A solution of the Boltzmann equations in the presence of three components and inelastic collisions

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ABSTRACT

A new algorithm for the solution of the system of three Boltzmann equations for three components in a mixture is developed. Binary collisions between molecules are taken into account assuming that these collisions are elastic or inelastic. The functionality testing of the algorithm is performed using a simple test problem of heat and mass transfer in the mixture of n-dodecane, p-dipropylbenzene and nitrogen between two infinite parallel walls. The mixture of n-dodecane and p-dipropylbenzene is chosen due to the fact that it can approximate realistic Diesel fuels reasonably well. It is concluded that the predictions of the new kinetic algorithm are qualitatively consistent with the predictions of more basic models of the phenomena for which it has been tested. The algorithm is ready for the analysis of a wider range of heat and mass transfer problems in which the contribution of three components in the mixture is essential.

1. Introduction

The limitations of widely used engineering approaches to modelling evaporation/condensation/ heat transfer processes based on the hydrodynamic approximation, even in the case when these processes take place at high pressures, have been discussed in a number of papers (see [1] for a review of the early models and [2] for a review of more recent developments). In a number of papers, including [3–7], the evaporation of n-dodecane $C_{12}H_{26}$ (an approximation for Diesel fuel) has been studied and a new model has been developed based on a combination of the kinetic and hydrodynamic approaches. In the immediate vicinity of droplet surfaces (up to about one hundred molecular mean free paths), the vapour and ambient gas dynamics have been studied based on the Boltzmann equation (kinetic region), while at larger distances the analysis has been based on the hydrodynamic equations (hydrodynamic region). Mass, momentum and energy fluxes have been conserved at the interface between these regions.

The analysis of [3] was based on the assumption that n-dodecane evaporates into its own vapour (the contribution of air in the kinetic region was ignored). Although this assumption is rather far from most conditions in which fuel droplets evaporate, it allowed the authors of [3] to avoid the numerical solution of the Boltzmann equation and base their analysis on its approximate analytical solution for the mass flux. The authors of [4,5] considered a more realistic problem of n-dodecane evaporation into air and developed a new numerical algorithm for the solution of a system of two Boltzmann equations for n-dodecane and air, taking into account elastic collisions between: n-dodecane molecules; air molecules; and between n-dodecane and air molecules. One of the main limitations of the analysis presented in [4,5] was that the effects of heat transfer in the kinetic region were ignored. The latter was taken into account in a more general model presented in [6].

The approaches of [4–6] were based on the assumption that all collisions between molecules are elastic. A new approach to taking into account the effects of inelastic collisions was developed in [7] and applied to the problem of n-dodecane droplet heating and evaporation in [8].

One of the important limitations of the approaches described in [3–8] is that they have been based on the assumption that Diesel fuel can be approximated by n-dodecane. A more detailed analysis of the composition of Diesel fuel showed that it includes hundreds

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Nomenclature

E	energy	x	distance or components of $\mathbf{X}$
f	molecular velocity distribution function	$\mathbf{X}$	N-dimensional vector
$\mathbf{j}$	molecular number flux		
J	collision integral	*Greek symbols*	
ℓ	mean free molecular path	θ	angle determining the direction of velocity
L	distance between walls	σ	diameters of molecules
M	total number of cells	ϕ	angle determining the direction of velocity
n	molecular number density		
N	number of degrees of freedom	*Subscripts*	
N_{int}	number of internal degrees of freedom	a	air
$\mathbf{q}$	heat flux	f	total
r	radius in the energy space	n	n-dodecane
$\mathbf{r}$	position	nt	nitrogen
t	time	p	p-dipropylbenzene
T	temperature		
$\mathbf{v}$	velocity		

of various hydrocarbon components [9,10]. These components can be subdivided into two main groups: alkanes and aromatics. The assumption that n-dodecane can approximate alkanes is a reasonable one (see [9,11]), while aromatics can be approximated by p-dipropylbenzene [11]. In this case a more accurate approximation of Diesel fuel, compared with the one based on its approximation by n-dodecane, could be its approximation by a mixture of n-dodecane and p-dipropylbenzene. Mass fractions of n-dodecane in this mixture vary from 0.8 to 0.7 [11,9].

To improve the accuracy of kinetic modelling of Diesel fuel droplet heating and evaporation, one would naturally expect that this modelling should take into account the contributions of both n-dodecane and p-dipropylbenzene. We cannot, however, perform this modelling before a kinetic algorithm of the solution of the system of three Boltzmann equations for n-dodecane, p-dipropylbenzene and air, taking into account the effects of inelastic collisions between respective molecules, has been developed. The results of the development of such an algorithm and its preliminary testing are presented in our paper.

The mathematical model, used in our analysis, is discussed in Section 2. In Section 3 this model is applied to the analysis of three test cases. The main results of the paper are summarised in Section 4 .

2. Mathematical models

The evolution of the molecular velocity distribution functions of air $f_a \equiv f_a(\mathbf{r}, t, \mathbf{v})$ (or any other neutral gas, including nitrogen), n-dodecane $f_n \equiv f_n(\mathbf{r}, t, \mathbf{v})$, and p-dipropylbenzene $f_p \equiv f_p(\mathbf{r}, t, \mathbf{v})$ is controlled by the corresponding Boltzmann equations:

$$\left. \begin{array}{l} \dfrac{\partial f_a}{\partial t} + \mathbf{v}_a \dfrac{\partial f_a}{\partial \mathbf{r}} = J_{aa} + J_{an} + J_{ap} \\[2mm] \dfrac{\partial f_n}{\partial t} + \mathbf{v}_n \dfrac{\partial f_n}{\partial \mathbf{r}} = J_{na} + J_{nn} + J_{np} \\[2mm] \dfrac{\partial f_p}{\partial t} + \mathbf{v}_p \dfrac{\partial f_p}{\partial \mathbf{r}} = J_{pa} + J_{pn} + J_{pp} \end{array} \right\} , \qquad (1)$$

where $J_{\alpha\beta}$ ($\alpha = a, n, p$; $\beta = a, n, p$) are collision integrals, taking into account the contribution of the collisions between molecules. Triple collisions are ignored.

Explicit expressions for the collision integrals $J_{\alpha\beta}$ can be presented as [4]:

$$J_{\alpha\beta} = \frac{\sigma_{\alpha\beta}^2}{2} \int_{-\infty}^{+\infty} d\mathbf{v_1} \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left(f_\alpha' f_{\beta 1}' - f_\alpha f_{\beta 1} \right) |\mathbf{v}_\alpha - \mathbf{v}_{\beta 1}|, \qquad (2)$$

where $\sigma_{\alpha\beta} = (\sigma_\alpha + \sigma_\beta)/2$, σ_α and σ_β are the corresponding diameters of molecules of air 'a', n-dodecane 'n' and p-dipropylbenzene

'p', θ and ϕ are angular coordinates of molecules β relative to molecules α, superscript $'$ indicates the velocities and the distribution functions after collisions, subscript $_1$ indicates that the function f_α is modified under the influence of collisions with molecules of the type $_\beta$. The first integral on the right hand side of (2) is calculated in the three dimensional velocity space. Expression (2) is the same as that used in [4], where the contribution of only 2 components in the kinetic region was taken into account. This is justified by the fact that triple collisions are ignored.

All collision integrals $J_{\alpha\beta}$ are calculated taking into account the contribution of internal degrees of freedom (inelastic collisions) as described in [7]. A degree of freedom is usually defined as a parameter corresponding to each independent variable necessary to describe the energy of a molecule [12]. A mono-atomic molecule has three degrees of freedom corresponding to its translational energies in x, y and z directions. Poly-atomic molecules have additional degrees of freedom corresponding to their rotational and vibrational motions (see [13] for the analysis of degrees of freedom of CO_2 molecules).

The main ideas of the approach used in [7] are summarised below.

Regardless of the nature of the collision between molecules, their centre of mass is not affected by this collision. During the collisions, the energy of each molecule is redistributed between the degrees of freedom, but the total number of degrees of freedom remains the same. If we assume that none of these degrees of freedom is preferable to any of the others we can consider the redistribution of energy between these degrees of freedom during the collision process as random (this follows from the equipartition-of-energy theorem [12]). For each of these degrees of freedom we allocate one dimension in the $N-$dimensional space describing all degrees of freedom and consider a sphere in this space with its centre at the origin (where energies of all degrees of freedom are equal to zero) and radius $r = \sqrt{\sum_{i=1}^{i=N} E_i}$, where E_i is the energy of the ith degree of freedom. Since r^2 gives the total energy of the system E_f, this equation can be considered as an equation for the conservation of energy. The location of the points on the surface of this sphere can be described by an $N-$dimensional vector $\mathbf{X} = (x_1, x_2, \ldots \ldots x_N)$ with the basis $(\mathbf{e_1}, \mathbf{e_2}, \ldots \mathbf{e_N})$ and the norm $||\mathbf{X}|| = r = \sqrt{E_f}$. The redistribution of energy between the degrees of freedom during the collision process can be described in terms of the random rotation of vector $\mathbf{X}$ in the $N-$dimensional space.

The numerical algorithm used in the analysis is based on the method of direct numerical solution of the Boltzmann equation.

Physical and velocity spaces are discretised along with time. Time and physical space are discretised as in conventional structured computational fluid dynamics (CFD) codes. The discretisation of the velocity space is performed similarly to that of the physical space by replacing continuous values of $\mathbf{v}$ with a discrete set $\{\mathbf{v}^k\}^M$, where k indicates the position of a velocity cell and M is the total number of cells. The numerical solution of the discretised system of equations is performed in two steps. Firstly, molecular displacements are calculated ignoring the effect of collisions ($J^k_{\alpha\alpha} = J^k_{\alpha\beta} = 0$). Secondly, the collisional relaxation is calculated under the assumption of spatial homogeneity.

3. Applications

3.1. Evaporation and condensation from flat walls

Let us consider two parallel walls kept at constant temperatures $T_{w1} = 1$ and $T_{w2} = 1$ as shown in Fig. 1. The distance between the walls L is equal to 10 mean free paths for n-dodecane ℓ_n at temperature T_{w2}. Space between the walls is filled with:

(1) a mixture of n-dodecane, p-dipropylbenzene and nitrogen (three component mixture);
(2) a mixture of n-dodecane and nitrogen (two component mixture);
(3) pure n-dodecane or p-dipropylbenzene (single component).

Initially, molar fractions of all components are assumed to be equal to 1. It is also assumed that the distribution functions of n-dodecane and p-dipropylbenzene at both walls are half-Maxwellian with densities $n_{s1} = 2$ and $n_{s2} = 1$, describing evaporated species. N-dodecane and p-dipropylbenzene molecules hitting the walls are removed from the domain (they are condensed), while for nitrogen molecules it is assumed that the flux of incoming molecules is equal to the flux of molecules reflected from the walls.

Note that although, strictly speaking, the above mentioned combination of parameters might not be realistic for practical applications it turned out to be useful for testing the code.

The space grid in the numerical analysis has been taken equal to $0.5\,\ell_n$, and $12 \times 12 \times 12$ velocity grid points have been used.

The predicted distributions of the number density of n-dodecane for three and two component mixtures and one component substance versus the distance from the first plate are shown in Fig. 2 (the distance x is normalised by ℓ_n). Two cases have been considered: the contribution of internal degrees of freedom (corresponding to rotational and vibrational movements of the constituent molecules) is ignored (a); the numbers of these degrees

Fig. 2. Plots of n-dodecane number density n_n versus the distance from the first plate x predicted by the model, taking into account the contributions of: three components, n-dodecane, p-dipropylbenzene and nitrogen (thick solid curves), two components: n-dodecane and nitrogen (thin solid curves), and a single component (n-dodecane) (dashed curves). The contribution of internal degrees of freedom is either ignored (a) or taken into account assuming that $N_{int} = 20$ for n-dodecane and p-dipropylbenzene and $N_{int} = 2$ for nitrogen (b).

for n-dodecane and p-dipropylbenzene are equal to 20, while nitrogen has 2 internal degrees of freedom (b). As follows from our previous analysis [7,8], only the first 20 internal degrees of freedom of such complex molecules as n-dodecane contribute to the results predicted by the kinetic calculations (the actual number of internal degrees of freedom of n-dodecane, taking into account translational, rotational and vibrational movements of the constituent molecules, is expected to be much more than 20). It is anticipated that the same conclusion should remain valid for p-dipropylbenzene. This is supported by our analysis presented later in this paper (see Fig. 5).

As follows from Fig. 2, the density distributions for three and two component mixtures are very close. They coincide within the accuracy of plotting when the contribution of internal degrees of freedom is taken into account (see Fig. 2b). Both these distributions differ considerably from the distribution for the one component substance. In all cases the expected concentration jumps near the walls are clearly seen. These jumps are noticeably larger for the one component substance compared with three or two component mixtures. The physical nature of these density jumps has been
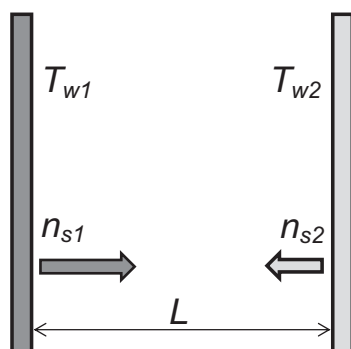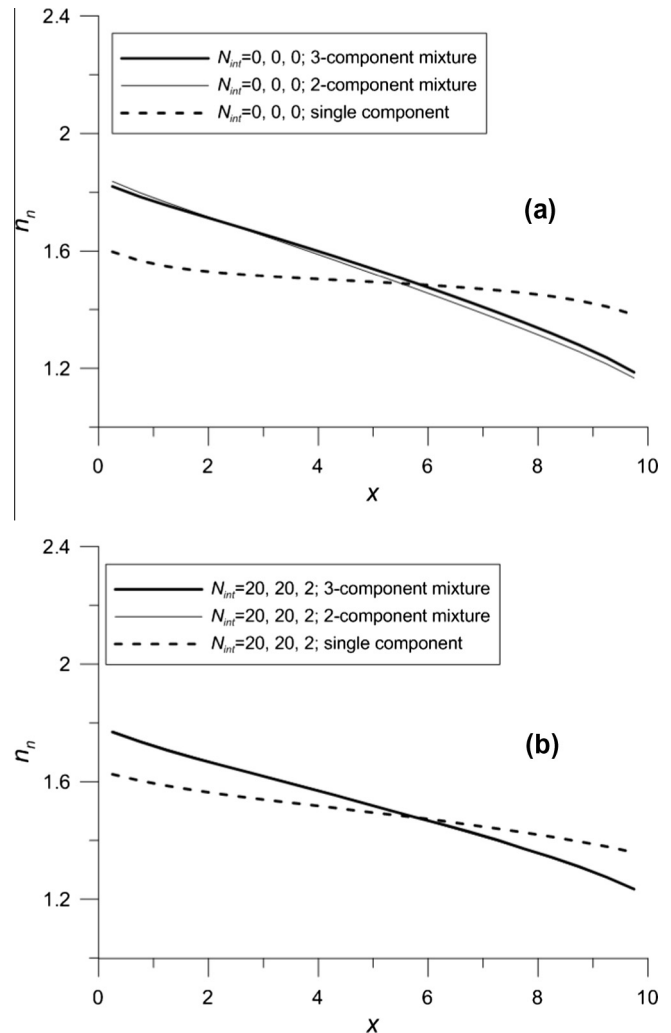

Fig. 1. A schematic presentation of the setup used for the analysis of mass/heat transfer processes in up to three component mixtures. The distance between the walls L is assumed to be equal to 10 mean free molecular paths of n-dodecane molecules ℓ at the temperature of the second wall (T_{w2}).

widely discussed in the literature, starting with a pioneering monograph [1]. In [14] it was shown that the introduction of these jumps into a conventional CFD code (FLUENT) enables this code to be used for modelling rarefied gases.

The contribution of internal degrees of freedom has little effect on the distribution of number densities of n-dodecane. It leads to an increase in number density jumps for three and two component mixtures and a slight decrease in these jumps for the case of a single component.

The distributions of the number densities of p-dipropylbenzene for a three component mixture and a one component substance are shown in Fig. 3. Comparing Figs. 2 and 3 one can see that the distributions of n-dodecane and p-dipropylbenzene are very close which is related to the closeness of masses and sizes of the corresponding molecules (see Table 1).

The distributions of the number density of nitrogen for three and two component mixtures are shown in Fig. 4. Comparing Fig. 4 with Figs. 2 and 3 one can see that in contrast to n-dodecane and p-dipropylbenzene, the number density of nitrogen increases from the first plate to the second one. This means that nitrogen molecules are expected to move from the region of high concentration of n-dodecane and p-dipropylbenzene to the region of low concentration of these molecules, which is consistent with the corresponding thermodynamics equations for the mixtures. In
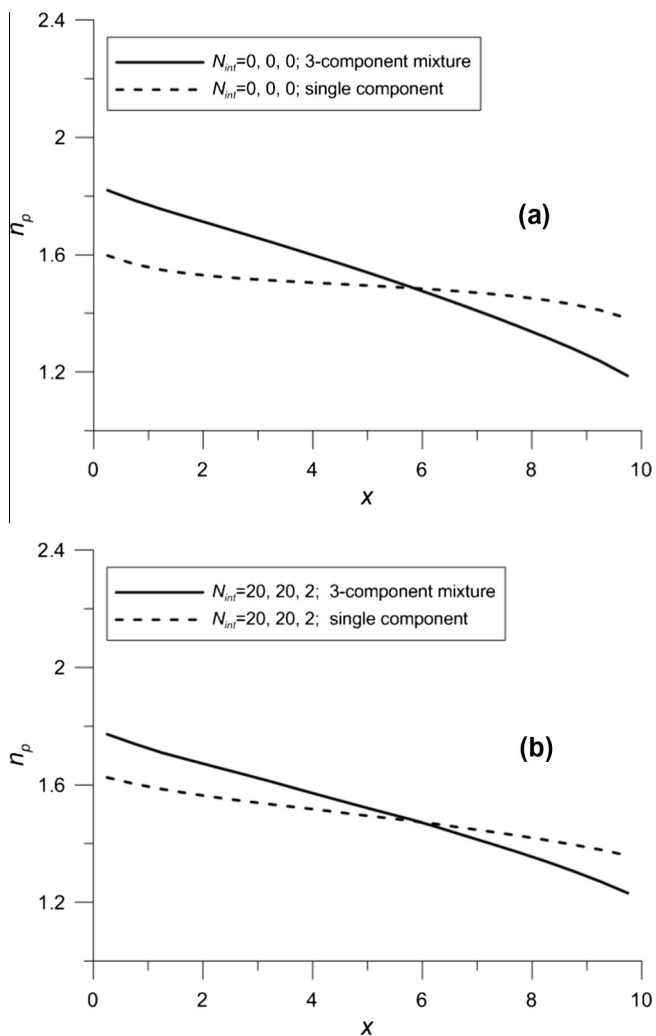
Table 1
Chemical formulae, molar masses and molecular diameters of n-dodecane, p-dipropylbenzene and nitrogen are given in Table 1.

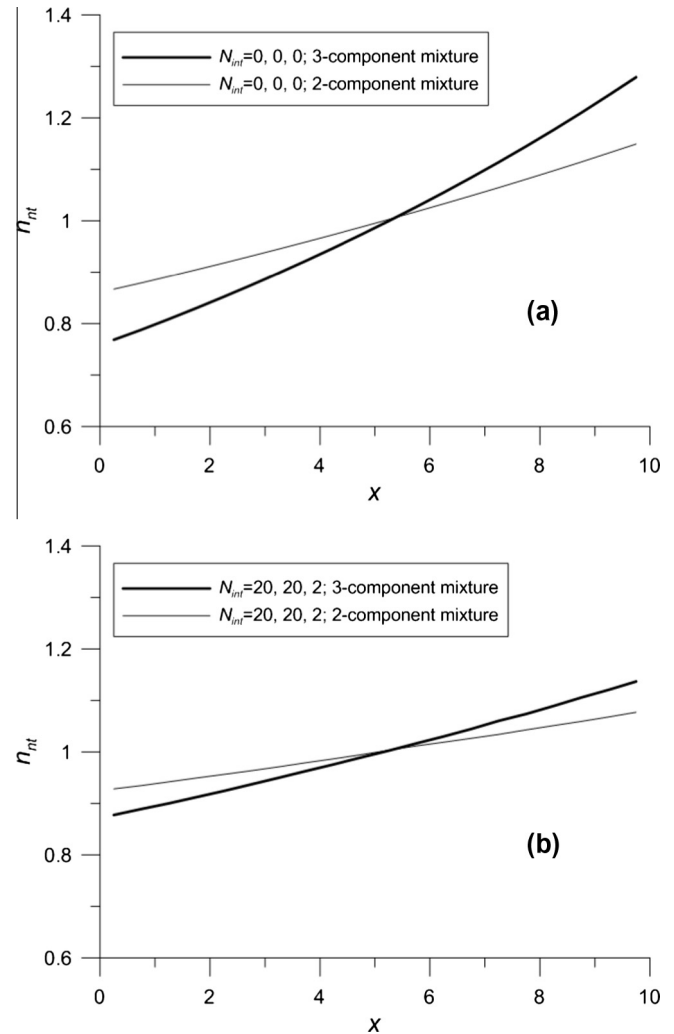| Component	Chemical formula	Molar mass (kg/kmol)	Molecular diameter
n-dodecane	$C_{12}H_{26}$	170.3	7.12 Å
p-dipropylbenzene	$C_{12}H_{18}$	162.27	6.73 Å
nitrogen	N_2	28.97	3.617 Å

Fig. 4. The same as Figs. 2 and 3 but for nitrogen, taking into account the contributions of: three components, n-dodecane, p-dipropylbenzene and nitrogen (thick solid curves); and two components, n-dodecane and nitrogen (thin solid curves).

Fig. 3. The same as Fig. 2 but for p-dipropylbenzene, taking into account the contributions of three components: n-dodecane, p-dipropylbenzene and nitrogen (thick solid curves) and a single component (p-dipropylbenzene) (dashed curves).

contrast to the case shown in Fig. 2, the distribution of nitrogen is rather different for three and two component mixtures. Since the number density of nitrogen at the walls is not specified we cannot infer any information about the number density jump in the vicinity of the walls for nitrogen. As in the cases shown in Figs. 2 and 3, the contribution of internal degrees of freedom produces only minor effects on the number density of nitrogen.

The number fluxes of n-dodecane and p-dipropylbenzene for the three component mixture and single components versus the number of internal degrees of freedom N_{int} are shown in Fig. 5. It is assumed that N_{int} for n-dodecane and p-dipropylbenzene are equal and N_{int} for nitrogen is equal to 2, except when N_{int} for
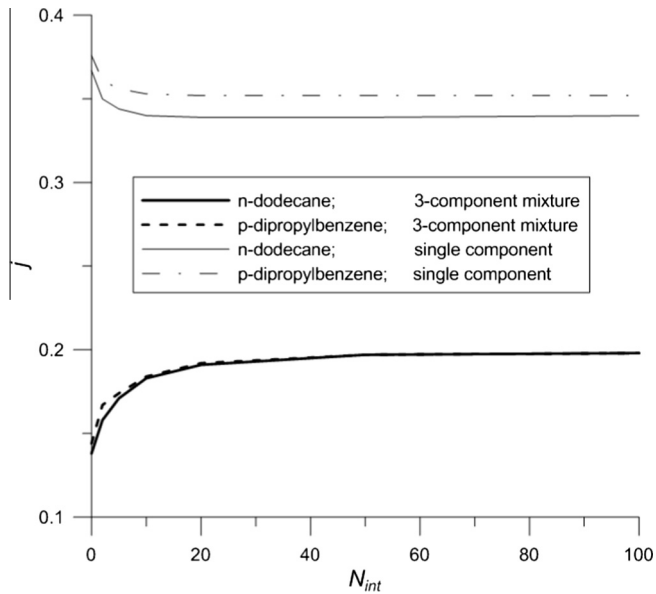
Fig. 5. Plots of number fluxes of n-dodecane and p-dipropylbenzene versus the number of internal degrees of freedom N_{int}, predicted by the model, taking into account the contributions of: three components, n-dodecane, p-dipropylbenzene and nitrogen and the models of single components (n-dodecane or p-dipropylbenzene).

Fig. 6. The same as Fig. 2 but for n-dodecane temperature, taking into account only heat transfer between the walls.

n-dodecane and p-dipropylbenzene are equal to 0. In the latter case N_{int} for nitrogen has been taken equal to 0 as well. As one can see from this figure, although the number densities of n-dodecane and p-dipropylbenzene are weak functions of the number of internal degrees of freedom, the dependence of number fluxes of these components on this number is rather strong, at least at $N_{int} \leqslant 20$. At larger N_{int} these fluxes do not depend on N_{int}, in agreement with our earlier results [7,8]. Mass fluxes of n-dodecane and p-dipropylbenzene are close for the three component mixture, but are noticeably different for the case of single components. Mass fluxes of n-dodecane and p-dipropylbenzene are both much larger for the single components than for the three component mixture as expected.

3.2. Heat conduction between two flat walls

Let us consider the same case as discussed in the previous section, but ignore the effects of evaporation and condensation and assume that $T_{w1} = 2$ and $T_{w2} = 1$ (see Fig. 1). In this case the processes between the walls will lead to pure heat conduction between them.

The distributions of temperature of n-dodecane for three and two component mixtures and one component substance versus the distance from the first plate are shown in Fig. 6. As in the case shown in Fig. 2, two cases have been considered: the contribution of internal degrees of freedom is ignored (a); the numbers of these degrees for n-dodecane and p-dipropylbenzene are equal to 20, while nitrogen has 2 internal degrees of freedom (b).

As follows from Fig. 6, the n-dodecane temperatures for three and two component mixtures and a single component are reasonably close, especially when the contribution of internal degrees of freedom is ignored (see Fig. 6a). In all cases the expected temperature jumps near the walls are clearly seen. The physical nature of these temperature jumps is similar to that of the density jumps; see [1,14] for details. The contribution of internal degrees of freedom has little effect on the distribution of temperatures of n-dodecane, as in the case of number densities shown in Fig. 2.
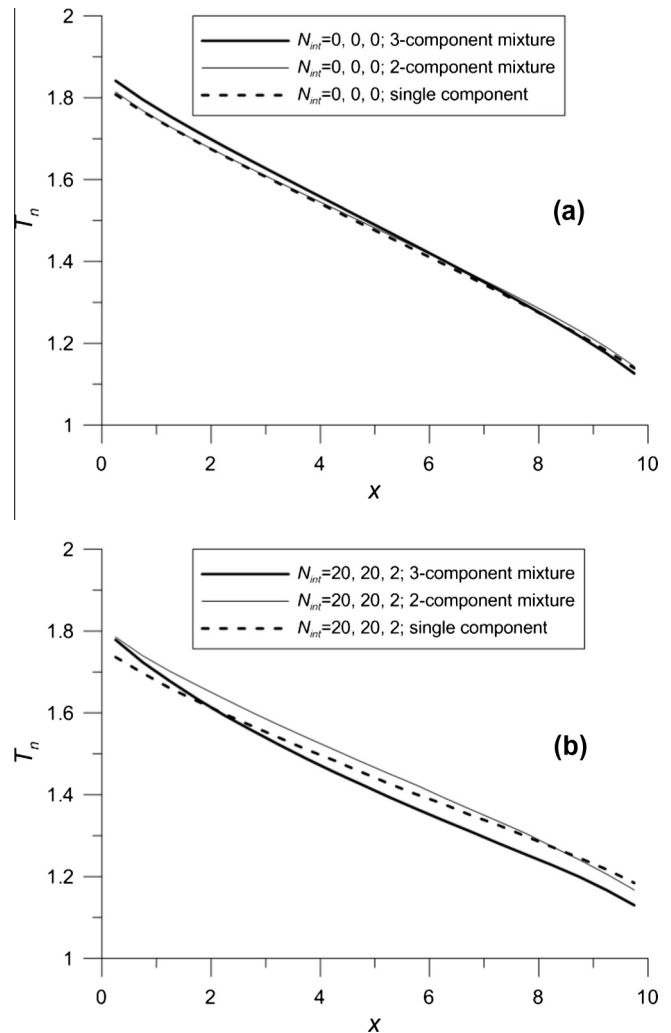
The distributions of the temperature of p-dipropylbenzene for the three component mixture and one component substance are shown in Fig. 7. Comparing Figs. 6 and 7 one can see that the distributions of temperature of n-dodecane and p-dipropylbenzene are very close which is related to the closeness of masses and sizes of the corresponding molecules (cf. the corresponding distributions of number densities shown in Figs. 2 and 3).

The distributions of the temperature of nitrogen for three and two component mixtures and a single component are shown in Fig. 8. Note that in contrast to the problem of evaporation and condensation, considered in the previous section, we considered the case when the space between the walls is filled with nitrogen alone. In contrast to the case of the distribution of mass densities, the distribution of temperatures of nitrogen is reasonably close to that of n-dodecane and p-dipropylbenzene. This shows that the system is close to local thermodynamic equilibrium as expected.

The heat fluxes of n-dodecane, p-dipropylbenzene and nitrogen, predicted for the three component mixture, and single components, versus the number of internal degrees of freedom N_{int} are shown in Fig. 9. As in the case shown in Fig. 5, it is assumed that N_{int} for n-dodecane and p-dipropylbenzene are equal and N_{int} for nitrogen is equal to 2, except when N_{int} for n-dodecane and p-dipropylbenzene are equal to 0. In the latter case N_{int} for nitrogen has been taken equal to 0 as well. As one can see from this figure,
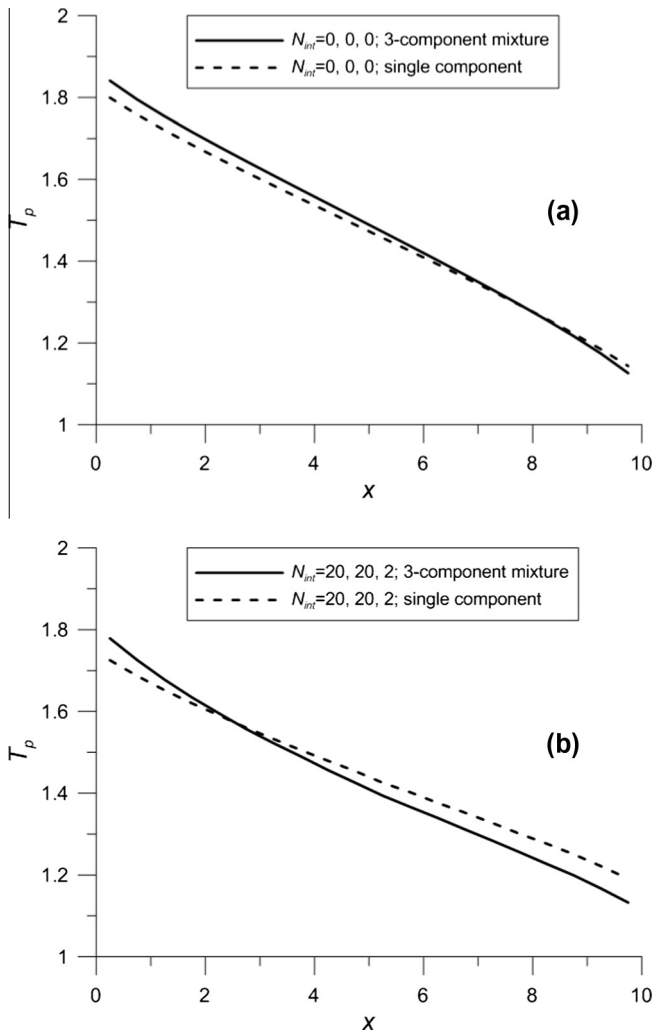
Fig. 7. The same as Fig. 3 but for p-dipropylbenzene temperature, taking into account only heat transfer between the walls.

Fig. 8. The same as Fig. 6 but for nitrogen temperature.

the dependence of heat fluxes of components on N_{int} is weaker than in the case of number fluxes (cf. Fig. 5). These heat fluxes remain practically unchanged for $N_{int} > 10$. For the three component mixture the total heat flux between the walls is equal to the sum of the heat fluxes due to individual components. The largest heat flux for single components is predicted for nitrogen which reflects its largest thermal conductivity.

3.3. Heat and mass transfer between two flat walls

Let us consider the case when heat and mass transfer between walls take place simultaneously. As in the case of evaporation and condensation considered in Section 3.1, it is assumed that the distribution functions of n-dodecane and p-dipropylbenzene at both walls are half-Maxwellian with densities $n_{s1} = 2$ and $n_{s2} = 1$, describing evaporated species. N-dodecane and p-dipropylbenzene molecules hitting the walls are removed from the domain (they are condensed), while for nitrogen molecules it is assumed that the flux of incoming molecules is equal to the flux of molecules reflected from the walls. Initially, molar fractions of all components are assumed to be equal to 1. In contrast to the case considered in Section 3.1, we took into account the difference between T_{w1} and T_{w2} and assumed that $T_{w1} = 2$ and $T_{w2} = 1$ (see Section 3.2). In all cases we have considered the three component mixture
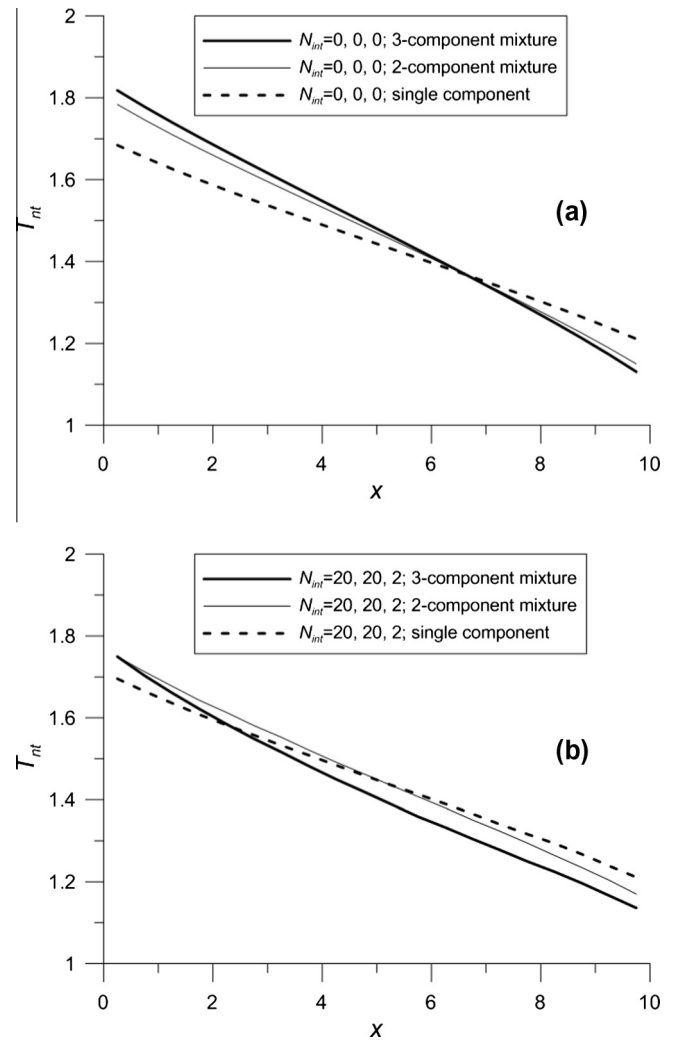
and assumed that $N_{int} = 20$ for n-dodecane and p-dipropylbenzene, and $N_{int} = 2$ for nitrogen.

The spatial distributions of the number densities of n-dodecane and nitrogen, predicted by the models taking into account both heat and mass transfer processes, only heat transfer process (see Section 3.2), and only mass transfer processes (see Section 3.1), are shown in Fig. 10. The plot n_n versus x for the case when only mass transfer is taken into account is identical to the corresponding plot shown in Fig. 2b (solid curve). The plot n_{nt} versus x for the case when only mass transfer is taken into account is identical to the corresponding plot shown in Fig. 4b (thick solid curve).

As follows from Fig. 10a, the distributions of n-dodecane, predicted by the models taking into account both heat and mass transfer processes and only mass transfer processes are qualitatively similar. Both models predict a decrease in n-dodecane number density with x. This can be attributed to the fact that the rate of evaporation of n-dodecane from the hotter wall is stronger than that from the cooler wall. In the case when only heat transfer is taken into account, the number density of n-dodecane increases with x. This is related to an increase of n-dodecane number density with a decrease in temperature. The number density jumps near the walls, predicted by the model taking into account both heat and mass transfer, are larger than the ones predicted by the model taking into account only the mass transfer process. For all three models the number density of nitrogen increases with x. This is related
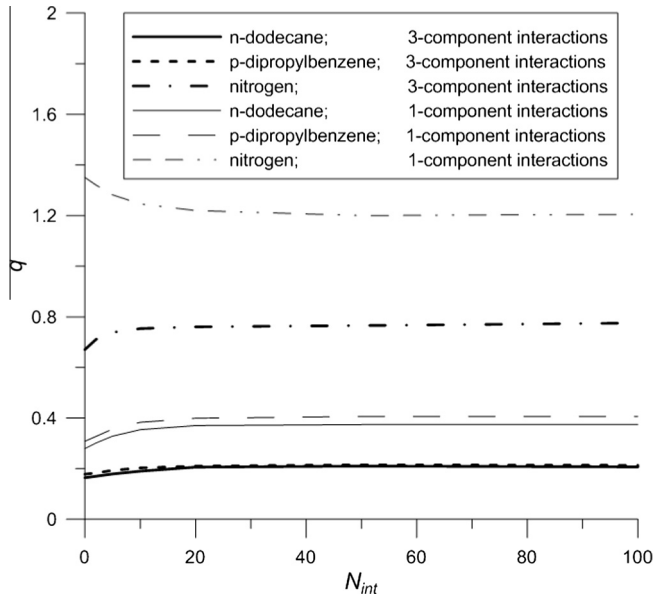
Fig. 9. The same as Fig. 5 but for heat fluxes due to various components, taking into account only heat transfer between the walls. The models, taking into account the contributions of three components (n-dodecane, p-dipropylbenzene and nitrogen) and single components (n-dodecane, p-dipropylbenzene or nitrogen) have been used.

to the fact that nitrogen does not evaporate and its number density decreases with increasing temperature.

The spatial distributions of the temperature of n-dodecane, predicted by the models taking into account both heat and mass transfer processes, only heat transfer process (see Section 3.2), and only mass transfer processes (see Section 3.1), are shown in Fig. 11. The plot T_n versus x for the case when only heat transfer is taken into account is identical to the corresponding plot shown in Fig. 6b (thick solid curve).

As follows from Fig. 11, the distributions of n-dodecane temperature, predicted by the models taking into account both heat and mass transfer processes and only the heat transfer process are qualitatively similar. Both models predict a decrease in n-dodecane temperature with x, as expected. The temperature jumps near the walls, predicted by the model taking into account both heat and mass transfer, are larger than the one predicted by the model taking into account only the heat transfer process. For the model taking into account only mass transfer processes, the n-dodecane temperature slowly increases with x, which can be related to the corresponding decrease in the n-dodecane number density (see Fig. 10a).

The velocity distribution functions of n-dodecane $f_n(v_x, \ v_y = 0, \ v_z = 0)$ at three positions x ($x = 0.25$, $x = 2.25$ and $x = 4.25$), predicted by the three component model taking into account both heat and mass transfer processes, are shown in Fig. 12. As can be seen from this figure, at all three positions these functions are close to Maxwellian. An increase in the peak value of this distribution function with x is related to the corresponding decrease in the n-dodecane temperature, as shown in Fig. 11. The integrals of f_n over v_x, v_y and v_z would give us number densities of n-dodecane in the corresponding points x (see thick solid curve in Fig. 10a).

Spatial distributions of the temperature of nitrogen, predicted by the models taking into account both heat and mass transfer processes, only heat transfer process (see Section 3.2), and only mass transfer processes (see Section 3.1), are shown in Fig. 13. The plot of T_{nt} versus x for the case when only heat transfer and only mass transfer are taken into account are qualitatively similar to the
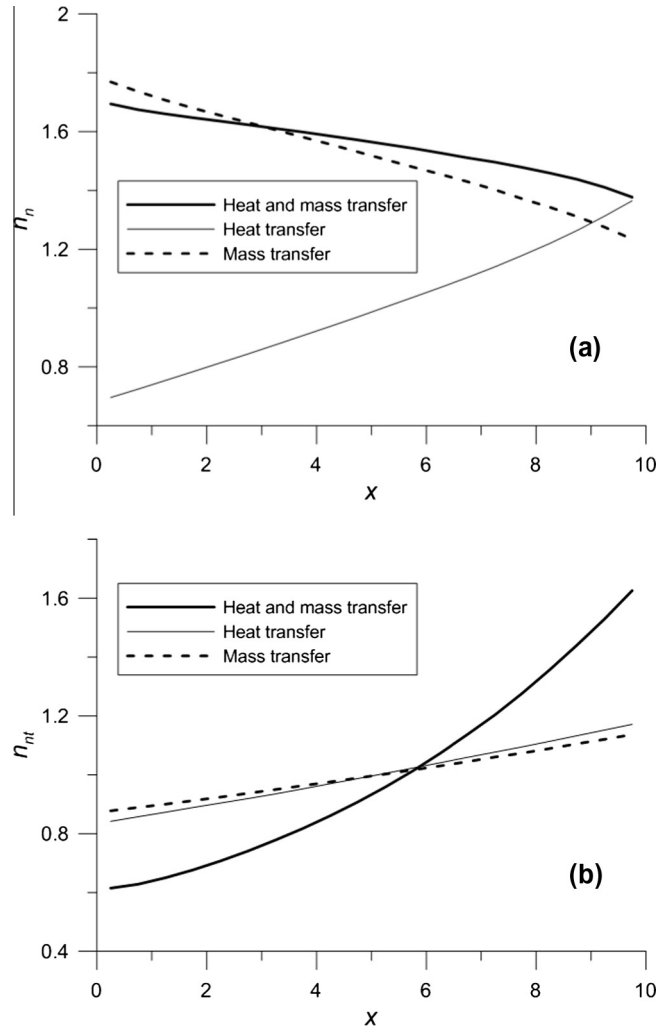

Fig. 10. The same as Fig. 2, but for n-dodecane (a) and nitrogen (b) number densities and the models taking into account both mass and heat transfer between the walls (thick solid curves), only heat transfer between them (thin solid curves), and only mass transfer between them (dashed curves). The model, taking into account the contributions of three components (n-dodecane, p-dipropylbenzene and nitrogen), and the contribution of internal degrees of freedom, assuming that $N_{int} = 20$ for n-dodecane and p-dipropylbenzene and $N_{int} = 2$ for nitrogen, has been used.
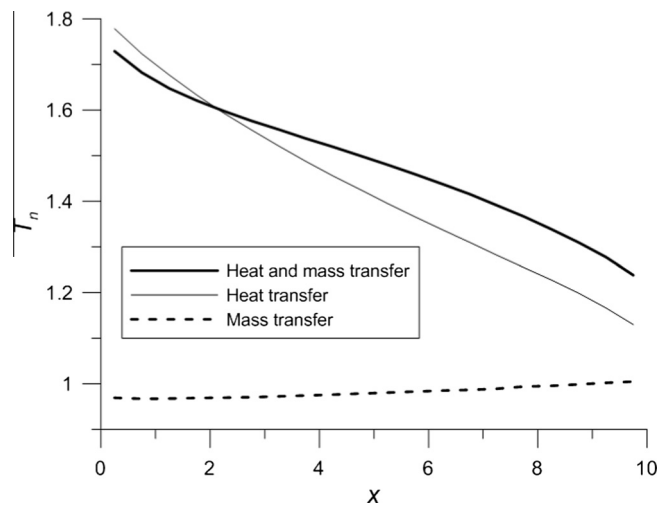

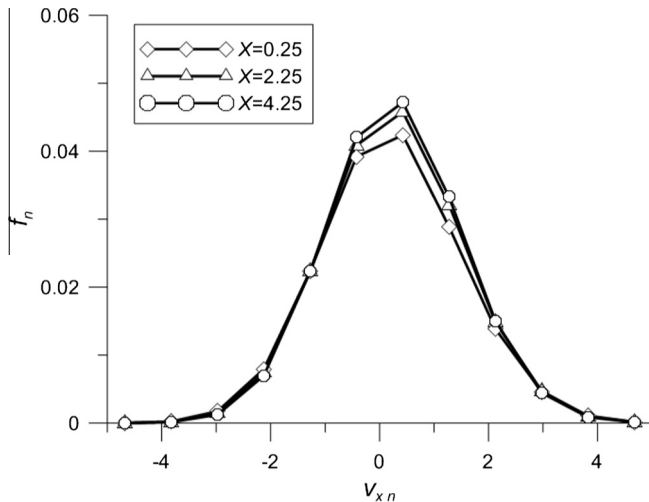**Fig. 11.** The same as Fig. 10 but for n-dodecane temperature.

Fig. 12. The velocity distribution functions of n-dodecane $f_n(v_x, v_y = 0, v_z = 0)$ at three positions x ($x = 0.25$, $x = 2.25$ and $x = 4.25$), predicted by the three component model taking into account both heat and mass transfer processes. As in the case of Figs. 10 and 11, the model, taking into account the contributions of three components (n-dodecane, p-dipropylbenzene and nitrogen), and the contribution of internal degrees of freedom, assuming that $N_{int} = 20$ for n-dodecane and p-dipropylbenzene and $N_{int} = 2$ for nitrogen, has been used.
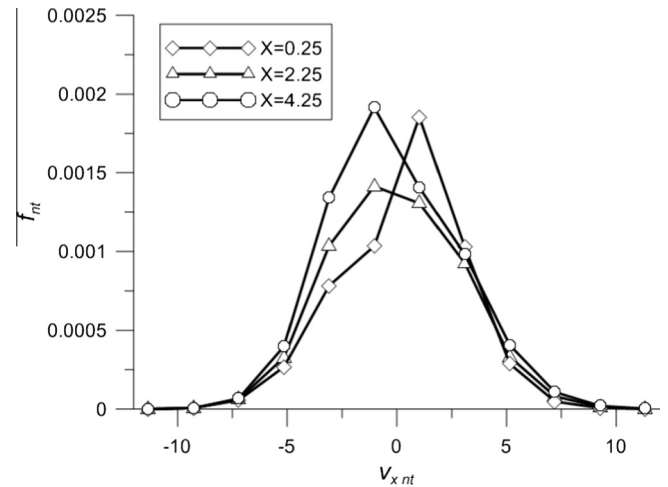

Fig. 14. The same as Fig. 12 but for the nitrogen velocity distribution functions.

velocities for nitrogen molecules shown in Fig. 14 is wider than in the case of n-dodecane molecules as shown in Fig. 12. This is attributed to the fact that nitrogen molecules are much lighter than n-dodecane molecules. Note that the dispersion of the distribution function, shown in Fig. 14, at $x = 2.25$ is noticeably larger than at other x which leads to increased temperature of nitrogen in the vicinity of this x as shown in Fig. 13. The integrals of f_{nt} over v_x, v_y and v_z would give us number densities of nitrogen in the corresponding points x (see thick solid curve in Fig. 10b).

4. Conclusions

A new algorithm for the solution of the system of three Boltzmann equations for three components in a mixture has been developed. Binary (but not triple) collisions between molecules have been taken into account; the collisions have been assumed to be elastic or inelastic and in the latter case they have been analysed based on the model described in [7].

The functionality testing of the model has been performed using three simple test problems of heat and mass transfer in the mixture of n-dodecane, p-dipropylbenzene and nitrogen between two infinite parallel walls. The mixture of n-dodecane and p-dipropylbenzene has been chosen due to the fact that it can approximate realistic Diesel fuels reasonably well [11]. It has been shown that in the case of pure mass transfer the predicted distribution of n-dodecane number density between the walls is almost unaffected by the presence of p-dipropylbenzene, and the effects of internal degrees of freedom on this distribution have been shown to be relatively weak. The distribution of nitrogen between the walls, however, has been shown to be visibly affected by the presence of n-dodecane and p-dipropylbenzene.

In the case of pure mass transfer, the number fluxes of components between walls have been shown to change noticeably with increasing numbers of internal degrees of freedom N_{int} when $N_{int} < 20$, but remain almost unchanged when $N_{int} > 20$. This result is consistent with the one presented in [7] for similar problems but based on the analysis of two component mixtures. In the case of pure heat transfer between the walls the distributions of temperatures of various components between the walls have been shown to be qualitatively similar.

It has been pointed out that the velocity distribution functions of n-dodecane remain almost Maxwellian at various positions between the walls when both heat and mass transfer processes are taken into account. Noticeable deviations from the Maxwellian
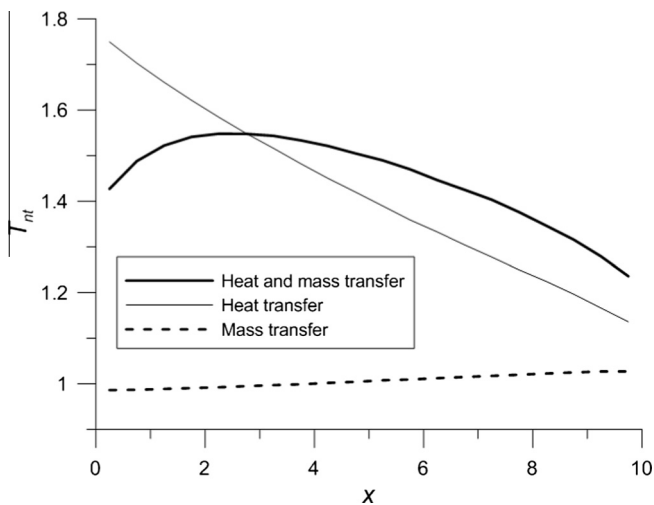

Fig. 13. The same as Fig. 11 but for the nitrogen temperature.

corresponding plots for n-dodecane temperatures shown in Fig. 11 (thin solid and dashed curves). In the case when both heat and mass transfer processes are taken into account, however, the behaviour of the curve T_{nt} versus x becomes more complex. At first T_{nt} increases with x until it reaches its maximal value. Then it decreases with x as in the case when only the heat transfer process is taken into account. The high nitrogen temperature jump near $x = 0$ can be related to the low number density of nitrogen near $x = 0$. Average temperature of the system decreases with increasing x as expected.

The velocity distribution functions of nitrogen $f_{nt}(v_x, v_y = 0, v_z = 0)$ at the same three positions x as in Fig. 12, predicted by the three component model taking into account both heat and mass transfer processes, are shown in Fig. 14. As can be seen from this figure, at all three positions these distributions are noticeably different from the Maxwellian ones. The range of

distributions have been observed for the corresponding distribution functions of nitrogen.

It is concluded that the predictions of the new kinetic algorithm are qualitatively consistent with the predictions of more basic models of the phenomena for which it has been tested. It is ready for the analysis of a wider range of heat mass transfer problems in which the contribution of three components in the mixture is essential.

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