To the Editor:

In a recent article, we presented a new solution to the Boltzmann equation for monatomic gases (Kerkhof and Geboers,[1] further indicated as KG-1). For this nonequilibrium approach we used a modification of the Enskog scheme. There are several errors in the derivation. As I was the author responsible for the derivation, I would like to point out those errors, and provide corrections and additions to the article to remedy them. In addition I indicate a number of typographical errors.

Derivation of the Transport Equations

There is an erroneous statement (Eq. 201) in that the expression is not equal to zero. Further in Eq. 213 the coefficients $a_i^{(0)}$, $a_j^{(0)}$ should be multiplied with the $\boldsymbol{w}_i$, $\boldsymbol{w}_j$ appropriately, and the result of Eq. 213 is, thus, not valid.

I have modified the derivation with an alternative Enskog-scheme. Details are given in the supplementary material. This results in a first-order approximation function

$$\phi_i = -\mathbf{C}_i \cdot \nabla \ln T - \mathbf{B}_i : \nabla \mathbf{v}_{i0} \tag{1}$$

This eliminates the treatment of the **A**-terms in the derivation, and results in the same expressions for the momentum balance Eq. 266, the equation of energy Eq. 268, the species stress tensor Eq. 245, and the species molecular heat flux Eq. 269. Also the expressions for the diffusion coefficients, the viscosity, the thermal conductivity, and the thermal diffusivity in terms of Ω-integrals are retained.

Equivalence of Old and new Bracket Integrals

My treatment of the equivalence of old and new bracket integrals in Appendix B was incorrect. In the supplementary material a modified treatment is given, which shows that the bracket integrals are not identical, but have very small numerical differences.

Extended Development of the B-Terms

In KG-1 the development of the **B**-terms was limited to those containing $\nabla \mathbf{v}_{i0}$. In the supplementary material the extension of the first-order approximation with terms $\nabla \mathbf{v}_{j0}$ is presented. This leads to a momentum balance with a more general expression for the shear term

$$\prod_i^{[1]} = -2\sum_l \eta_{il}\mathbf{S}_l \tag{2}$$

$$\mathbf{S}_l = \frac{1}{2}\left(\nabla \mathbf{v}_{l0} + (\nabla \mathbf{v}_{l0})^T - \frac{2}{3}(\nabla \mathbf{v}_{l0} : \mathbf{I})\mathbf{I}\right) \tag{3}$$

and an associated extended set of partial viscosities η_{il}, for which expressions are given in terms of Ω-integrals in the supplementary material. It is shown that the expressions for the viscosity of mixtures give identical results as in KG-1. The equation of energy is also extended in the shear term.

Binary Transport in Pores and Capillaries with the Extended Shear Expression

The mathematical descriptions for binary transport in pores and capillaries with the extended shear expression are presented in the supplementary material. A first exploratory numerical evaluation shows that velocity profiles and averaged fluxes are close to those from the previous work, thus, allowing the previous theory to be used for good engineering estimates.

Additional Corrections

On p. 98 (top) in Eq. 182, there should not be a dot multiplication.

On p. 98, in Eq. 184, the $\frac{1}{3}$ should be replaced by $\frac{2}{3}$.

At the top of page 101, the “2” should be deleted.

On p.101, in the second term of Eq. 224 there should be a quadruple integral instead of a triple.

On p. 102, Eq. 244 should read $\prod_i^{[1]} = -m_i b_i^{(0)} \int \mathbf{u}_i\mathbf{u}_i[\mathbf{w}_i\mathbf{w}_i - \frac{1}{3}w_i^2\mathbf{I}] : \nabla \mathbf{v}_{i0} h_i^{[0]} d\mathbf{v}_i$

On p. 102, Eq. 250 should read $\prod_{mix} = \sum_i \prod_i = p\mathbf{I} - 2\sum_i \eta_i \mathbf{S}_i$.

On p. 104, top of second column, the reference to Eq. 173 should be to Eq. 171.

On p. 110, Eq. 322b should read $K_{12} = \frac{D_1^K}{p_1}\frac{\eta_1}{\eta_t}h + \frac{D_1^K D_2^K(1-h)}{p\mathrm{D}_{12}}$.

Equation 322c should read $K_{21} = \frac{D_2^K}{p_2}\frac{\eta_2}{\eta_t}h + \frac{D_1^K D_2^K(1-h)}{p\mathrm{D}_{12}}$.

On p. 111, Eq. 326 should read $\lambda r_p = \sqrt{\frac{8}{\varphi}}$.

On p. 112, Eq. 334 should read $g_D = \dfrac{[1-(1-h)\zeta_{12}]Q}{d_1 d_2 + (d_1+d_2)Q}$, $Q = Q_{12}\dfrac{p x_1 x_2}{\mathcal{D}_{12}}$.

In Eqs. 335a and 335b the symbol Q_{12} should be replaced by Q

$$f_{1m} = \frac{x_2}{\mathcal{D}_{12}} d_2 \frac{1+(1-h)\zeta_{12}}{d_1 d_2 + (d_1+d_2)Q}$$

$$f_{2m} = \frac{x_1}{\mathcal{D}_{12}} d_2 \frac{1+(1-h)\zeta_{12}}{d_1 d_2 + (d_1+d_2)Q}.$$

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Literature Cited

1. Kerkhof PJAM, Geboers MAM. Toward to a unified theory of isotropic molecular transport phenonena. *AIChE J*. 2005;51:79–121.

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