0.8-0.1-0.1 and at 25 °C.

	$D'_{T,1} \times 10^{-12}$ (m^2/s K)	$D'_{T,3} \times 10^{-12}$ (m^2/s K)
Ground conditions	0.68 ± 0.05	-0.48 ± 0.04
	$\widehat{D_1} \times 10^{-10}$ (m^2/s)	$\widehat{D_2} \times 10^{-10}$ (m^2/s)
Ground conditions	5.48 ± 0.03	6.61 ± 0.03
	$S'_{T,1} \times 10^{-3}$ (K^{-1})	$S'_{T,3} \times 10^{-3}$ (K^{-1})
Ground conditions	1.17 ± 0.06	-0.88 ± 0.05
Microgravity conditions	1.38 ± 0.05	-0.61 ± 0.03
Combined conditions	1.28 ± 0.04	-0.70 ± 0.03

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References

1. M.M. Bou-Ali, J.K. Platten, J. Non-Equilib. Thermodyn. **30**, 385 (2005).
2. A. Mialdun, V. Shevtsova, J. Chem. Phys. **138**, 161102 (2013).
3. J.K.G. Dhont, S. Wiegand, S. Duhr, D. Braun, Langmuir **23**, 1674 (2007).
4. H. Tello Alonso, A.C. Rubiolo, S.E. Zorrilla, J. Food Eng. **109**, 490 (2012).
5. F. Montel, Entropie **184/185**, 86 (1994).
6. M. Touzet, G. Galliero, V. Lazzeri, M.Z. Saghir, F. Montel, J.C. Legros, C.R. Méc. **339**, 318 (2011).
7. F. Montel, J. Bickert, A. Lagisquet, G. Galliero, J. Petrol. Sci. Eng. **58**, 391 (2007).
8. A. Mialdun, V. Yasnou, V. Shevtsova, A. Königer, W. Köhler, D. Alonso de Mezquia, M.M. Bou-Ali, J. Chem. Phys. **136**, 244512 (2012).
9. P. Blanco, P. Polyakov, M.M. Bou-Ali, S. Wiegand, J. Phys. Chem. B **112**, 8340 (2008).
10. A. Perronance, C. Leppla, F. Leroy, B. Rousseau, S. Wiegand, J. Chem. Phys. **116**, 3718 (2002).
11. P.A. Artola, B. Rousseau, G. Galliero, J. Am. Chem. Soc. **130**, 10963 (2008).
12. M. Eslamian, M.Z. Saghir, Phys. Rev. E **80**, 011201 (2009).
13. F. Croccolo, H. Bataller, F. Scheffold, J. Chem. Phys. **137**, 234202 (2012).
14. J.K. Platten, M.M. Bou-Ali, P. Costeséque, J. Dutrieux, W. Köhler, C. Leppla, S. Wiegand, G. Wittko, Philos. Mag. **83**, 1965 (2003).
15. G. Wittko, W. Köhler, Philos. Mag. **83**, 1973 (2003).
16. C. Leppla, S. Wiegand, Philos. Mag. **83**, 1989 (2003).
17. J.K. Platten, M.M. Bou-Ali, J.F. Dutrieux, Philos. Mag. **83**, 2001 (2003).
18. M.M. Bou-Ali, J.J. Valencia, J.A. Madariaga, C. Santamaría, O. Ecenarro, J.F. Dutrieux, Philos. Mag. **83**, 2011 (2003).
19. P. Costesèque, J.-C. Loubet, Philos. Mag. **83**, 2017 (2003).
20. K. Ghorayeb, A. Firoozabadi, AlChE J. **46**, 883 (2000).
21. L. Kempers, J. Chem. Phys. **90**, 6541 (1989).
22. J.P. Larre, J.K. Platten, G. Chavepeyer, Int. J. Heat Mass Transfer **40**, 545 (1997).
23. S. Srinisvasan, M.Z. Saghir, J. Non-Equilib. Thermodyn. **36**, 243 (2011).
24. P. Blanco, M.M. Bou-Ali, J.K. Platten, D. Alonso de Mezquía, J.A. Madariaga, C. Santamaría, J. Chem. Phys. **132**, 114506 (2010).
25. M. Larrañaga, D.A.S. Rees, M.M. Bou-Ali, J. Chem. Phys. **140**, 054201 (2014).
26. A. Königer, H. Wunderlich, W. Köhler, J. Chem. Phys. **132**, 174506 (2010).
27. A. Mialdun, V. Sechenyh, J.C. Legros, J.M. Ortiz de Zárate, V. Shevtsova, J. Chem. Phys. **139**, 104903 (2013).
28. A. Leahy-Dios, M.M. Bou-Ali, J.K. Platten, A. Firoozabadi, J. Chem. Phys. **122**, 234502 (2005).
29. A. Ahadi, S. Van Vaerenbergh, M.Z. Saghir, J. Chem. Phys. **138**, 204201 (2013).
30. Q. Galand, S. Van Vaerenbergh, F. Montel, Energy Fuels **22**, 770 (2008).
31. V. Sechenyh, J.-C. Legros, V. Shevtsova, J. Chem. Thermodyn. **62**, 64 (2013).
32. S. Mazzoni, V. Shevtsova, A. Mialdun, D. Melnikov, Yu. Gaponenko, T. Lyubimova, M.Z. Saghir, Europhys. News **41**, 14 (2010).
33. A. Mialdun, C. Minetti, Y. Gaponenko, V. Shevtsova, F. Dubois, Micrograv. Sci. Technol. **25**, 83 (2013).