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# AN APPROACH TO CALCULATION OF THE VISCOSITY OF DISSOCIATED GAS MIXTURES FORMED FROM OXYGEN, NITROGEN, AND CARBON

**V. V. Gorskii and S. N. Fedorov**

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*The results of the solution of an optimization problem on coordination of the widely used data on the viscosity of individual substances and air as a whole are presented. The proposed method of correction of literature data on the viscosity of the components of air mixtures is used to estimate the possible alteration of similar data for a number of carbon-containing compounds.*

At the present time among the best approaches to calculation of the viscosity of pure substances is the procedure which is based on extensive literature data and which was suggested in [1], where the following formula is recommended to calculate the coefficient of the dynamic viscosity of the $i$th component of a gas mixture:

$$\mu_i = 0.1 \exp \left[ (A_i \ln T + B_i) \ln T + C_i \right] . \tag{1}$$

For the set of components considered in the present work the numerical values of the vectors **A**, **B**, and **C** are given in Table 1. At the same time, for qualitative calculation of the viscosity of gas mixtures the Hirschfelder formulas are most often used in practice [2] in which the following relation is used to calculate the viscosity of each individual substance:

$$\mu_i = 0.26693 \cdot 10^{-5} \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega^{(2,2)*} (Tk/\varepsilon)} \tag{2}$$

in combination with the potential function of the Lennard-Jones intermolecular interaction of the form [2]

$$\varphi (r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] . \tag{3}$$

The tabulated dependence of the integral $\Omega^{(2.2)*}$ on the relative temperature $T^* = Tk/\varepsilon$ given in [2] for the potential function (3) can be approximated by the formulas

$$\log \Omega^{(2,2)*} = \begin{cases} \sum\limits_{j=1}^{5} a_j (\log T^*)^{5-j} , & \log T^* < 1 ; \\ \sum\limits_{j=1}^{2} b_j (\log T^*)^{2-j} , & \log T^* \geq 1 , \end{cases} \tag{4}$$

where

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Federal State Unitary Enterprise "Scientific-Research Association of Machine Building", 33 Gagarin Str., Reutov-6, Moscow Region, 143966, Russia; email: fnpc@npomash.ru. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 80, No. 5, pp. 97–101, September–October, 2007. Original article submitted May 17, 2006.

TABLE 1. Coefficients for Calculating the Viscosity of Individual Substances

| Component | **A** | **B** | **C** |
|---|---|---|---|
| $CO_2$ | –0.019527387 | 1.04781800 | –14.3221200 |
| CO | –0.019527394 | 1.01329500 | –13.9787300 |
| $N_2$ | 0.0268142000 | 0.31778380 | —11.3155513 |
| $O_2$ | 0.0449290000 | –0.0826158 | –9.20194750 |
| NO | 0.04363780000 | –0.0335511 | –9.57674300 |
| $C_2$ | –0.008431100 | 0.78760600 | –13.0268000 |
| $C_3$ | –0.008431200 | 0.78760900 | –12.8240000 |
| CN | –0.008381100 | 0.78603300 | –12.9406000 |
| C | –0.008328500 | 0.77032400 | –12.7378000 |
| N | 0.0115572000 | 0.60316790 | –12.4327495 |
| O | 0.0203144000 | 0.42944040 | –11.6031403 |

TABLE 2. Optimum Values of the Coefficients Used in Calculation of the Parameters of the Potential Function of the Lennard-Jones Intermolecular Interaction for the Set of Individual Substances Considered

| Component | $T_{\text{sup}}$ | $\varepsilon/k$ | $\varepsilon_{\text{lit}}/k$ | $D_1$ | $D_2\cdot 10$ | $D_3\cdot 10$ | $D_4\cdot 100$ |
|---|---|---|---|---|---|---|---|
| $CO_2$ | 3150 | 195.2 | 190.0 [2] | 4.0423 | –3.5962 | 4.1681 | 0.0000 |
| CO | 0 | 91.69 | 110.0 [2] | 3.8140 | –3.3515 | 1.6440 | 1.9172 |
| $N_2$ | 15 | 91.45 | 91.50 [2] | 3.8488 | –5.1473 | 1.5572 | –0.67045 |
| $O_2$ | 3150 | 113.2 | 113.2 [2] | 3.5226 | 0.62378 | –1.9822 | 0 |
| NO | 15 | 119.0 | 119.0 [2] | 3.6957 | –1.2910 | 0.0000 | –3.1749 |
| $C_2$ | 3150 | 78.80 |  | 3.8700 | –0.33627 | 1.1266 | 0.0000 |
| $C_3$ | 3150 | 107.9 |  | 3.7813 | –0.24455 | 0.75374 | 0.0000 |
| CN | 3150 | 75.00 | 100.0 [4] | 3.8134 | –0.30582 | 1.0960 | 0.0000 |
| C | 3150 | 30.59 | 33.00 [4] | 3.2320 | 0.23097 | 0.42886 | 0.0000 |
| N | 10 | 38.00 | 38.00 [4] | 3.1788 | –5.6364 | 1.9394 | 1.1652 |
| O | 3150 | 44.00 | 44.00 [4] | 2.9867 | –2.7484 | 1.5700 | 0.0000 |

$$\mathbf{a} = \begin{vmatrix} -0.150150 \\ +0.225178 \\ +0.130334 \\ -0.486090 \\ +0.200868 \end{vmatrix} ; \quad \mathbf{b} = \begin{vmatrix} -0.150500 \\ +0.070635 \end{vmatrix} . \tag{5}$$

The application of formulas (4) and (5) ensure the continuity and differentiability of the calculated function as well as the condition that the value of the error of calculation does not exceed 1% in the entire region of its determination considered in [2].

In order to use the data on the viscosity of individual substances from [1] within the temperature range 300–6000 K for the Hirschfelder method of calculation of the viscosity of a gas mixture the problem of optical approximation of the functional dependence (1) by formula (2) has been solved. Moreover, it was assumed that the value of the parameter of the potential function of intermolecular interaction $\sigma$ may depend on temperature as

$$\sigma = \sum_{j=1}^{3} D_j \left( \frac{T - T_{\text{sup}}}{5000} \right)^{j-1} + D_4 \frac{5000}{T - T_{\text{sup}}} . \tag{6}$$

TABLE 3. Comparison of the Values of the Parameter $\sigma$ of the Potential Function of Intermolecular Interaction for the Considered Set of Individual Substances Calculated by Eqs. (6) (Numerator) and (7) (Denumerator) with Literature Data

| Component | $T$, K | | | | | | | | $\sigma_{\text{lit}}$ |
|---|---|---|---|---|---|---|---|---|---|
| | 300 | 500 | 1000 | 2000 | 3000 | 4000 | 5000 | 6000 | |
| $CO_2$ | $\frac{4.3827}{4.3827}$ | $\frac{4.3500}{4.3291}$ | $\frac{4.274}{4.2022}$ | $\frac{4.1471}{3.9779}$ | $\frac{4.0535}{3.7908}$ | $\frac{3.9932}{3.6386}$ | $\frac{3.9663}{3.5189}$ | $\frac{3.9728}{3.4293}$ | 3.996 [2] |
| CO | $\frac{4.1140}{4.1140}$ | $\frac{3.9738}{3.9603}$ | $\frac{3.8494}{3.8036}$ | $\frac{3.7542}{3.6457}$ | $\frac{3.7040}{3.5340}$ | $\frac{3.6750}{3.4439}$ | $\frac{3.6624}{3.3698}$ | $\frac{3.6645}{3.3094}$ | 3.590 [2] |
| $N_2$ | $\frac{3.7023}{3.7023}$ | $\frac{3.7312}{3.7185}$ | $\frac{3.7194}{3.6751}$ | $\frac{3.6521}{3.5465}$ | $\frac{3.5857}{3.4212}$ | $\frac{3.5290}{3.3070}$ | $\frac{3.4836}{3.2053}$ | $\frac{3.4501}{3.1158}$ | 3.681 [2] |
| $O_2$ | $\frac{3.4227}{3.4227}$ | $\frac{3.4339}{3.4222}$ | $\frac{3.4592}{3.4180}$ | $\frac{3.4978}{3.3967}$ | $\frac{3.5206}{3.3590}$ | $\frac{3.5275}{3.3056}$ | $\frac{3.5186}{3.2374}$ | $\frac{3.4938}{3.1552}$ | 3.433 [2] |
| NO | $\frac{3.1314}{3.1314}$ | $\frac{3.3559}{3.3445}$ | $\frac{3.5091}{3.4674}$ | $\frac{3.5645}{3.4655}$ | $\frac{3.5655}{3.4018}$ | $\frac{3.5530}{3.3295}$ | $\frac{3.5351}{3.2527}$ | $\frac{3.5146}{3.1741}$ | 3.470 [2] |
| $C_2$ | $\frac{3.9258}{3.9258}$ | $\frac{3.9195}{3.9061}$ | $\frac{3.9053}{3.8588}$ | $\frac{3.8837}{3.7715}$ | $\frac{3.8711}{3.6934}$ | $\frac{3.8675}{3.6243}$ | $\frac{3.8730}{3.5635}$ | $\frac{3.8874}{3.5107}$ | — |
| $C_3$ | $\frac{3.8198}{3.8198}$ | $\frac{3.8155}{3.7972}$ | $\frac{3.8058}{3.7418}$ | $\frac{3.7909}{3.6363}$ | $\frac{3.7821}{3.5371}$ | $\frac{3.7794}{3.4437}$ | $\frac{3.7826}{3.3559}$ | $\frac{3.7919}{3.2732}$ | — |
| CN | $\frac{3.8665}{3.8665}$ | $\frac{3.8604}{3.8473}$ | $\frac{3.8468}{3.8011}$ | $\frac{3.8263}{3.7157}$ | $\frac{3.8144}{3.6394}$ | $\frac{3.8114}{3.5717}$ | $\frac{3.8171}{3.5121}$ | $\frac{3.8316}{3.4603}$ | 3.500 [4] |
| C | $\frac{3.2328}{3.2328}$ | $\frac{3.2318}{3.2268}$ | $\frac{3.2300}{3.2124}$ | $\frac{3.2290}{3.1862}$ | $\frac{3.2314}{3.1633}$ | $\frac{3.2372}{3.1438}$ | $\frac{3.2464}{3.1274}$ | $\frac{3.2591}{3.1142}$ | 2.800 [4] |
| N | $\frac{3.3476}{3.3476}$ | $\frac{3.2243}{3.2392}$ | $\frac{3.1336}{3.1165}$ | $\frac{3.0144}{2.9745}$ | $\frac{2.9306}{2.8688}$ | $\frac{2.8671}{2.7844}$ | $\frac{2.8211}{2.7177}$ | $\frac{2.7916}{2.6676}$ | 2.880 [4] |
| O | $\frac{3.1944}{3.1944}$ | $\frac{3.1765}{3.1715}$ | $\frac{3.1339}{3.1168}$ | $\frac{3.0582}{3.0177}$ | $\frac{2.9951}{2.9320}$ | $\frac{2.9445}{2.8596}$ | $\frac{2.9065}{2.800}$ | $\frac{2.8811}{2.7530}$ | 2.960 [4] |
| Ar | $\frac{3.4180}{3.4180}$ | $\frac{3.4180}{3.4127}$ | $\frac{3.4180}{3.3993}$ | $\frac{3.4180}{3.3727}$ | $\frac{3.4180}{3.3460}$ | $\frac{3.4180}{3.3194}$ | $\frac{3.4180}{3.2927}$ | $\frac{3.4180}{3.2660}$ | 3.418 [4] |

Here **D** is the vector of unknown coefficients; $T_{\text{sup}}$ is the reference value of temperature. In turn, the value of the parameter of intermolecular interaction $\varepsilon$ was taken constant, since numerical experiments showed that the introduction of the dependence of this parameter on temperature into calculation does not improve the quality of the solution of the approximation problem considered.

The optimal values of the vector of coefficients **D** and of the parameter $\varepsilon$ were determined with the aid of one of the variants of the Hook–Jeeves heuristic method of direct search [3]. The results found were compared with the literature data of [2, 4] and presented in Tables 2 and 3.

The solution obtained within the framework of the given optimization approach has a high enough accuracy as evidenced by the results of comparison (Fig. 1) between the viscosities of individual substances calculated by this technique and by the method of [1].

The problem of calculation of the transfer properties of gas mixtures is dealt with most fully and qualitatively in the literature on air in a state of thermochemical equilibrium. Here, mention should be made first of all of works [4, 5] that contain the most currently reliable information on the properties of air. In this connection, it is of great interest to carry out investigation aimed at comparing the data on the viscosity of air components from [1] with the data on air viscosity on the whole from [4, 5].

To solve this problem, in the present work we use the viscosities of gas mixtures calculated by the Hirschfelder equations [2] and the results of the solution of the above-described optimization problem for air compo-

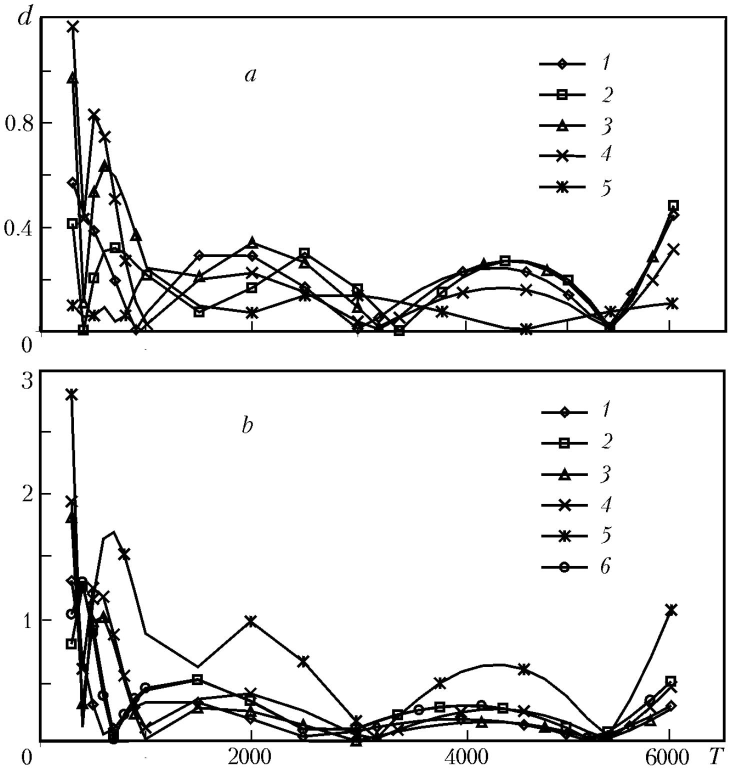

Fig. 1. Difference between the coefficients of the dynamic viscosities of individual substances calculated by Eqs. (6) and (1): a) air components: 1) O; 2) $O_2$; 3) N; 4) $N_2$; 5) NO; b) carbon-containing substances: 1) C; 2) $C_2$; 3) $C_3$; 4) CO; 5) $CO_2$; 6) CN. *d*, %; *T*, K.

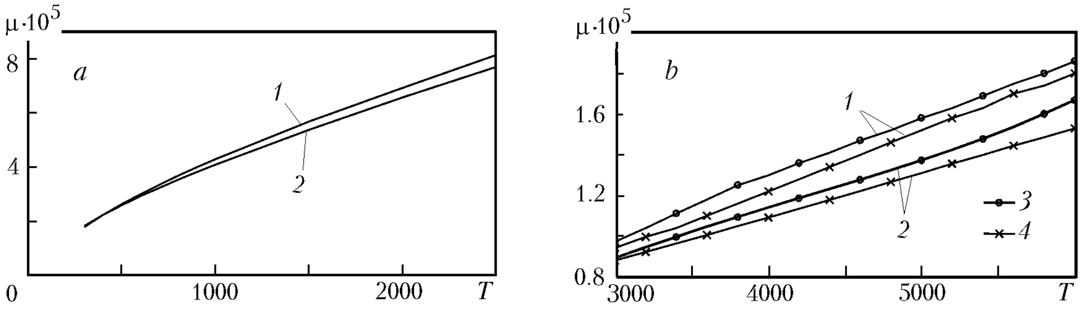

Fig. 2. The values of the coefficient of dynamic viscosity of air calculated by Eq. (6) and those presented in [4, 5]: a) $P = 1$ atm, $T \leq 2500$; b) $T \geq 3000$; 1) literature data; 2) results of calculations; 3) $P = 0.1$; 4) 100 atm. μ, kg/(m·sec); *T*, K.

nents. The investigations were carried out in the ranges of temperatures from 300 to 6000 K and pressures from 0.1 to 100 atm respectively.

For argon, the mass concentration of which in air does not exceed 1.5%, the values of the parameters of the potential function of intermolecular interaction were taken from [2], i.e., it was assumed that $\sigma_{Ar} = 3.418$ and $\varepsilon_{Ar}/k = 124$. The results of comparison of the coefficients of the dynamic viscosity of air calculated with the use of the data of [1] and those published in [4, 5] are given in Fig. 2, and the difference between then is shown in Fig. 3. As is seen, the difference between the calculated and literature data is insignificant at low temperatures, but as the tempera-

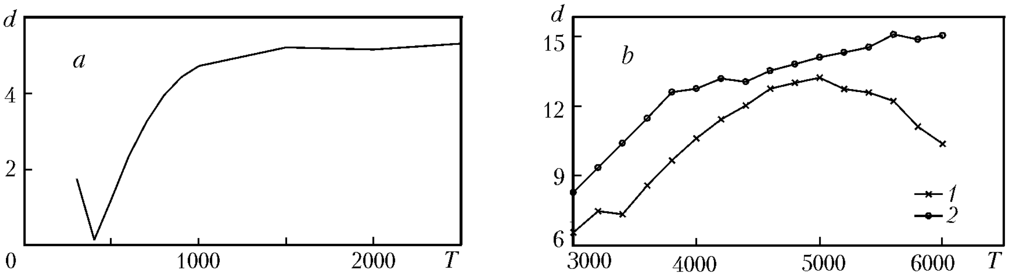

Fig. 3. Errors of calculation of air viscosity found by Eq. (6) with reference to the literature data from [4, 5]: a) $P = 1$ atm, $T \leq 2500$; b) $T \geq 3000$; $P \in [0.3, 100]$: 1) maximal error; 2) minimal error. $d$, %; $T$, K.

ture rises, the difference increases and attains 15%. We solved the problem of minimization of this mismatch within the framework of the least-square method for the case, where Eq. (6) is replaced by a relation of the form

$$\sigma = \left(1 - G_m \frac{T-300}{5000}\right)\left[\sum_{j=1}^{3} D_j \left(\frac{T-T_{\text{sup}}}{5000}\right)^{j-1} + D_4 \frac{5000}{T-T_{\text{sup}}}\right], \tag{7}$$

where **G** is understood to be the vector of the coefficients whose values depend only on the number of atoms in a molecule of species considered. According to the foregoing, for argon $D_1 = 3.418$ and $D_2 = D_3 = D_4 = 0$.

The solution found with the aid of the data of [4, 5] for the problem of searching for the optimum values of these correction factors is as follows: $G_1 = 0.039$ and $G_2 = 0.085$, whereas the values of the parameter $\sigma$ of the potential function of intermolecular interaction found with the aid of Eq. (7) for the air components are given in Table 3. The application of the indicated optimization approach makes it possible to decrease the value of the analyzed mismatch to 1%, which is acceptable for the majority of practical applications.

Table 3 lists also the values of the parameter $\sigma$ calculated with the aid of the proposed approach for a number of carbon-containing substances. In view of the fact that in the obtained solution of the optimization problem the value of the correction factor $G_m$ depends virtually linearly on the number of atoms in a molecule, $G_3$ was assumed equal to 0.12 in the present calculations.

## CONCLUSIONS

1. With the aid of optimization procedures, a correction of the well-known literature data on the viscosity of air components is made to calculate the viscosity of air in the state of thermodynamic equilibrium with an error not exceeding 1% in wide ranges of temperatures and pressures.

2. The article presents information on possible changes in the parameters of intermolecular interaction for a number of carbon-containing substances when refining the corresponding predicted relations within the framework of the same approach which was used in calculations of air components.

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## NOTATION

**A**, **a**, **B**, **b**, **C**, **D**, and **G**, vectors of coefficients in optimum approximation dependences; $d$, relative mismatch, %; $k$, Boltzmann constant, J/K; $m$, number of atoms in a molecule; $M$, molar mass, kg/kmole; $P$, pressure, atm; $r$, distance of the calculated point from the molecule center, Å; $T$, temperature, K; $\varepsilon$, parameter of the function of intermolecular interaction equal to the maximum energy of attraction (the depth of a potential well), J; $\varphi$, potential function, J; $\mu$, coefficient of dynamic viscosity, kg/(m·sec); $\sigma$, parameter of the function of intermolecular interaction equal to the distance from the molecule at which the potential function is equal to zero, Å; $\Omega^{(2.2)*}$, ratio of the values of one of the integrals of intermolecular interaction $\Omega^{(2.2)}$ calculated for the potential function considered and within the framework of the model of solid spheres. Subscripts: lit, literature data; sup, supporting value; $i$, mixture component. Superscript: *, relative value.

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