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## COMPUTATION OF GASDYNAMIC AND KINETIC PROCESSES IN HYPERSONIC WAKES BEHIND AEROSOL PARTICLES

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In many technical problems one is interested in achieving fast mixing of the reacting components in times comparable with the characteristic chemical reaction time. One possible method of achieving fast mixing of reacting substances is that described in [1], where one of the components is sprayed as an aerosol into a hypersonic stream of the other reacting component.

The chemical and gaskinetic processes occurring in the wakes behind aerosol particles are difficult to describe theoretically.

The difficulties stem from the fact that the flow of a gas mixture behind the particles, because of the small particle size, comparable with the molecular mean free path, varies over wide limits, from continuum flow described by the Navier-Stokes equations, to free-molecular flow described by the Boltzmann equation. The flow region near the particle and behind it is conventionally divided into two zones (Fig. 1, 1) a particle; 2) shock wave; 3) wake). In Zone I the flow is described by the Boltzmann equation, and in Zone II by the continuum equations. At a sufficient distance from the particle ( $x \gg d$ ) the transverse velocity components will be much less than the longitudinal, and in that case in Zone II the flow is described by equations of boundary layer type.

If we neglect the variation in particle velocity due to stagnation, on a scale in which the perturbations behind the particles in the gas are damped, then, in the coordinate system moving with the particle, the equations have the form [2]

$$\begin{aligned} \frac{\partial p}{\partial r} = 0, \quad \frac{1}{r} \frac{\partial}{\partial r}(\rho v r) + \frac{\partial}{\partial x}(\rho u) = 0, \\ \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r}(\mu r \frac{\partial u}{\partial r}), \\ \rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ \frac{\mu}{Pr} r \left[ \frac{\partial H}{\partial r} + (Pr - 1) \frac{\partial}{\partial r}(u^2/2) + \sum_i \left( \frac{\rho D_i}{\mu} Pr - 1 \right) T c_{p_i} M_i \frac{\partial F_i}{\partial r} \right] \right\} + \sum_j Q_j. \end{aligned} \quad (1)$$

Equations (1) must be supplemented by the transfer equations for the various components of the mixture

$$\rho u \frac{\partial F_i}{\partial x} + \rho v \frac{\partial F_i}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left( \rho D_i r \frac{\partial F_i}{\partial r} \right) + \rho W_i \quad (2)$$

and the equations of state

$$p = \rho R T \sum_i F_i, \quad \sum_i M_i F_i = 1. \quad (3)$$

The enthalpy H is determined by the relation

$$H = \sum_i M_i F_i c_{p_i} T + u^2/2. \quad (4)$$

In addition, the terms appearing in Eqs.(1) and (2)  $-Q_j$ , corresponding to the heat release per unit volume due to the reaction of type j, and  $W_i$ , corresponding to the variation in the component  $F_i$  due to all the chemical reactions – must be determined from the chemical kinetic equations.

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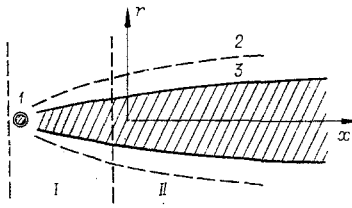
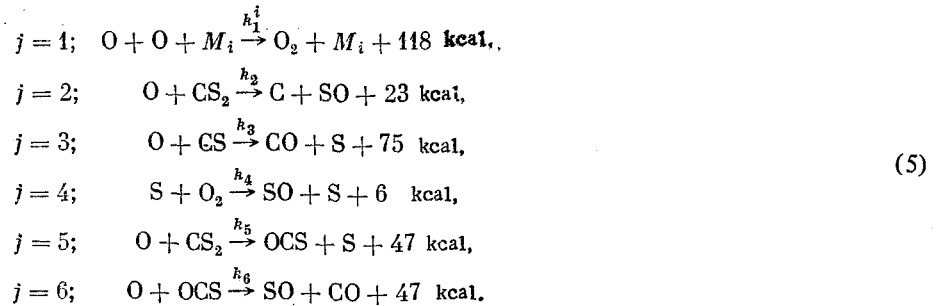


Fig. 1

We illustrate the analysis of the processes below by the example of calculating combustion of  $\text{CS}_2$  in the aerodynamic wake formed behind an individual particle of liquid (or solid)  $\text{CS}_2$  in hypersonic flow of the mixture  $\text{He} + \text{O} + \text{O}_2$  (3.9:0.1:1). Here we use the following basic chemical reactions, occurring in the mixture  $\text{CS}_2 + \text{O}_2 + \text{O} + \text{He}$  [3]:



Here  $M_i$  ( $i = 1, \dots, 9$ ) denote particles (molecules or atoms) of, respectively,  $\text{O}_2$ ,  $\text{CS}_2$ ,  $\text{CS}$ ,  $\text{SO}$ ,  $\text{OCS}$ ,  $\text{CO}$ ,  $\text{O}$ ,  $\text{He}$ ,  $\text{S}$ .

The rate constants for the chemical reactions  $k_j^i$ ,  $k_j$  ( $i = 1, \dots, 9$ ,  $j = 2, \dots, 6$ ) are taken from [3]. The quantities  $Q_j$  in Eq. (1) can be expressed in terms of the concentration  $F_i$  as follows:

$$Q_1 = c^3 \sum_{i=1}^9 k_1^i F_i F_7^2 e_i / N_A, \quad Q_j = c^2 k_j \frac{e_j}{N_A} F_i F_k, \quad j = 2, \dots, 6, \quad c = \rho N_A. \tag{6}$$

Expressions for  $W_i \sim (dF_i/dt)_{\text{chem}}$  were given in [3]. In Eq. (6) the quantities  $e_j$  are the heat of reaction  $j$ , in J/kmole.

To solve Eqs. (1)-(6) we need to know the transport coefficients ( $\mu$ ,  $\text{Pr}$ ,  $D_i$ ) in the mixture, and their dependence on temperature and pressure. The coefficients  $D_i$  in the mixture were determined from the relations [4]

$$D_i = \frac{1 - \bar{c}_i}{N \sum_{\substack{j=1 \\ j \neq i}} \bar{c}_j / D_{ij}}, \tag{7}$$

where  $D_{ij}$  are binary diffusion coefficients. The values of  $D_{ij}$  were given in [6] for the mixtures  $\text{He}-\text{O}$ ,  $\text{He}-\text{CO}$ ,  $\text{He}-\text{O}_2$ ,  $\text{CO}-\text{O}_2$ ,  $\text{O}-\text{O}_2$ . In the remaining cases the coefficients  $D_{ij}$  were calculated from the relations [5]

$$D_{ij} = \text{const} \left[ \frac{M_i + M_j}{M_i M_j} \right]^{1/2} T^{3/2} / p \left( \frac{\sigma_i + \sigma_j}{2} \right)^2 \Omega_D. \tag{8}$$

Values of the effective diameters  $\sigma_i$  of the molecules and of the collision integrals  $\Omega_D$  for the Lennard-Jones potential, obtained from data on viscosity in pure gases, were given in [4]. For the components  $\text{CS}$ ,  $\text{SO}$ ,  $\text{S}$  (for which the present authors know of no viscosity data), the force constants of the Lennard-Jones potential were assumed to be the same as for  $\text{CO}$ ,  $\text{O}_2$ ,  $\text{O}$ .

The dependence of the coefficients  $D_{ij}$  on temperature was approximated by the function  $T^{1.7}$  [5]. Values of  $D_{ij}$ , calculated for  $T = 300^\circ\text{K}$  and  $p = 10^5 \text{ N/m}^2$ , are shown in Table 1.

The mixture viscosity  $\mu$  was calculated from the formula [6]

$$\mu = \left( \sum_{i=1}^N \bar{c}_i / \mu_i \right)^{-1}, \tag{9}$$

and the dependence  $\mu_i(T)$  was approximated by the function  $T^{0.65}$ . In cases where no experimental values of  $\mu_i$  were known, they were computed from the recommendations in [4]. The Prandtl number was assumed to be 0.75 in the calculations. The contribution of molecular oscillations to the specific heats  $c_{p_i}$  in Eq. (4) was not accounted for, since the characteristic temperatures considered here did not exceed  $600^\circ\text{K}$ .

Thus, with Eqs. (1)-(9) we can describe completely the transport processes and the kinetics in the aerodynamic wake behind the particles.

To solve this system of equations we require initial values of the parameters  $p$ ,  $\rho(r)$ ,  $u(r)$ ,  $H(r)$ ,  $F_1(r)$ , which can be obtained, in general, only by solving the Boltzmann equation in Region I. However, approximate values of these parameters can be determined by using the integral conservation laws. To do this we shall seek values of  $H(r)$ ,  $\rho u(r)$ ,  $\rho_{CS_2}(r)$  at the initial section in the form of the Gaussian profiles:

$$\begin{aligned} \rho(r) u(r) &= \rho_e u_e + \xi \exp(-br^2), \quad H(r) = H_e + \eta \exp(-br^2), \\ \frac{\rho_{CS_2}}{\rho} &= \gamma \exp(-br^2). \end{aligned} \quad (10)$$

Using the conservation integrals for flux of  $\rho_{CS_2}$ ,  $u$ ,  $\rho u$ ,  $\rho u H$  between boundary sections of Region I, and assuming that  $\rho_e \simeq \rho_0$ ,  $H_e \simeq H_0$ ,  $u_e \simeq u_0$ , we can obtain the following expressions relating the quantities  $\xi$ ,  $\eta$ ,  $b$ ,  $\gamma$ :

$$\xi = \frac{\rho_0 u_0 \eta}{q + c_{pm} T_m + H_0 - \eta/2}, \quad b = \frac{\pi}{m}, \quad \gamma = \frac{\xi}{\rho_0 u_0 + \xi/2}. \quad (11)$$

Postulating hypersonic free-molecular flow, the rate of evaporation of the aerosol particle mass,  $\dot{m}$ , can be determined from the expression [1]

$$\dot{m} = \frac{\rho_0 u_0^3}{2} \alpha \cdot S/q. \quad (12)$$

The value of  $a$  in the calculations was taken to be 0.5, and the value of  $q = 5 \cdot 10^5$  J/kg.

In determining the initial conditions below we shall assume that the gas composition at the initial section, apart from the component  $CS_2$ , remains the same as in the oncoming stream. This assumption is valid if the characteristic chemical reaction times are less than the resistance time of the gas in Zone I, and will be valid after the final computations are made. For known values of the coefficients  $\xi$ ,  $\eta$ ,  $\gamma$ ,  $b$  from Eqs. (3), (4), and (10), and the evident relation  $F_{CS_2} = \frac{\rho_{CS_2}}{\rho} \frac{1}{M_2}$  we can find the initial profiles of all the variables. However, Eqs. (11) are not sufficient to find 4 unknown constants, and one needs an additional physical condition, which we take to be the following relation

$$H(0, 0) \ll H_e, \quad (13)$$

which results from the fact that, because of the low initial rate of evaporation of  $CS_2$ , the total enthalpy  $H(0, 0)$  on the wake axis in the initial section is much less than that of the oncoming stream. The indeterminacy in the choice of  $H(0, 0)$  from Eq. (13) corresponds to indeterminacy in the distance of the initial section from the particle, and therefore, within the limits of Eq. (13) the quantity  $H(0, 0)$  was given parametrically, and, as was confirmed by the calculations, for variation of  $H(0)$  in the range 0.1 He–0.5 He, the wake parameters at sufficient distance from the initial section are independent (to an accuracy of  $\sim 10\%$ ) of the quantity  $H(0, 0)$ , a feature which evidently stems from the similarity properties of the flow in the wake [7].

In order not to vary the finite-difference subdivision mesh with respect to the coordinate  $r$  when changing the wake radius, we write Eqs. (1) and (2) in the new coordinates  $x'$ ,  $r'$ :

$$x' = x, \quad r' = r/R(x) \quad (14)$$

with the aid of the transformations

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'} - \frac{r'}{R(x)} \frac{dR}{dx} \frac{\partial}{\partial r'}, \quad \frac{\partial}{\partial r} = \frac{1}{R(x)} \frac{\partial}{\partial r'}. \quad (15)$$

Equations (1) and (2), transformed with the help of Eqs. (14) and (15), were written in a form ready for the use of a numerical method of solving the system of parabolic equations [8, 9]:

$$a_i \frac{\partial f_i}{\partial x} + b_i \frac{\partial f_i}{\partial r'} = g_i \frac{\partial}{\partial r'} \left( c_i \frac{\partial f_i}{\partial r'} \right) + e_i f_i + d_i, \quad (16)$$

where we take the quantities  $f_i$  to be any of the functions  $H(r', x)$ ,  $u(r', x)$ ,  $F_1(r', x)$ . In using the transformations of Eqs. (14) and (15) we must assign the dependence  $R(x)$ , which, generally speaking, can be chosen as an arbitrary monotonically increasing function, e.g., subject to the condition  $R(x) = \delta(x)$ , where  $\delta(x)$  is the diameter of the wake, determined from conservation of momentum (momentum displacement thickness).

TABLE 1

| $i \backslash j$ | CO   | O    | CS <sub>2</sub> | CS   | SO   | O <sub>2</sub> | S    | OCS  |
|------------------|------|------|-----------------|------|------|----------------|------|------|
| He               | 0,73 | 1,09 | 0,49            | 0,71 | 0,72 | 0,74           | 1,04 | 0,53 |
| CO               |      | 0,33 | 0,11            | 0,22 | 0,21 | 0,23           | 0,31 | 0,13 |
| O                |      |      | 0,24            | 0,31 | 0,30 | 0,32           | 0,33 | 0,25 |
| CS <sub>2</sub>  |      |      |                 | 0,09 | 0,10 | 0,11           | 0,19 | 0,06 |
| CS               |      |      |                 |      | 0,19 | 0,21           | 0,25 | 0,11 |
| SO               |      |      |                 |      |      | 0,24           | 0,31 | 0,10 |
| O <sub>2</sub>   |      |      |                 |      |      |                | 0,32 | 0,12 |
| S                |      |      |                 |      |      |                |      | 0,21 |

In the present calculations the function  $R(x)$  was assigned as follows:

$$R^2(x) \int_0^1 F_2(r', x) \rho u r' dr' = R^2(0) \int_0^1 F_2(r', 0) \rho(r', 0) u(r', 0) r' dr'. \quad (17)$$

It is clear that the value of  $R(x)$  calculated from Eq. (17), will be larger than the radius of the diffusive wake for the CS<sub>2</sub> component, determined by Eq. (17) with no chemical reactions in the wake. The boundary conditions for the system of equations (1) and (2) (or Eq. (16)) are written in the form

$$\begin{aligned} \text{for } r' = 0 \quad \partial/\partial r' &= 0, \\ \text{for } r' = 1 \quad F_i(1, x) &= F_{ie} = F_{i\infty}, \quad H(1, x) = H_e, \quad u(1, x) = u_e. \end{aligned}$$

The values of  $H_e$ ,  $u_e$  (which are close to  $H_\infty$ ,  $u_\infty$ ) are determined from the properties of the solutions of Eq. (1) as  $r \rightarrow \infty$  (this is derived in the Appendix).

For numerical integration of the system of equations of the type (16) we used the method described in [9]. The step size of the finite difference mesh with respect to the  $r'$  axis was chosen to be  $h_r = 1/30$ , and the integration step size along the  $x$  axis was variable, and ranged from  $h_x = 0.05 R(0)$  at  $x = 0$  to  $h_x = 0.2 R(x)$  at  $x \gg R(0)$ .

Values of the radial component  $v$  were determined by means of a recurrence method from the conservation integral for mass flux in an annular volume bounded by the coordinates  $x$ ,  $x + h_x$  and  $r' - h_r$ ,  $r' + h_r$ . The number of iterations required to establish the solutions  $f_i$ , to a given relative accuracy ( $10^{-3}$ ) in the layer  $x + h_x$ , from the known solutions in the layer  $x$ , did not exceed 6. The solution time on the scale  $x = 1000d$  was 6-8 min on the BESM-6 computer.

Figure 2 shows characteristic profiles of concentrations, temperature, and enthalpy at distances  $x = 0$  and  $830d$  for the example with injected particles of  $d = 1.5 \cdot 10^{-5}$  m, particle velocity relative to the flow 3000 m/sec, and flow parameters  $p = 10^4$  N/m<sup>2</sup>,  $T_\infty = 300$  K ( $1 - H/H_\infty$ ;  $2 - T/T_\infty$ ;  $3 - \bar{F}_{CS_2, \rho_\infty RT_\infty/p_\infty}$ ;  $4 - F_{CO, \rho_\infty RT_\infty/p_\infty}$ ).

Figure 3 shows the dependence of the wake axis temperature, the enthalpy  $H$ , and the CO concentration on the wake axis as a function of distance  $x$  for various values of  $\eta = H_e - H(0, 0)$  ( $1 - H/H_\infty$ ;  $2 - T/T_\infty$ ;  $3 - \bar{F}_{CS_2, \rho_\infty RT_\infty/p_\infty}$ ;  $4 - F_{CO, \rho_\infty RT_\infty/p_\infty}$  for  $p_\infty = 10^4$  N/m<sup>2</sup>,  $T_\infty = 300$  K,  $d = 15 \mu$ ; the broken curves correspond to  $H(0, 0) = 0.1 H_e$ , and the solid curves to  $H(0, 0) = 0.3 H_e$ ).

It can be seen from the profiles presented that the wake parameters at large distances  $x \gg R(0)$  depend very little on the assumed initial profiles  $H(r', 0)$ . Also, the characteristic dimension in which the chemical reactions occur turns out to be larger than the dimension for the gasdynamic processes.

We are also interested in the efficiency of the CS<sub>2</sub> combustion process in the wake behind an evaporating particle. Figure 4 shows the dependence of the quantity

$$\beta = 2\pi \int_0^\infty \rho_{CS_2}(r) u(r) r dr / \dot{m},$$

the fraction of nonreacted CS<sub>2</sub> at large distances  $x$ , where the reaction slows down due to cooling of the gas in the wake, as a function of the gas temperature and pressure in the oncoming stream [1)  $p = 5 \cdot 10^3$  N/m<sup>2</sup>; 2)  $p = 10^4$  N/m<sup>2</sup>; 3)  $p = 2 \cdot 10^4$  N/m<sup>2</sup>; the broken curves correspond to  $T_\infty = 250^\circ$ K, and the solid curves to  $T_\infty = 300^\circ$ K,  $d = 15 \mu$ ]. As expected, the combustion efficiency depends appreciably on the temperature and pressure, but comparison with the results of calculated CS<sub>2</sub> combustion in the same mixture in an expanding nozzle, with postulated instantaneous mixing [3] shows that the combustion efficiency in the wake can be the same as in the case [3].

Thus, mixing achieved by injecting one of the active components in the form of aerosol particles into a hypersonic gas stream of the other component is an efficient method of obtaining nonequilibrium components in chemically reacting gas flows.

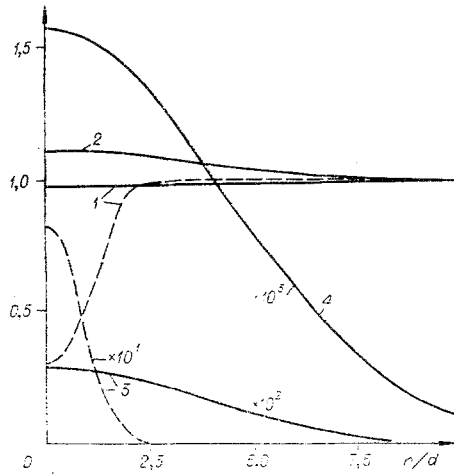


Fig. 2

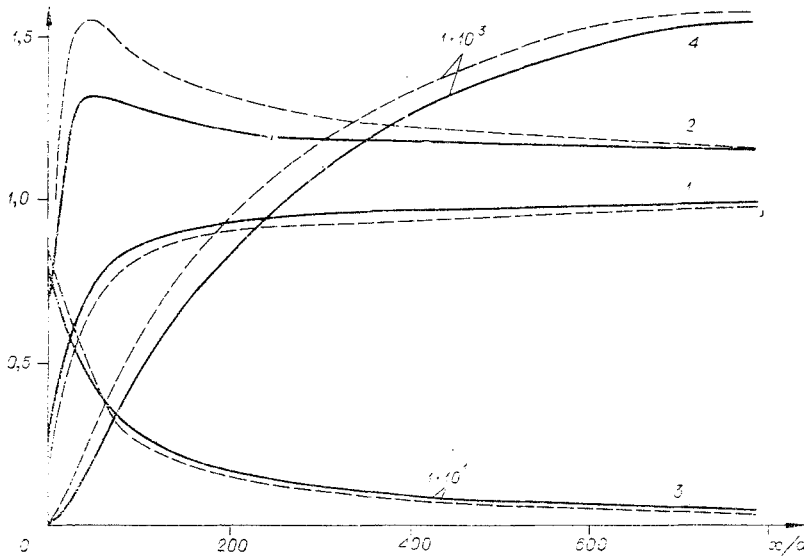


Fig. 3

APPENDIX

In the general case, where the quantity  $R(x)$  is chosen independently of the momentum displacement thickness  $\delta$  in the wake (e.g., it can be shown that  $R(x) < \delta$ ), to increase the solution accuracy one must "correct" the boundary conditions for  $H$  and  $u$ . One can improve these conditions using the asymptotic properties of solutions of Eq. (1). Using the equations for conservation of momentum and mass in (1), one can write the following integrals:

$$\int_0^{R(x)} \frac{\partial}{\partial x} (\rho u^2) r dr = \left( \mu r \frac{\partial u}{\partial r} - \rho v u r \right) \Big|_{r=R(x)}, \tag{A.1}$$

$$\int_0^{R(x)} \frac{\partial}{\partial x} (\rho u) r dr = -(\rho v r) \Big|_{r=R(x)}.$$

Since, as  $r \rightarrow \infty$ , the right sides of Eq. (A.1) go to zero, from Eq. (A.1), taking into account that for  $r \geq R(x)$   $|u - u_\infty| \ll u_\infty$ , and  $|\rho u - \rho_\infty u_\infty| \ll \rho_\infty u_\infty$ , we can obtain the linearized equation

$$\rho_\infty u_\infty \frac{d}{dx} \int_{R(x)}^\infty (u - u_\infty) r dr = \left[ -\mu r \frac{\partial u}{\partial r} + \rho_\infty r (u - u_\infty) \left( v - u_\infty \frac{dR}{dx} \right) \right] \Big|_{r=R(x)}. \tag{A.2}$$

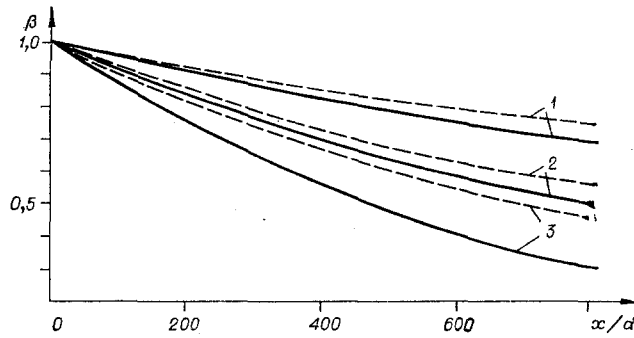


Fig. 4

If we seek a local solution for  $r \geq R(x)$  in the form

$$\varepsilon(r, x) = u - u_\infty = c(x) \exp(-br^2), \quad (\text{A.3})$$

then, it follows from Eqs. (A.2) and (A.3) that

$$\begin{aligned} \rho_\infty u_\infty \frac{d\varepsilon_e}{dx} \frac{1}{b} &= -\mu R(x) \left. \frac{\partial u}{\partial r} \right|_{r=R(x)} + \varepsilon_e \rho_\infty R(x) \left( v_e - \frac{dR}{dx} u_\infty \right), \\ 2bR(x) \varepsilon_e &= - \left. \frac{\partial u}{\partial r} \right|_{r=R(x)}. \end{aligned} \quad (\text{A.4})$$

With the differential relations (A.4) we can express the quantity  $\varepsilon_e = u_e - u_\infty$  in terms of the values of  $\partial u / \partial r$  ( $r = R(x), x$ ),  $v_e$ ,  $R(x)$  and thereby include an improved value of  $u_e$  in the iteration process at each section  $x + h_x$ . The quantity  $H_e$  is determined from the known value  $u_e$  using the relation

$$H_e = H_\infty + (u_e - u_\infty) u_e.$$

In the case where  $R(x)$  is determined, e.g., from the momentum conservation integral (i.e.,  $R(x) \equiv \delta(x)$ ), and the diffusive wake scale is larger than  $R(x)$ , the boundary values for the  $F_{ie}$  concentrations can be improved analogously.

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