Comment on "A Multicomponent Boundary Layer Chemically Coupled to an Ablating Surface"

PAUL A. LIBBY[*]
University of California, San Diego, La Jolla, Calif.

IN Ref. 1 there is presented inter alia an approximation which pertains to the binary diffusion coefficients $\mathcal{D}_{ij}$, which is claimed to lead to convenience in the numerical treatment of multicomponent diffusive flows and which was apparently proposed first by Bird in a relatively inaccessible publication.[2] The approximation involves writing

$$\mathcal{D}_{ij} \simeq \bar{D}(T,p)/F_iF_j \tag{1}$$

where F_i and F_j are at most weak functions of the temperature T. The accuracy of the approximation has been assessed in both Refs. 1 and 2 by comparing calculations based thereon with exact values of $\mathcal{D}_{ij}$ for a variety of chemical systems and for those systems shown to lead to errors of less than roughly 17%. The apparent convenience achieved by the approximation is that there results an explicit relation for the mass flux of species i in terms of the gradient of concentration of species i and of a sum over gradients of all species.

It is the purpose of this comment to make two observations about the approximation of Eq. (1); the first concerns the absence of any fundamental basis for it. Note that according to the rigid sphere model (the treatment of F_i and F_j as constants appears analogous to the use of such a model)

$$\mathcal{D}_{ij} \sim \frac{T^{3/2}}{p}\left[\left(\frac{m_i + m_j}{m_i m_j}\right)^{1/2} \frac{1}{(\sigma_i + \sigma_j)^2}\right] \tag{2}$$

where m_i and σ_i denote the molecular weight and diameter of species i, respectively. Now comparison with Eq. (1) permits $\bar{D}$ to be identified and we can ask when may the [ ] quantity be approximated by a product F_iF_j. Clearly, if either $m_j \ll m_i$ and if $\sigma_j \ll \sigma_j$, or if the opposite inequalities apply, the approximation holds in the limit; it also holds if $m_j \simeq m_i$, $\sigma_i \simeq \sigma_j$ again in the limit but in general the answer must be that it does not hold! The strictly empirical nature of Eq. (1) is not made clear in Ref. 1 except by implication that the agreement with exact calculations is "surprisingly good."

The second observation pertains to the need for the approximation when detailed calculations of boundary-layer flows involving multicomponent diffusion are being performed. In these cases extensive numerical analysis is called for; depending on the method used it is convenient to have an explicit relation either for the gradient of concentration of species i in terms of the diffusive fluxes of all species and of the temperature gradient if thermal diffusion is included or for the diffusive flux of species i in terms of the gradients of concentration and of temperature. However either of these can be obtained numerically by multiplication of the general matrix system relating the diffusional fluxes, the gradients of concentration, and the temperature gradient by an appropriate inverse matrix which may be obtained for any order of interest from a standard subroutine. It is thus not evident to us that someone embarking on a large-scale computation of boundary layers with complex composition will wish to employ Eq. (1) which may introduce unnecessary empiricism.

References

[1] Kendall, R. M., Rindal, R. A., and Bartlett, E. P., "A Multicomponent Boundary Layer Chemically Coupled to an Ablating Surface," *AIAA Journal*, Vol. 5, No. 6, June 1967, pp. 1063–1071.

[2] Bird, R. B., "Diffusion in Multicomponent Gas Mixtures," presented at the 25th Anniversary Congress of the Society of Chemical Engineers (Japan), November 6–14, 1961; published in abbreviated form in *Kagaku Kogaku*, Vol. 26, 1962, pp. 718–721.

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[*] Professor of Aerospace Engineering, Department of the Aerospace and Mechanical Engineering Sciences. Associate Fellow AIAA.

Reply by Authors to P. A. Libby

R. M. KENDALL,[*] R. A. RINDAL,[†]
AND E. P. BARTLETT[†]
Aerotherm Corporation, Palo Alto, Calif.

IN his comment, Professor Libby has advanced two observations, both relating to the approximation for binary diffusion coefficients proposed by Professor Bird[‡] and later by ourselves. The first observation has to do with whether the approximation has a "fundamental basis"; the second pertains to the "need for the approximation." These two items will be discussed in that order.

Whether a fundamental basis exists depends primarily on the definition of "fundamental." Professor Libby seems to imply by this word the existence of a physical and associated mathematical model. Certainly no such model was advanced in our paper nor has one been developed subsequently to rationalize the success of the approximation. The fact that this approximation is not mathematically consistent with the rigid sphere model, or any other physical model for that matter, does not seem to be germane. It is, as we hoped we had clarified in the paper, a correlation equation. It permits the inexact replacement of sets of binary diffusion coefficients, whether measured or calculated, by smaller sets of parameters (the diffusion factors). Thus, the physical models upon which the original data are based are retained in the approximation, granted with some error. One cannot prove that such a correlation will always be successful. It is significant, therefore, that correlations have been performed for a variety of systems and have consistently resulted in little loss of accuracy[1] (as illustrated in Table 1 of our paper, errors are typically from 1 to 5% and seldom exceed 10%). It is also significant that all errors in $\mathcal{D}_{ij}$ are known, and, furthermore, are known in advance. Thus, the approximation does not have to be employed in the event that some errors are unacceptably large.

In his comment, Professor Libby has related the proposed correlation expression with the rigid sphere model [his Eq. (2)]. We would like to state for the record that we see no significant analogy between "the treatment of F_i and F_j as constants" and "the use of such a (rigid sphere) model" as stated parenthetically in the comment. Furthermore, the arguments associated with Eq. (2) of the comment are ambiguous and demand some clarification. It has been well established that bifurcation can be accomplished exactly for any binary or ternary system and therefore his Eq. (2) and the associated arguments can only be viewed from the standpoint of a multicomponent system. Certainly if all $\mathfrak{M}_i$ and σ_i are equal, the bifurcation of the bracketed term will be precise. However, the large inequality postulate presented is insufficient to describe a multicomponent system, and, furthermore, *no* system including such an inequality permits an exact bifurcation of the bracketed term. It

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[*] Manager, Analytical Services Division. Member AIAA.

[†] Staff Engineer, Analytical Services Division. Member AIAA.

[‡] Professor Bird's paper cited in our original paper is now available in English as NASA TT F-10, 925.

should be recognized that the correlation requires satisfying, with least-square errors, $I(I-1)/2$ simultaneous relations for I coefficients, not an isolated equation such as that examined in the comment.

Professor Libby questions "the need for the approximation when detailed calculations of boundary-layer flows involving multicomponent diffusion are being performed." It would seem that the primary consideration here is the tradeoff between accuracy and computational conveniences (in particular, speed, storage, and input requirements). Although not having performed large-scale boundary-layer computations utilizing the approach suggested by Professor Libby, our experience to date leads us to believe that substantial computation convenience is achieved with little loss of accuracy. The boundary-layer equations proposed in our paper have recently been programmed[2] and solutions have been obtained considering 30 molecular species.[3] Philco 212 computer time required for a nonsimilar boundary-layer solution over an ablating body in this case was 6 min. This included the evaluation of edge conditions, a similar solution at the stagnation point, and nonsimilar solutions at 19 additional stations. However, as pointed out in our paper, the primary motivation for introducing the approximation was to develop a transfer-coefficient model to be used in lieu of large-scale boundary-layer computations. In constructing a film coefficient model considering unequal diffusion effects, a convenient alternative approach of equivalent accuracy does not exist.

References

[1] Bartlett, E. P., Kendall, R. M., and Rindal, R. A., "A Unified Approximation for Mixture Transport Properties for Multicomponent Boundary-Layer Applications," Rept. 66-7, Part IV, March 1967, Aerotherm Corp.

[2] Kendall, R. M. and Bartlett, E. P., "Nonsimilar Solution of the Multicomponent Laminar Boundary Layer by an Integral Matrix Method," Paper 67-218, Jan. 1967, AIAA; also, Rept. 66-7, Part III, March 1967, Aerotherm Corp.

[3] Kendall, R. M., Bartlett, E. P., Rindal, R. A., and Moyer, C. B., "An Analysis of the Coupled Chemically Reacting Boundary Layer and Charring Ablator" Rept. 66-7, Part I, March 1967, Aerotherm Corp.

Comment on "Dynamics of a Radiating Gas with Application to Flow Over a Wavy Wall"

M. S. Wecker*
General Applied Science Laboratories Inc., Westbury, N. Y.

IN his excellent exposition of the application of the spherical-harmonic approximation to the radiation-transport equation, Cheng found [Ref. 1, Eq. (6.11)] the velocity potential for the linearized flow of a nonscattering grey gas over a small-amplitude wavy wall to be

$$\varphi(x_1,x_2) = \frac{U_\infty l}{2\pi} Re \left\{ \sum_{j=1}^{2} A_j \exp\left[\frac{2\pi}{l}(c_j x_2 + i x_1)\right]\right\}$$

$$= U_\infty \epsilon \sum_{j=1}^{2} e^{-2\pi\delta_j(x_2/l)} \left[a_j \cos 2\pi \left(\frac{x_1 - \lambda_j x_2}{l}\right) - b_j \sin 2\pi \left(\frac{x_1 - \lambda_j x_2}{l}\right)\right]$$

where the wall shape was given by

$$X_2 = \epsilon \sin 2\pi x_1/l$$

and A_j, c_j, δ_j, λ_j, a_j, and b_j could be found from his Eqs. (6.8–6.10).

From this velocity potential, it should follow that the normal velocity perturbation may be written as

$$\frac{u_2'}{U_\infty} = \frac{1}{U_\infty}\frac{\partial\varphi}{\partial x_2} = -\frac{2\pi\epsilon}{l}\sum_{j=1}^{2} e^{-2\pi\delta_j(x_2/l)} \times \left\{(a_j\delta_j - b_j\lambda_j)\cos\frac{2\pi}{l}(x_1 - \lambda_j x_2) - (a_j\lambda_j + b_j\delta_j)\sin\frac{2\pi}{l}(x_1 - \lambda_j x_2)\right\}$$

However, Cheng, in writing this expression in his Eq. (6.13b), included only the first term; the second, sine, term was omitted. In addition, through a typographical error, the coefficient of the cosine term was incorrectly given as $(a_j\delta_j + b_j\lambda_j)$.

It should be noted that where $x_2 = 0$, the coefficient of the sine term is identically zero. This is a consequence of Cheng's Eq. (6.9):

$$\sum_{j=1}^{2} A_j c_j = 2\pi \frac{\epsilon}{l}$$

Thus, on the wall surface, the omitted term equals zero. However, since Cheng's solution should be valid throughout the flow, the omitted sine term must be included in any calculation of u_2' for x_2 not identically zero.

Reference

[1] Cheng, P., "Dynamics of a Radiating Gas with Application to Flow Over a Wavy Wall," *AIAA Journal*, Vol. 4, No. 2, 1966, pp. 238–245.

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* Supervisor, Technical Staff; now with IBM, Washington, D.C. Member AIAA.

Comment on "Computation of Stress Resultants from the Element Stiffness Matrices"

Fernando Venâncio Filho*
Instituto Tecnológico de Aeronáutica, São José dos Campos, São Paulo, Brazil

THE general form of Eq. (1), Ref. 1, to take into account not only continuous distributed loads, but also discontinuous and concentrated loads applied outside the nodes, was presented in a previous work.[2] The partitioning of Eq. (5) of Ref. 2 relative to the structural elements of the structural system results, for each element, in an equation exactly like Eq. (3), Ref. 1 (with the exception of the inertia term which was not considered in Ref. 2). The generalized forces $-\{Q_i\}^1$ are precisely the component submatrices of $[s]$ [Eq. (5) of Ref. 2]. The generalized forces $-\{Q_i\}$ of the second equation of the example are simply the fixed-end bending moments and shear forces of the elements. This concept was already introduced in Refs. 2 and 3.

From the final results of the example and the final paragraph of the Note a misleading conclusion may be drawn that the method discussed is approximate. In reality the method is theoretically an exact one as the generalized displacements are obtained from the equilibrium equations relative to the nodes, and these are exactly satisfied (except for computational er-

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* Head, Aeronautical Engineering Department.