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Numerical method for multicomponent diffusion with a posteriori evaluation of calculation accuracy on the basis of mass balance

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ABSTRACT

The new method of computational modeling for multicomponent diffusion with evaluation of calculation accuracy on the basis of mass balance is suggested. Results of proposed method applied for the modeling of diffusion separation of air species (nitrogen and oxygen) in multicomponent boundary layer on permeable flat plate at helium injection have been presented. Efficiency analysis of proposed method has been carried out and compared to the known calculation method allowing to exclude one of diffusion differential equations. Numerical results of diffusion separation of air species (nitrogen and oxygen) obtained with the controllable calculation accuracy have been presented.

1. Introduction

Many actual problems of gas dynamics and heat and mass transfer lead to the necessity of multicomponent flow modeling including these with chemical reactions [1]. These are, for instance, evaporation of complex fluids into gas flow, hypersonic flow over an aircraft plates, flows in the jet engines nozzles, combustion process, etc. Gas flow composition in some cases numbers thousands of various substances. At that, modeling result often depends on the determination accuracy of substance fraction which content in the flow is insignificant. Serving as an example hydrogen–xenon mixture has Prandtl number decreasing three times already at the mass fraction of hydrogen 1% [2].

As it is known, precision of the results obtained by numerical methods mainly depends on the accuracy of physical models designed-in the calculation algorithm and precision of applied numerical method.

Accuracy evaluation of the physical model used for numerical study of the particular problem is possible by means of a posteriori comparison of obtained results and experimental data. However, it is possible only when applied numerical method does not cause significant errors in the obtained solution.

To identify numerical method error there are *a priori* (presupposed prior to calculations) and *a posteriori* (evaluated after complete calculation or its part) methods. For example, evaluation method of approximation order for differential equations can be reckoned among *a priori* methods [3]. Comparison with standard experiments results, results of analytical solutions, standard results of numerical modeling (obtained on the basis of more common equations, on grids with greater nodes, with the use of higher order schemes) can be reckoned among *a posteriori* methods [4].

One of the most frequently used *a posteriori* methods for accuracy evaluation is examination of obtained numerical solution for accomplishment of one or several additional conditions. For example, to model flow in the tube (nozzle) examination of integral condition of the mass balance in the channel [1] is carried out, to model heat transfer in closed cavity integral balance of heat flows [5] is examined. All these additional conditions are, as a matter of fact, excess data and their mathematical formulations redefine initial closed equation system describing the considered problem.

This work offers method of *a posteriori* evaluation of computational accuracy for numerical study of multicomponent diffusion with the use of excess information on the gas flow compound. Possibility of calculation correction on the basis of the mass balance equation in the process of numerical integration of equations of the boundary layer is studied. Accuracy and speed of the calculation of the proposed method is analyzed.

2. Problem statement

Consider laminar flow of gas mixture along the permeable flat plate at the injection of foreign gas into the main flow. Flow scheme is presented in Fig. 1. Temperatures of the main flow and injected gas are equal to each other. Ignore thermo-diffusion and diffusion-thermo effects.

Considered problem can be solved on the basis of the boundary layer theory. System of differential equations can be presented as follows:

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Nomenclature

D_{ij}	binary diffusion coefficient for species i–j (m^2/s)
J	mass flux of component related to mass average mean velocity (kg/(m^2s))
j_w	intensity of gas injection through the porous plate (kg/(m^2s))
K	mass fraction of component
M	molecular weight of mixture (kg/kmol)
M_i	molecular weight of component i (kg/kmol)
P	pressure (Pa)
R	universal gas constant (8314.41 J/(kmol K))
u and v	mass average mean velocity along and across the plate, accordingly (m/s)
x and y	coordinates along and across the plate, accordingly (m)
X	molar fraction of component

Greek symbols

α	weight factor for calculation error correction
δ	boundary layer thickness (m)
δK	computational modeling error of the mass balance
Δx	step along the plate (m)
μ	dynamic viscosity of the gas mixture (Pa s)
μ_i	dynamic viscosity of the component i (Pa s)
ρ	density of the mixture (kg/m^3)

Subscripts

i, j and k	gas mixture component number
n	number of gas mixture component
N	number of computational grid nodes across the boundary layer
w	conditions on the wall
0	conditions in the main flow
' (apostrophe)	conditions in the injected gas
*	iteration approximation
**	corrected iteration approximation

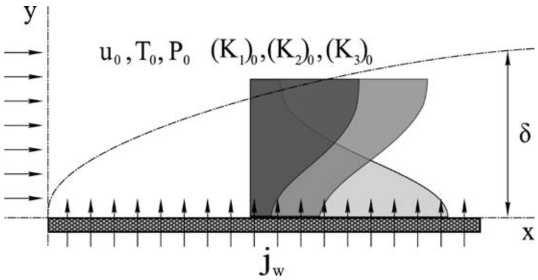

Fig. 1. Flow scheme in the multicomponent boundary layer on the permeable plate.

Continuity equation:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0, \tag{1}$$

Momentum equation:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right), \tag{2}$$

Diffusion equations:

$$\rho u \frac{\partial K_i}{\partial x} + \rho v \frac{\partial K_i}{\partial y} = \frac{\partial(-J_i)}{\partial y}, \quad i = 1 \ldots n, \tag{3}$$

where n is the number of species J_i is the mass flow of i-component.

To calculate diffusion flows of species we use iterative model by Lapin and Strelets based on Maxwell–Stefan correlations [1]:

$$J_i = -\frac{\rho}{B_i}\frac{\partial K_i}{\partial y} + \frac{MK_i}{B_i}\sum_{j=1, j\neq i}^{n}\left(\frac{J_j}{M_j D_{ij}}\right) - \frac{\rho K_i}{B_i M}\frac{\partial M}{\partial y}; \quad B_i = \sum_{j=1, j\neq i}^{n}\left(\frac{MK_j}{M_j D_{ij}}\right). \tag{4}$$

To close the equation system (1)–(3) we use the ideal gas law:

$$\rho = PM/RT, \tag{5}$$

correlation determining dynamic viscosity of multicomponent gas mixture Gordon and McBride [6]:

$$\mu = \sum_{j=1}^{n} K_j \mu_j \left(K_j + \sum_{k=,k\neq j}^{n} K_k F_{jk}\right)^{-1};$$

$$F_{jk} = 0.25\left(1 + \left(\frac{\mu_j}{\mu_k}\right)^{0.5}\left(\frac{M_k}{M_j}\right)^{0.25}\right)^2 \left(\frac{2M_k}{M_j + M_k}\right)^{0.5} \tag{6}$$

and formula for molecular weight of mixture:

$$M = \left(\sum_{j=1}^{n} \frac{K_j}{M_j}\right)^{-1}. \tag{7}$$

To solve differential Eqs. (1)–(3) it is necessary to write down boundary conditions. On the porous plate (at $y = 0$) longitudinal velocity $u_w = 0$ (adhesion hypothesis), transverse velocity is determined by the specified injection intensity $v_w = j_w/\rho_w$, and gas mixture components fractions are determined on the balance:

$$(J_i)_w = j_w(K_i' - K_{iw}), \tag{8}$$

where $(J_i)_w$ is intensity of the diffusion flow of i – substance on the surface of porous plate determined by the correlation (4); K_{iw}, K_i' is mass fraction of i – substance on the surface of porous plate and in injected gas mixture. At the outer of the boundary layer (at $y = \delta$) longitudinal velocity and component fraction are considered constant and equal to u_0 and K_{i0}, accordingly.

Eqs. (1)–(7) along with the boundary conditions completely describe the considered problem. Moreover, solutions of Eq. (3) must satisfy the equation of mass balance:

$$\sum_{i=1}^{n} K_i = 1, \tag{9}$$

containing excess information on the gas flow compound and redefining the equation system (1)–(7). As a rule, this equation is used for the elimination of one of differential diffusion equations. Besides, it can be used for accuracy evaluation of computational modeling results.

3. Numerical method for multicomponent diffusion with *a posteriori* evaluation of calculation accuracy on the basis of mass balance

In this work, we used numerical integration method for boundary layer equations in physical coordinates on the Crank–Nikolson scheme [4] in the nonuniform Cartesian grid with the compression close to high velocity gradients. Calculation area was adapted on the thickness of the dynamic boundary layer. Nonlinearity of differential equations was eliminated by simple iteration method at every integration step with the accuracy within 0.001%. Number of computational grid nodes on the thickness of the boundary layer, N amounted to 100 and, in specified cases, 400.

To evaluate the results accuracy of numerical integration of Eqs. (1)–(3) and correction of calculation error the algorithm was changed as follows:

(1) Calculation of the first iteration approximation for the mass fraction profiles and gas mixture components on Eq. (3) – K_i^*.
(2) Evaluation of the fraction calculation accuracy for every profile node from the balance (9) according to the formula:

$$\delta K = 1 - \sum_{i=1}^{n} K_i^* \tag{10}$$

(3) Correction of the gas flow in every profile node according to the formula $K_i^{**} = K_i^* + \delta K \cdot \alpha_i$, where α_i is the weight factor.
(4) Use of the fraction profile K_i^{**} for new iteration approximation.

Weight factor α_i in this case influences prospective share in the error at mass balance determination obtained in the solution of i – equation of diffusion. If $\alpha_i = 1,\ \alpha_j = 0$, for $j = 1 \ldots i-1,\ i+1 \ldots n$ the algorithm turns out to be the solution algorithm $n-1$ of the diffusion equation with determination of the fraction of i – component on the mass balance at the same time supposing maximum error for fraction of this component. Weight factor values can be selected at random from 0 to 1 under the condition: $\sum_{i=1}^{n}\alpha_i = 1$. One of the most efficient (on the iteration convergence velocity) is correlation $\alpha_i = K_i^*/(1-\delta K)$, use of which implicates error distribution proportionate to the mass fraction of species [7]. Brief description and calculation samples of the proposed method can be found in the paper [8].

4. Results and discussion

To analyze efficiency of the proposed numerical method we modeled helium injection into the laminar boundary layer of air. Air was assumed as the 2-component mixture of nitrogen (N_2) and oxygen (O_2) with the mass fraction 74.9% and 25.1%, accordingly. Thermodynamic and transfer gas properties were identified according to the data of the work [9]. Flow velocity was assumed equal to 2 m/s, air and injected gas temperature was 22.5 ° C, pressure in the flow coincided with the atmospheric pressure, intensity of gas injection was 0.00307 kg/(m^{2}s), that coincided with the experiment conditions [10].

Fig. 2 demonstrates calculation results for the mole fraction profiles N_2, O_2, and He, on the thickness of the boundary layer 80 mm beyond the front edge of the plate. Lines mark results of numerical modeling on the proposed method (with error evaluation and correction of the composition proportionate to mass fraction of the components). Modeling results with determination of oxygen on the correlation (9) are marked with black triangles. Circles – experimental data of the work [10]. As it is seen, the modeling results for both cases are close to each other and correspond with the results of the experiment within the error of 5 mol % that conforms with the accuracy of the experimental method applied by the authors [10]. Obtained result, as it seems at the first glance, proved that new calculation method doe not provide any advantages. However, it is wrong.

Fig. 3 shows changing correlation of mass fractions of nitrogen and oxygen on the thickness of the boundary layer caused by the multicomponent character of the diffusion processes. Authors of works [8,10] denote this effect as diffusion separation effect. Reduction to dimensionless value was carried out in relation to nitrogen and oxygen fractions in the main flow. Modeling results of diffusion separation effect are compared with experimental data of the work [10], where chromatography analysis served to obtain the value $(X_{N_2}/X_{O_2})/(X_{N_2}/X_{O_2})_0 = (K_{N_2}/K_{O_2})/(K_{N_2}/K_{O_2})_0$ in each profile point with the correction not exceeding 0.2%.

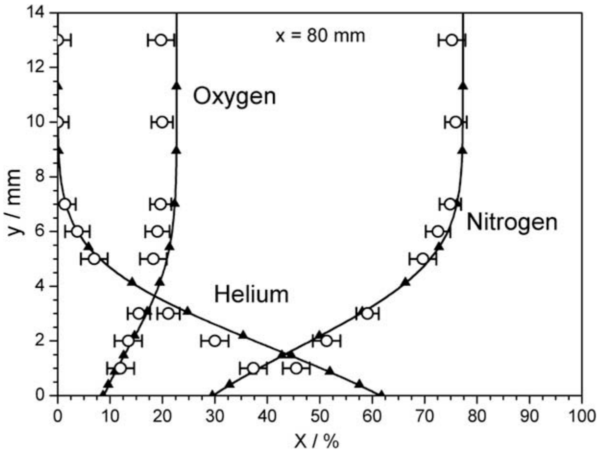

Fig. 2. Distribution profiles of mole fraction of nitrogen, oxygen and helium on the thickness of the boundary layer 80 mm beyond the plate edge: lines and triangles are results of numerical modeling and circles are experimental data of the work [10].

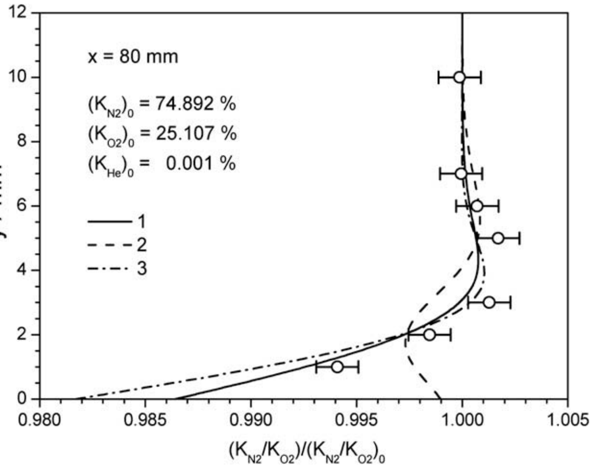

Fig. 3. Effect of diffusion separation of air components in the boundary layer on the permeable plate at helium injection 80 mm beyond the front edge of the plate: circles are experimental data of the work [10], lines are results of numerical modeling (1, on the proposed method and; 2 and 3, determined on the correlation (9) fractions of oxygen and nitrogen, accordingly).

It is clear that the results of numerical modeling on the proposed method (full line) are maximum close to the experimental points and show 1.5% increase of oxygen fraction in relation to nitrogen fraction near the porous plate. Results of modeling with determination of oxygen on Eq. (9) demonstrate inverse effect. If we determine nitrogen fraction on Eq. (9) relative increase of oxygen fraction will be equal to 2%.

Advantage of the proposed method becomes apparent if we consider the modeling results of diffusion separation effect in the sections of the boundary layer down along the plate. Fig. 4 shows distribution profiles $(K_{N_2}/K_{O_2})/(K_{N_2}/K_{O_2})_0$ on the thickness of the boundary layer in sections 190 and 400 mm, and Fig. 5 (lines 3 and 4) demonstrates distributions of the same value along the plate length. It can be seen that the growing interval from the front edge of the plate or as it is demonstrated in the work [10], growing fraction of the injected gas cause increase of relative oxygen content near the porous plate. Again results of modeling obtained from the determination of oxygen fraction on correlation (9), vice versa show increase of relative nitrogen content for more than 10%.

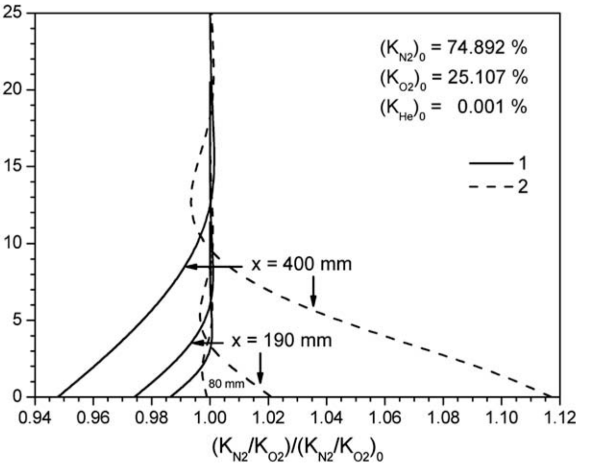

Fig. 4. Profiles of dimensionless ratio of nitrogen and oxygen fractions 80, 190 and 400 mm beyond the front edge of the plate: results of numerical modeling: 1, on the proposed method and 2, with determination of oxygen fraction on correlation (9).

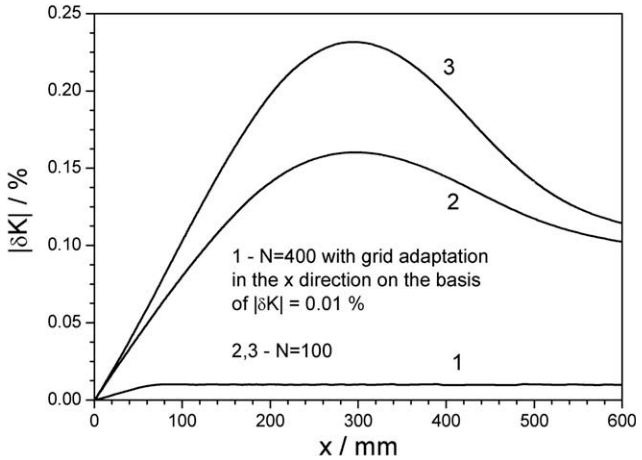

Fig. 6. Error evaluation on the mass balance (9) for different calculation methods: 1 and 2, on the proposed method $N = 400$ and 100, accordingly; and 3, without correction, determining on correlation (9) nitrogen fraction.

Figs. 5 and 6 present two options of calculation results for the diffusion separation effect on the proposed method. In the first option (Fig. 5, line 2) number of grid nodes in the transverse direction is $N = 100$; step $\Delta x = \delta/100$ in the longitudinal direction changed in proportion to the thickness of the dynamic boundary layer. Calculation error evaluation performed according to Eq. (10), is presented in Fig. 6, line 2. It is seen that maximum value $|\delta K|$ is reached in the middle of the plate and amounts to 0.16%. It is interesting to note that iteration convergence accuracy amounted to 0.001% that is two orders less than the one obtained by the error evaluation on the mass balance. Thus, it can be said that iteration process convergence with specified accuracy in the multicomponent diffusion problems does not guarantee that the obtained solution would have the same accuracy. Different calculation options demonstrated that notable increase of the modeling accuracy could be achieved only by increasing the number of computational grid nodes both in the longitudinal and transverse directions. At the same time, it turned out that the proposed method serves to control numerical modeling error and to adapt computational grid reaching specified calculation accuracy with the lowest possible consumption of computer time.

Second calculation option (Fig. 5, line 1 and Fig. 6, line 1) is realized on the grid with the number of nodes in transverse direction $N = 400$; the step in the longitudinal direction was calculated on the basis of maximum error, $\delta K = 0.01\%$ in the previous integration step. As it is seen from the Fig. 5, calculation results obtained for these two options are close to each other along the whole plate length but significantly differ from the modeling results with the fraction calculation for one of the mixture species on the mass balance.

Efficiency of the proposed method in terms of consumed computer time can be evaluated on the table data (Table 1). Average number of iterations for every integration step of the boundary layer equations along the plate on the basis of the proposed method is twice less than in the methods determining one of the components fraction on the balance (9). At the same time, the proposed method requires additional differential equation of diffusion and correction procedure that increases total calculation time. Still, *ceteris paribus* consumed computer time is 30% less than in the fastest calculation option with determination of nitrogen fraction on mass balance and maximum correction $|\delta K|$ is almost twice less. We can assume that with the increase of the mixture components number the efficiency of the method shall increase since the share of consumed computer time spending to the solution of one additional diffusion equation decreases.

5. Conclusions

The method of *a posteriori* evaluation of calculation accuracy at the numerical study of the multifunctional diffusion on the basis of the mass balance equation has been proposed. Algorithm of error evaluation for calculation of the gas mixture species allowing for correction of calculation results has been developed.

Numerical modeling of multicomponent diffusion in the air laminar boundary layer on the flat plate at helium injection through the

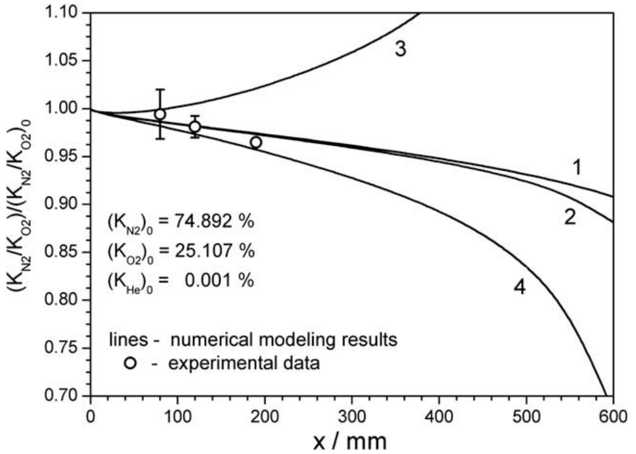

Fig. 5. Effect of diffusion separation of the air components on the surface of permeable plate depending on the distance along the plate. Results of numerical modeling: 1 and 2, on the proposed method $N = 400$ and 100, accordingly; 3 and 4, determining on correlation (9) fractions of oxygen and nitrogen, accordingly, circles are experimental data of the work [10].

Table 1
Efficiency of different methods of numerical modeling.

Method	Iterations[a]	Time[b] (s)	$\|\delta K\|$[c] (%)
$N = 100$[d]	16	74	0.16
$N = 400$[d]	32	1106	0.01
$N = 100$, N_2[e]	32	110	0.24
$N = 100$, O_2[e]	38	240	0.23

[a] Average number of iterations for u, v, K_i profile calculation in one section on x.
[b] Time of field u, v, K_i calculation in the specified flow area.
[c] Maximum calculation error evaluated on Eq. (10).
[d] Proposed method with correction.
[e] Without correction, fraction of mentioned component on balance (9).

porous plate has been carried out. On the basis of the numerical modeling results it has been shown that the calculation error of the component fraction is determined by the size of the computational grid cell and can exceed in orders specified iteration convergence accuracy. It has been shown that the calculation error evaluation obtained in accordance with the proposed method can serve a criterion of the computational grid adaptation. The computational grid adaptation allows obtaining the gas flow composition with any specified accuracy. Use of the proposed method for the component fraction calculation in the boundary layer proved its higher efficiency despite the large number of the computational operations related to the calculation of additional differential equation and the correction procedure. It is related to the number of iterations that is significantly less at each integration step than at the normal method of diffusion modeling excluding one of the differential equations for the mixture components fraction.

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