

ferent shapes of the feeding stream are very close. Considering the fact that the computations were performed in the region where \mathbf{X} does not depends on δ_0 , it shows that the shape of the feeding stream can affect the product distribution only for very slow feeding rates.

One can conclude that the proposed model of micromixing enables prediction of influence of main processing parameters such as $\overline{\mathbf{Da}}$, θ , \mathbf{a} and \mathbf{F}_i on the course of mixing and reaction. The model gives also the possibility to relate the shape and size of the reaction zone to the product distribution. Contrary to the lamellar structure model [22,23], the present approach takes into account not only mixing within separated fluid elements but also mass exchange between the fluid elements and their surrounding. This is due to the fact that the volume of the reaction zone grows because of molecular diffusion, accelerated by deformation. However, it should be pointed out that the model relates the growth of the volume of the reaction zone only to the diffusion coefficient of the reactant initially contained in the reaction zone. Thus, the model estimations are correct provided that an initial concentration of this reactant is much higher than the concentrations of other reactants in the environment.

5.2. An Integral Method for Mixing and Chemical Reaction in Deformed Diffusion Layers.

When mixing in a local frame of reference proceeds between species reacting instantaneously, the reaction zone is reduced to a plane and the process is completely controlled by molecular diffusion. In the case of single irreversible reaction



one has to solve the system of two equations of type:

$$\frac{\partial c_i}{\partial t} - \alpha \cdot x \frac{\partial c_i}{\partial x} = D_i \cdot \frac{\partial^2 c_i}{\partial x^2} \quad (5.51a)$$

with the condition linking species fluxes at the reaction plane:

$$\nu_A \cdot D_A \frac{\partial c_A}{\partial x} + \nu_B \cdot D_B \cdot \frac{\partial c_B}{\partial x} = 0 \quad (5.51b)$$

Solution of equations (5.51) is difficult due to the presence of the moving boundary. Only in a specific case $\mathbf{D}_A = \mathbf{D}_B$ can system (5.51) be reduced to

$$\frac{\partial c}{\partial t} - \alpha \cdot x \frac{\partial c}{\partial x} = D \cdot \frac{\partial^2 c}{\partial x^2} \quad (5.52)$$

where

$$c = v_B \cdot c_A - v_A \cdot c_B \quad (5.53)$$

is a new composition variable. After solution of equation (5.52) the concentrations of real reactants can be obtained from the composition variable:

$$c_A = \frac{|c| + c}{2 \cdot v_B}, \quad (5.54a)$$

$$c_B = \frac{|c| - c}{2 \cdot v_A}. \quad (5.54b)$$

At this point a simple integral method is proposed, allowing simple estimation of reactants conversions for the general case $D_A \neq D_B$ or $D_A = D_B$. A starting point for this formulation is a proposition by Tryggvason and Dahm [74].

These authors considered a single, combustion reaction of type (5.50) with the second-order, temperature dependent kinetics

$$R_i = \pm v_i \cdot k_0 \cdot e^{-\frac{E}{RT}} \cdot c_A \cdot c_B, \quad i = A, B, P, \quad (5.55)$$

where the minus sign is appropriate when $i = \{A, B\}$ and the plus sign when $i = \{P\}$. The process is considered in a local frame of reference following the reaction zone movement (with x axis pointed perpendicularly to the initial interface between **A** and **B**). Applying the usual assumption that in the vicinity of the coordinate origin the velocity field is given by the pure strain flow $\{v_x, v_y, v_z\} = \{-\alpha_x x, \alpha_y y, \alpha_z z\}$, Tryggvasson and Dahm [74] formulated dimensionless transport equations for species concentrations and temperature:

$$\frac{\partial C_i}{\partial \Gamma} - (U_x + A_x \cdot X) \cdot \frac{\partial C_i}{\partial X} = \frac{1}{Re \cdot Sc_i} \cdot \frac{\partial^2 C_i}{\partial X^2} \pm v_i \cdot Da \cdot e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B, \quad i = A, B, P, \quad (5.56a)$$

$$\frac{\partial \theta_T}{\partial \Gamma} - (U_x + A_x \cdot X) \cdot \frac{\partial \theta_T}{\partial X} = \frac{1}{Re \cdot Pr} \cdot \frac{\partial^2 \theta_T}{\partial X^2} + v_P \cdot Da \cdot He \cdot e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B. \quad (5.56b)$$

Dimensionless variables in equations (5.56) are defined with respect to characteristic reference values L^* , u^* , T^* and c^* for length, velocity, temperature and concentration:

$$X = \frac{x}{L^*}, \quad \Gamma = \frac{t \cdot u^*}{L^*}, \quad U_i = \frac{v_i}{u^*}, \quad C_i = \frac{c_i}{c^*}, \quad \theta_T = \frac{T}{T^*}, \quad A_x = \frac{\alpha_x \cdot L^*}{u^*}. \quad (5.57)$$

The dimensionless parameters in equations (5.56) are given by:

$$Re \cdot Sc_i = u^* \cdot L^* / D_i, \quad (5.58a)$$

$$Re \cdot Pr = u^* \cdot L^* / D_T, \quad (5.58b)$$

- Damköhler number $Da = k_0 \cdot c^* L^* / u^*$, (5.58c)

- Heat release parameter $He = \frac{q}{c_v \cdot T^*}$, (5.58d)

- Zel'dovich number $Ze = \frac{E}{R \cdot T^*}$, (5.58e)

where D_T , c_v and q are thermal diffusivity, constant volume specific heat and heat release per unit mass of fuel respectively. Symbol U_x in equations (5.56) is the normal velocity at which the local reference system follows the reaction zone.

If the diffusion layers are so thin that C_i and θ_T reach their far field values before encountering another layer, equations (5.56) can be integrated with weight functions X^j [74]. Assuming that $X^j \cdot (\partial C_i / \partial X)$ for $i=\{A,B\}$, $X^j \cdot C_p$ and $X^j \cdot (\theta_T - \theta_T^\infty)$ go to zero sufficiently fast far away from the reaction plane, so that the moments defined below:

$$M_j^i = \int_{-\infty}^{+\infty} X^j \cdot \frac{\partial C_i}{\partial X} dX , \quad i=A,B , \quad (5.59a)$$

$$M_j^P = \int_{-\infty}^{+\infty} X^j \cdot C_p dX , \quad (5.59b) \quad M_j^T = \int_{-\infty}^{+\infty} X^j \cdot (\theta_T - \theta_T^\infty) dX \quad (5.59c)$$

are convergent, Tryggvason and Dahm [74] expressed the results of integration of equations (5.56) in terms of M_j^i , M_j^P and M_j^T :

$$\frac{dM_0^i}{d\Gamma} = 0 , \quad (5.60a)$$

$$\frac{dM_1^i}{d\Gamma} = \pm U_x \cdot C_i^\infty - A_x \cdot M_1^i + v_i \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B dX , \quad (5.60b)$$

$$\frac{dM_2^i}{d\Gamma} = -2 \cdot U_x \cdot M_1^i - 2 \cdot A_x \cdot M_2^i \mp \frac{2 \cdot C_i^\infty}{Re \cdot Sc_i} + 2 \cdot v_i \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X dX , \quad (5.60c)$$

$$\frac{dM_0^P}{d\Gamma} = -A_x \cdot M_0^P + v_P \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B dX , \quad (5.61a)$$

$$\frac{dM_1^P}{d\Gamma} = -U_x \cdot M_0^P - 2 \cdot A_x \cdot M_1^P + v_P \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X dX , \quad (5.61b)$$

$$\frac{dM_2^P}{d\Gamma} = -2 \cdot U_x \cdot M_1^P - 3 \cdot A_x \cdot M_2^P + \frac{2 \cdot M_0^P}{Re \cdot Sc_P} + v_P \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X^2 dX , \quad (5.61c)$$

$$\frac{dM_0^T}{d\Gamma} = -A_x \cdot M_0^T + v_P \cdot He \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B dX , \quad (5.62a)$$

$$\frac{dM_1^T}{d\Gamma} = -U_x \cdot M_0^T - 2 \cdot A_x \cdot M_1^T + v_P \cdot He \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X dX , \quad (5.62b)$$

$$\frac{dM_2^T}{d\Gamma} = -2 \cdot U_x \cdot M_1^T - 3 \cdot A_x \cdot M_2^T + \frac{2 \cdot M_0^T}{Re \cdot Pr} + v_P \cdot He \cdot Da \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X^2 dX . \quad (5.62c)$$

The symbols \pm or \mp in equations (5.60) always relate the sign on the top to reactant A and that on the bottom to B. Symbols C_i^∞ and θ_T^∞ denote the far field values of concentrations and temperature.

Equations (5.60)÷(5.62) involve temperature and reactant profiles only through the "reaction integrals". Tryggvason and Dahm [74] suggested that to find the "reaction integrals" and consequently determine the evolution of moments (5.59) one can use "relatively crude representation for the actual temperature and concentration profiles".

Let us first discuss the problem of selection of U_x . In the simplest case, one can set U_x equal to zero and then the local frame of reference is fixed at the initial position of the interface between A and B. If the reaction zone is supposed to move far away from the system origin, moments (5.59) can grow considerably, which can affect accuracy of calculated conversion. Tryggvason and Dahm [74] proposed to chose U_x in such a way that the first moment of temperature profile vanishes. In this case one obtains from equation (5.62b):

$$U_x = v_P \cdot \frac{He \cdot Da}{M_0^T} \cdot \int_{-\infty}^{+\infty} e^{-\frac{Ze}{\theta_T}} \cdot C_A \cdot C_B \cdot X dX . \quad (5.63)$$

Then the system of equations (5.60)÷(5.62) was closed assuming that concentration and temperature profiles are self similar and can be characterized by a family of simple functions. These functions may not satisfy mass transfer equations in their differential form but can be sufficient to estimate the "reaction integrals". Tryggvason and Dahm [74] implemented in computations two type of functions.

The first group of functions called "linear" (sketched at figures 5.7ab) is defined as:

$$\frac{C_i(X)}{C_i^\infty} = \begin{cases} 1 & \text{if } X \leq \Delta_i - \delta_i/2 \\ 1/2 \pm (\Delta_i - X)/\delta_i & \text{if } \Delta_i - \delta_i/2 < X < \Delta_i + \delta_i/2 \\ 0 & \text{if } X \geq \Delta_i + \delta_i/2 \end{cases} \quad (5.64)$$

$$C_P(X) = \begin{cases} 0 & \text{if } X \leq -\delta_P/2 \\ C_M & \text{if } -\delta_P/2 < X < \delta_P/2 \\ 0 & \text{if } X \geq \delta_P/2 \end{cases} \quad (5.65)$$

$$\theta_T(X) - \theta_T^\infty = \begin{cases} 0 & \text{if } X \leq -\delta_T/2 \\ \theta_M & \text{if } -\delta_T/2 < X < \delta_T/2 \\ 0 & \text{if } X \geq \delta_T/2 \end{cases} \quad (5.66)$$

where Δ_i are displacements of the reactant gradient profiles from the coordinate origin and δ_i their widths. θ_M and C_M represent in equations (5.65) and (5.66) uniform temperature rise and product concentration levels.

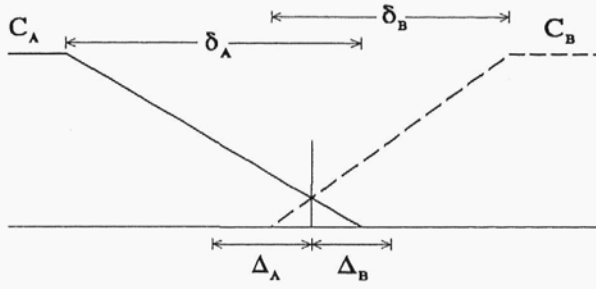


Figure 5.7a.

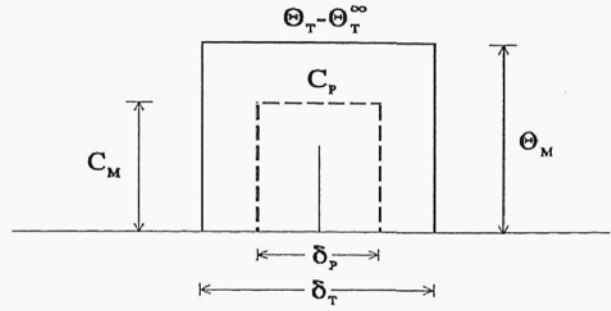


Figure 5.7b.

"Linear" concentration profiles.

Each function (5.64)-(5.66) is dependent on two parameters and thus moments (5.59) become:

$$M_1^i = \mp C_i^\infty \cdot \Delta_i, \quad M_2^i = \mp C_i^\infty \cdot (\delta_i^2/12 + \Delta_i^2), \quad (5.67)$$

$$M_0^P = C_M \cdot \delta_P, \quad M_2^P = C_M \cdot \delta_P^3/12, \quad (5.68)$$

$$M_0^T = \theta_M \cdot \delta_T, \quad M_2^T = \theta_M \cdot \delta_T^3/12. \quad (5.69)$$

The second group of "smooth" functions (shown in figures 5.8ab) is defined by:

$$\frac{C_i(X)}{C_i^\infty} = \frac{1}{2} \mp \frac{1}{2} \cdot \frac{(X \pm \Delta_i)^3 + 1.5 \cdot \delta_i^2 \cdot (X \pm \Delta_i)}{[(X \pm \Delta_i)^2 + \delta_i^2]^{3/2}}, \quad (5.70)$$

$$C_P(X) = C_M \cdot \frac{\delta_P^5}{(X^2 + \delta_P^2)^{5/2}}, \quad (5.71)$$

$$\theta_T(X) - \theta_T^\infty = \theta_M \cdot \frac{\delta_T^5}{(X^2 + \delta_T^2)^{5/2}} \quad (5.72)$$

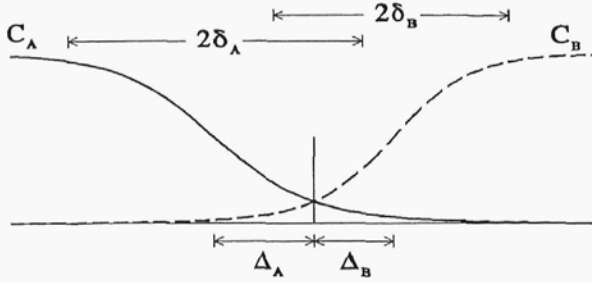


Figure 5.8a.

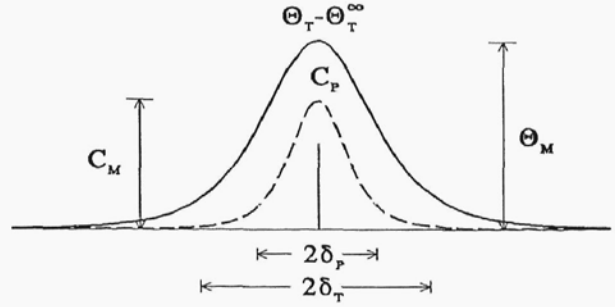


Figure 5.8b.

"Smooth" concentration profiles.

In this case moments (5.59) become:

$$M_1^i = \mp C_i^\infty \cdot \Delta_i, \quad M_2^i = \mp C_i^\infty \cdot (\delta_i^2/2 + \Delta_i^2), \quad (5.73)$$

$$M_0^P = \frac{4}{3} \cdot C_M \cdot \delta_P, \quad M_2^P = \frac{2}{3} \cdot C_M \cdot \delta_P^3, \quad (5.74)$$

$$M_0^T = \frac{4}{3} \cdot \theta_M \cdot \delta_T, \quad M_2^T = \frac{2}{3} \cdot \theta_M \cdot \delta_T^3. \quad (5.75)$$

The correctness of these approximations was verified by Tryggvason and Dahm [74] and Chang et al. [75] by comparison of results of full numerical solution of equations (5.56) with the results obtained using the integral method. It was found that both "linear" and "smooth" profiles are quite sufficient to determine quantities such as the total temperature rise, the total reaction rate or the total product amount with a few percent error. Moreover, the integral method was proved to be increasingly valid as Schmidt and Damköhler numbers increase; one should, however, remember that the convergence of full numerical simulation is very difficult to achieve.

In the present work the integral method by Dahm and co-workers [74,75] was adapted to model a local mixing with instantaneous chemical reaction $A + B \rightarrow P$, occurring in isothermal conditions. Assuming that the considered diffusion layer is isolated from other diffusion layers one can describe mixing in Lagrangian frame of reference using system of transport equations (5.51a) with boundary conditions:

- at the reaction plane (5.51b) and

$$c_A = c_B = 0 , \quad (5.76a)$$

- in the far field:

$$c_A(x \rightarrow -\infty, t) = c_{A0} , \quad (5.76b)$$

$$c_B(x \rightarrow +\infty, t) = c_{B0} \quad (5.76c)$$

and with initial conditions:

$$c_A(x, 0) = \begin{cases} c_{A0} & \text{if } x < 0 \\ 0 & \text{if } x \geq 0 \end{cases} , \quad (5.77a)$$

$$c_B(x, 0) = \begin{cases} 0 & \text{if } x \leq 0 \\ c_{B0} & \text{if } x > 0 \end{cases} . \quad (5.77b)$$

Using for simplicity the dimensionless variables:

$$\xi = \sqrt{\frac{\alpha}{D_A}} \cdot e^{\alpha t} \cdot x , \quad (5.78a)$$

$$\tau = \frac{1}{2} \cdot (e^{2\alpha t} - 1) , \quad (5.78b)$$

$$C_i = \frac{c_i}{c_{A0}} , \quad (5.78c)$$

and assuming that $\nu_A = \nu_B$ one can transform equations (5.51), (5.76) and (5.77) into:

$$\frac{\partial C_A}{\partial \tau} = \frac{\partial^2 C_A}{\partial \xi^2} , \quad (5.79a)$$

$$\frac{\partial C_B}{\partial \tau} = \frac{D_B}{D_A} \cdot \frac{\partial^2 C_B}{\partial \xi^2} , \quad (5.79b)$$

$$\left. \frac{\partial C_A}{\partial \xi} \right|_{\xi_R} + \frac{D_B}{D_A} \cdot \left. \frac{\partial C_B}{\partial \xi} \right|_{\xi_R} = 0 , \quad (5.79c)$$

$$C_A = C_B = 0 \quad \text{at } \xi = \xi_R , \quad (5.79d)$$

$$C_A(\xi \rightarrow -\infty, \tau) = 1 , \quad (5.79e)$$

$$C_B(\xi \rightarrow +\infty, \tau) = c_{B0}/c_{A0} , \quad (5.79f)$$

$$C_A(\xi, 0) = \begin{cases} 1 & \text{if } \xi < 0 \\ 0 & \text{if } \xi \geq 0 \end{cases} , \quad (5.79g)$$

$$C_B(\xi, 0) = \begin{cases} 0 & \text{if } \xi \leq 0 \\ c_{B0}/c_{A0} & \text{if } \xi > 0 \end{cases} , \quad (5.79h)$$

where ξ_R is the position of the reaction plane; the reaction plane is from definition perpendicular to ξ axis. Equations (5.79) present so-called Neumann's problem. The analytical solution of this problem is given by Carslaw and Jaeger [65, p.288]:

$$C_A(\xi, \tau) = 1 - \frac{1 + \operatorname{erf} \left[\xi / (2 \cdot \sqrt{\tau}) \right]}{1 + \operatorname{erf}(\lambda)} , \quad (5.80a)$$

$$C_B(\xi, \tau) = \frac{c_{B0}}{c_{A0}} - \frac{c_{B0}}{c_{A0}} \cdot \frac{1 - \operatorname{erf} \left[\xi / (2 \cdot \sqrt{\tau \cdot D_B/D_A}) \right]}{1 - \operatorname{erf}(\lambda / \sqrt{D_B/D_A})} , \quad (5.80b)$$

$$\xi_R = 2 \cdot \lambda \cdot \sqrt{\tau} , \quad (5.80c)$$

where constant λ can be determined from the following expression:

$$\frac{e^{-\lambda^2}}{1 + \operatorname{erf}(\lambda)} = \frac{c_{B0}}{c_{A0}} \cdot \sqrt{\frac{D_B}{D_A}} \cdot \frac{e^{-\frac{D_A}{D_B} \lambda^2}}{1 - \operatorname{erf}\left(\lambda \cdot \sqrt{D_A/D_B}\right)} . \quad (5.81)$$

Let us now solve Neumann's problem using an integral method and compare the results of calculations with the analytical solution. This will show how exact is the integral method by Dahm and co-workers [74,75].

The gradient concentration moments are defined as follows:

$$M_j^i = \int_{a_i(\tau)}^{b_i(\tau)} \xi^j \cdot \frac{\partial C_i}{\partial \xi} d\xi \quad i = A, B, \quad (5.82)$$

where the integration limits according to the boundary conditions (5.79def) are:

$$\text{-- for reactant A} \quad a_A = -\infty, \quad b_A = \xi_R, \quad (5.83a)$$

$$\text{-- for reactant B} \quad a_B = \xi_R, \quad b_B = +\infty. \quad (5.83b)$$

Differentiation of (5.82) with respect to the dimensionless time yields:

$$\frac{dM_j^i}{d\tau} = b_i^j \cdot \frac{db_i}{d\tau} \cdot \frac{\partial C_i}{\partial \xi} \Big|_{\xi=b_i} - a_i^j \cdot \frac{da_i}{d\tau} \cdot \frac{\partial C_i}{\partial \xi} \Big|_{\xi=a_i} + \int_{a_i}^{b_i} \xi^j \cdot \frac{\partial}{\partial \xi} \left(\frac{\partial C_i}{\partial \tau} \right) d\xi . \quad (5.84)$$

Integrating by parts the last term in equation (5.84) and using relation:

$$\frac{dC_i}{d\tau} \Big|_{\xi=\gamma} = \frac{d\gamma}{d\tau} \cdot \frac{\partial C_i}{\partial \xi} \Big|_{\xi=\gamma} + \frac{\partial C_i}{\partial \tau} \Big|_{\xi=\gamma} \quad (5.85)$$

one receives:

$$\frac{dM_j^i}{d\tau} = b_i^j \cdot \frac{dC_i}{d\tau} \Big|_{\xi=b_i} - a_i^j \cdot \frac{dC_i}{d\tau} \Big|_{\xi=a_i} - j \cdot \int_{a_i}^{b_i} \xi^{j-1} \cdot \left(\frac{\partial C_i}{\partial \tau} \right) d\xi . \quad (5.86)$$

Substituting equations (5.79ab) into equation (5.86) and using relations (5.79def) and (5.83) one obtains for $j=1$:

$$\frac{dM_1^A}{d\tau} = - \frac{\partial C_A}{\partial \xi} \Big|_{\xi=\xi_R}, \quad (5.87a)$$

$$\frac{dM_1^B}{d\tau} = \frac{D_B}{D_A} \cdot \frac{\partial C_B}{\partial \xi} \Big|_{\xi=\xi_R}. \quad (5.87b)$$

Notice that the right sides of equations (5.87) determine the rate of consumption of reactants in the instantaneous reaction. The numbers of moles consumed for unit time and per unit area

of the reaction plane are given by:

$$J_i = \mp D_i \cdot \frac{\partial c_i}{\partial x} \Big|_{x=x_R} = \mp D_i \cdot c_{A0} \cdot \sqrt{\frac{\alpha \cdot (2 \cdot \tau + 1)}{D_A}} \cdot \frac{\partial C_i}{\partial \xi} \Big|_{\xi=\xi_R} \quad i = A, B, \quad (5.88)$$

where the minus and plus signs refer to reactant A and B respectively.

Let us now approximate the concentration profiles by two-parameter "linear" functions as defined by equations (5.64) with X replaced by ξ . In this case the first order, gradient concentration moments (5.82) become:

$$M_1^A = -\Delta_A, \quad (5.89a)$$

$$M_1^B = \frac{c_{B0}}{c_{A0}} \cdot \Delta_B \quad (5.89b)$$

and equations (5.87) take the form:

$$-\frac{d\Delta_A}{d\tau} = \frac{1}{\delta_A}, \quad (5.90a)$$

$$\frac{d\Delta_B}{d\tau} = \frac{D_B}{D_A} \cdot \frac{1}{\delta_B} \quad (5.90b)$$

with the boundary condition:

$$\frac{1}{\delta_A} = \frac{D_B}{D_A} \cdot \frac{c_{B0}}{c_{A0}} \cdot \frac{1}{\delta_B}. \quad (5.91)$$

The reactants cannot coexist, so the concentration profiles cannot overlap, as shown in figure 5.9. Consequently one has:

$$\Delta_A + \delta_A/2 = \Delta_B - \delta_B/2. \quad (5.92)$$

The initial condition for differential equations (5.90) is

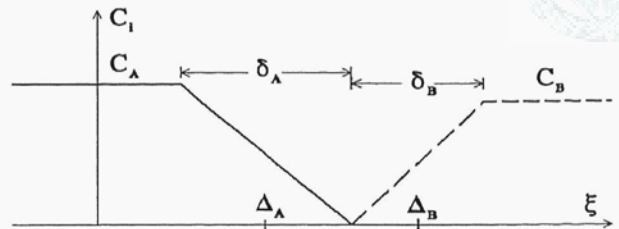


Figure 5.9. Linear concentration profiles - instantaneous reaction.

$$\tau = 0 \quad \delta_A = \delta_B = \Delta_A = \Delta_B = 0. \quad (5.93)$$

The analytical solution of the system of equations (5.90)÷(5.93) reads:

$$\delta_A = \sqrt{v \cdot \tau}, \quad (5.94a)$$

$$\delta_B = \frac{D_B}{D_A} \cdot \frac{c_{B0}}{c_{A0}} \cdot \sqrt{v \cdot \tau}, \quad (5.94b)$$

$$\Delta_A = -2 \cdot \sqrt{\tau/v}, \quad (5.94c)$$

$$\Delta_B = 2 \cdot \frac{c_{B0}}{c_{A0}} \cdot \sqrt{\tau/v}, \quad (5.94d)$$

where

$$v = 4 \cdot \left(1 + \frac{c_{A0}}{c_{B0}} \right) \left/ \left(1 + \frac{D_B}{D_A} \cdot \frac{c_{B0}}{c_{A0}} \right) \right. . \quad (5.95)$$

To evaluate the accuracy of the integral method let us compare the total numbers of moles of reactant A consumed per unit area of the reaction plane:

$$\dot{N}_A = \int_0^t J_A dt = -c_{A0} \cdot \sqrt{\frac{D_A}{\alpha}} \cdot \int_0^\tau \frac{\partial C_A}{\partial \xi} \frac{d\tau'}{\sqrt{2 \cdot \tau' + 1}} , \quad (5.96)$$

as computed from exact solution (5.80) and by the integral method.

From exact solution (5.80) and (5.81) one has:

$$\left. \frac{\partial C_A}{\partial \xi} \right|_{\xi=\xi_R} = - \frac{e^{-\lambda^2}}{1 + \operatorname{erf}(\lambda)} \cdot \frac{1}{\sqrt{\pi \cdot \tau}} \quad (5.97a)$$

and

$$\dot{N}_A = c_{A0} \cdot \sqrt{\frac{2 \cdot D_A}{\pi \cdot \alpha}} \cdot \frac{e^{-\lambda^2}}{1 + \operatorname{erf}(\lambda)} \cdot \ln(\sqrt{2 \cdot \tau + 1} + \sqrt{2 \cdot \tau}) . \quad (5.97b)$$

From approximate solution (5.94) and (5.95) one has:

$$\left[\left. \frac{\partial C_A}{\partial \xi} \right|_{\xi=\xi_R} \right]' = - \frac{1}{\delta_A} = - \frac{1}{\sqrt{v \cdot \tau}} \quad (5.98a)$$

and

$$\dot{N}_A' = c_{A0} \cdot \sqrt{\frac{2 \cdot D_A}{v \cdot \alpha}} \cdot \ln(\sqrt{2 \cdot \tau + 1} + \sqrt{2 \cdot \tau}) . \quad (5.98b)$$

Expressions (5.97b) and (5.98b) were plotted in figures (5.10abcd) for different values of ratios c_{B0}/c_{A0} and D_B/D_A .

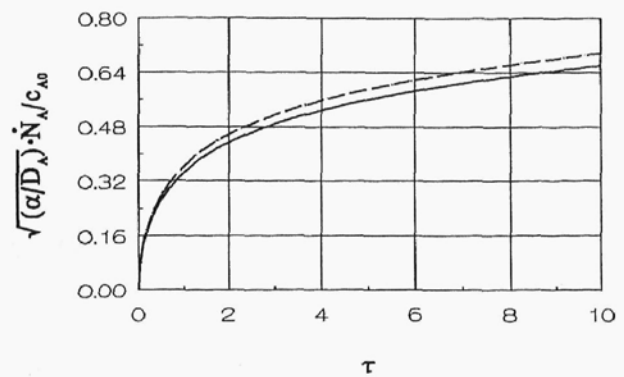
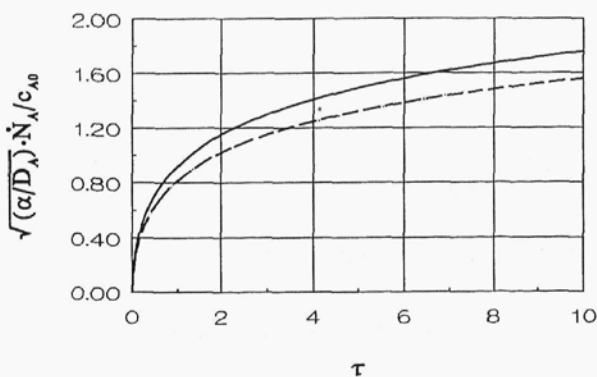


Figure 5.10a. $c_{B0}/c_{A0}=1$, $D_B/D_A=1$. Figure 5.10b. $c_{B0}/c_{A0}=0.2$, $D_B/D_A=1$.

Comparison between the analytical solution (—) and the integral method (---).

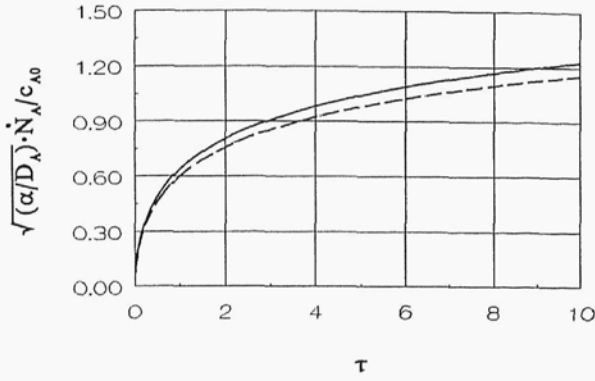


Figure 5.10c. $c_{B0}/c_{A0}=1$, $D_B/D_A=0.1$.

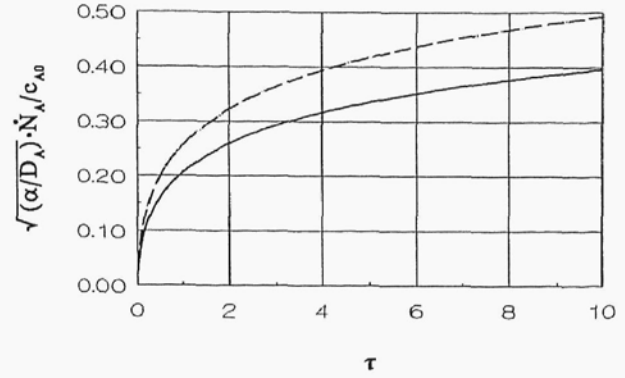


Figure 5.10d. $c_{B0}/c_{A0}=0.1$, $D_B/D_A=1$.

Comparison between the analytical solution (—) and the integral method (- - -).

Analysis of these figures indicates that for $D_A=D_B$ and $0.2 \leq c_{B0}/c_{A0} \leq 5$ the error of integral method is not higher than 11.4% (figures 5.10ab). The integral method also well estimates reactants consumption when c_{B0}/c_{A0} ratio is close to unity and $0.1 \leq D_B/D_A \leq 10$ (figure 5.10c). However, it should be noted that the accuracy of the integral method rapidly deteriorates when either $c_{B0}/c_{A0} \leq 0.1$ or $c_{B0}/c_{A0} \geq 10$ (figure 5.10d).

The method of the gradient concentration moments can also be applied in the case of two interacting diffusion layers, forming a deformed and reacting slab, as shown in figure 5.11.

Mixing and instantaneous reaction between species A and B initially forming a slab of thickness s_0 is now considered.

The layer is stretched in two dimensional stagnation flow, in the same way as

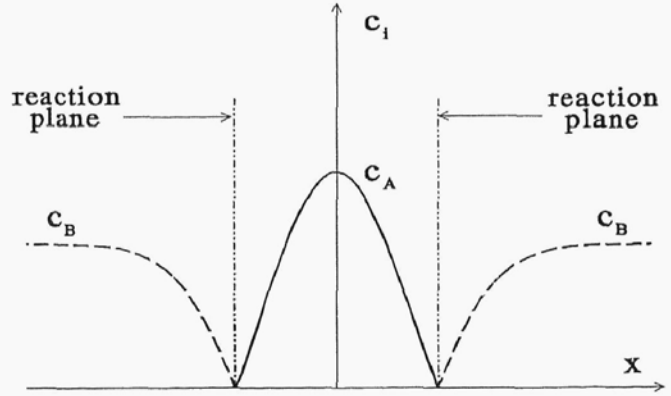


Figure 5.11. Two interacting diffusion layers.

shown in figure 3.2. Also in this case the material transport equations are given by (5.51a),

whereas the boundary and initial conditions are now:

- at the coordinate origin $\frac{\partial c_A}{\partial x} = 0$, (5.99)
- at the reaction plane equations (5.51b) and (5.76a) ,
- in the far field equation (5.76c) .

The initial conditions are:

$$c_A(x,0) = \begin{cases} c_{A0} & \text{if } 0 \leq x < s_0/2 \\ 0 & \text{if } x \geq s_0/2 \end{cases}, \quad (5.100a)$$

$$c_B(x,0) = \begin{cases} 0 & \text{if } x \leq s_0/2 \\ c_{B0} & \text{if } x > s_0/2 \end{cases}. \quad (5.100b)$$

Using for the dimensionless variables:

$$\xi = \frac{x}{s}, \quad (5.101a)$$

$$\tau = D_A \cdot \int_0^t \frac{dt'}{s(t')^2}, \quad (5.101b)$$

$$C_i = \frac{c_i}{c_{A0}}, \quad (5.101c)$$

one obtains again differential balances in the form of equations (5.79ab) with the boundary conditions given by (5.79cd), plus additionally:

$$\left. \frac{\partial C_A}{\partial \xi} \right|_{\xi=\xi_R} = 0, \quad (5.102a)$$

$$C_B(\xi \rightarrow +\infty, \tau) = \frac{c_{B0}}{c_{A0}} \quad (5.102b)$$

and with the initial conditions:

$$C_A(\xi,0) = \begin{cases} 1 & \text{if } 0 \leq \xi < 1/2 \\ 0 & \text{if } \xi \geq 1/2 \end{cases}, \quad (5.103a)$$

$$C_B(\xi,0) = \begin{cases} 0 & \text{if } \xi \leq 1/2 \\ c_{B0}/c_{A0} & \text{if } \xi > 1/2 \end{cases}. \quad (5.103b)$$

The analytical solution in the considered case exists only for $D_A = D_B$ and can be obtained from solution of equations (3.8) derived for an inert tracer - equation (3.9). The discussed above method of moments can be easily adopted to describe a general case including $D_A = D_B$ and $D_A \neq D_B$. Defining now the moments for reactants A and B as:

$$M_j^A = \int_0^{\xi_R} \xi^j \cdot \frac{\partial C_A}{\partial \xi} d\xi, \quad (5.104a)$$

$$M_j^B = \int_{\xi_R}^{+\infty} \xi^j \cdot \frac{\partial C_B}{\partial \xi} d\xi, \quad (5.104b)$$

leads to the same expression for time evolution of M_j^i as (5.87). In the first stage of the process, the reactant profiles can be approximated by equations (5.64) with X replaced by ξ , so the moments and governing equations (5.90)-(5.92) remain unchanged, whereas the initial conditions become:

$$\tau = 0 \quad \delta_A = \delta_B = 0, \quad \Delta_A = \Delta_B = 1/2. \quad (5.105)$$

The first stage of the process ends when the diffusion layers start to interact, or when

$$\Delta_A - \delta_A/2 = 0. \quad (5.106)$$

In the second stage of the process the "linear" concentration profile for reactant A (5.64) is replaced by

$$C_A(\xi, \tau) = \begin{cases} C_{AM} \cdot (1 - \xi/\delta_A) & \text{if } 0 \leq \xi < \delta_A \\ 0 & \text{if } \xi \geq \delta_A \end{cases}, \quad (5.107)$$

as shown in figure 5.12 and consequently

$$M_1^A = -C_{AM} \cdot \delta_A . \quad (5.108)$$

Notice that in the profile (5.107) the parameter representing the position of the diffusion layer Δ_A disappears but one need to know the concentration of reactant A at the system origin C_{AM} , so there are also two parameters.

In this case the equations (5.90a), (5.91)

and (5.92) become:

$$-\frac{d}{dt}(C_{AM} \cdot \delta_A) = \frac{C_{AM}}{\delta_A} , \quad (5.109)$$

$$\frac{C_{AM}}{\delta_A} = \frac{D_B}{D_A} \cdot \frac{c_{B0}}{c_{A0}} \cdot \frac{1}{\delta_B} , \quad (5.110)$$

$$\delta_A = \Delta_B - \delta_B/2 , \quad (5.111)$$

whereas equation (5.90b) is unchanged.

The backward Euler scheme was applied to solve the governing equations (5.90)÷(5.92) in the first stage and (5.90b) and (5.109)÷(5.111) in the second stage of the process. Figures 5.13abc show a comparison between the exact conversion values of reactant A and these given by the integral method for the case when $D_A=D_B$. As it can be seen, there is quite good agreement between the analytical and numerical results. However, it should be pointed out that the conversions of reagent A were slightly underestimated in all cases.

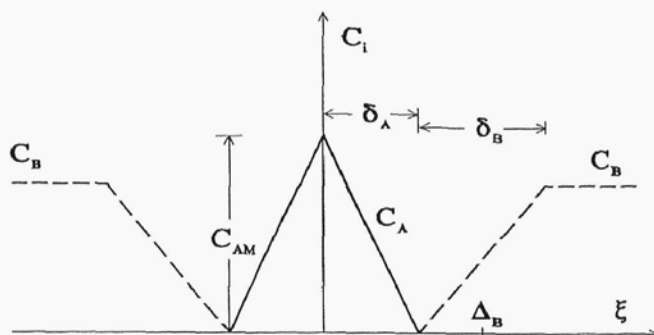


Figure 5.12. Linear concentration profiles; instantaneous reaction, second stage.

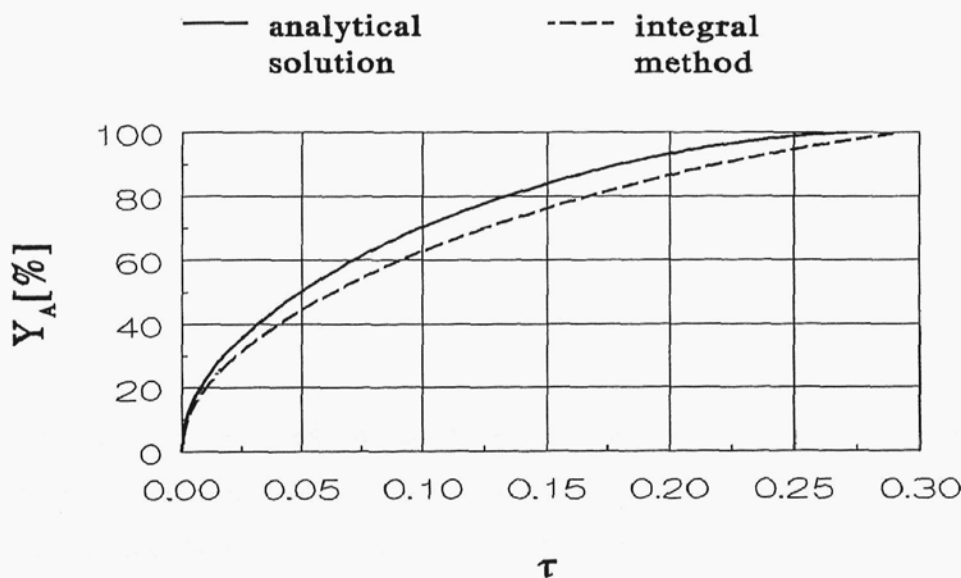


Figure 5.13a. Conversion of reagent A in instantaneous reaction; $c_{A0}=c_{B0}$, $D_A=D_B$.

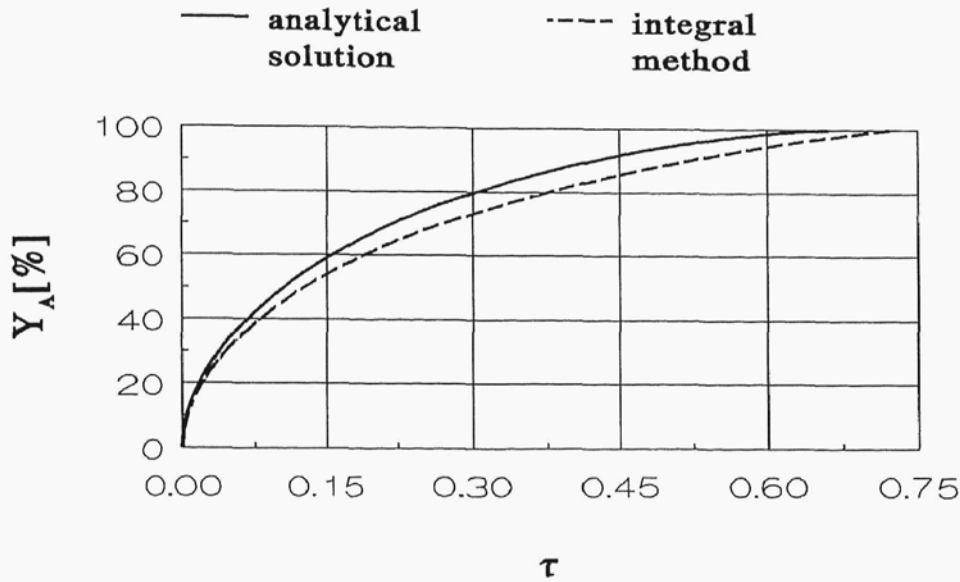


Figure 5.13b. Conversion of reagent A in instantaneous reaction; $c_{B0}/c_{A0}=0.5$, $D_A=D_B$.

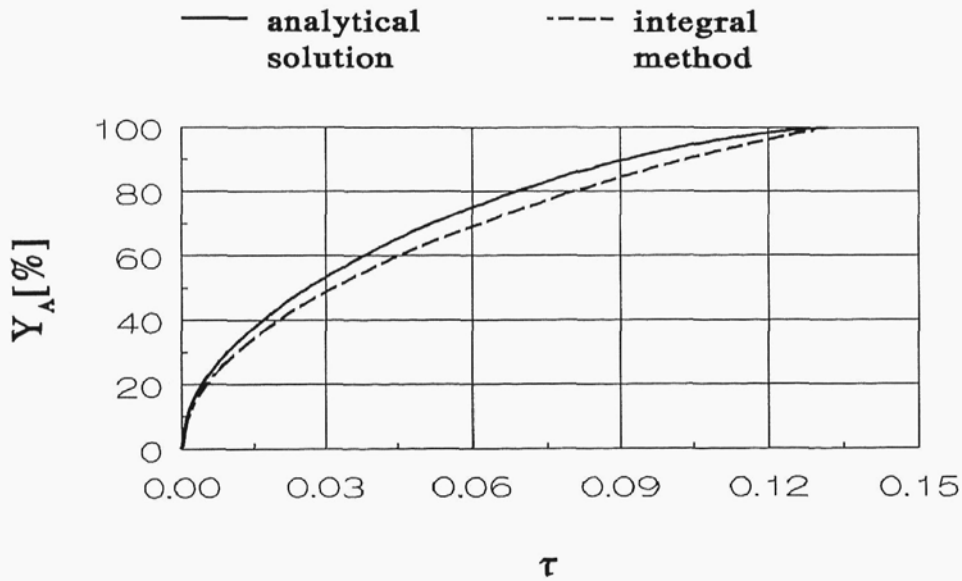


Figure 5.13c. Conversion of reagent A in instantaneous reaction; $c_{B0}/c_{A0}=2$, $D_A=D_B$.

Recapitulating the above considerations, one can see that the integral method similar to that proposed by Dahm and co-workers [74,75] can be very useful in modelling of local mixing with instantaneous chemical reaction. The method is very simple and easy to use. On the contrary to the method proposed in the previous point, it allows to take into account differences in diffusivity coefficients of reacting species. Although the method can only be used when the concentrations of reactants are initially not very different; for the concentration ratio higher than 5 or lower than 0.2 the first integral method gives better results.