

THE EFFECT OF AXIAL DISPERSION ON THE CONVERSION OF A SECOND-ORDER IRREVERSIBLE REACTION IN A TUBULAR REACTOR WITH COMPLETELY SEGREGATED FLOW¹

János SAWINSKY and András DEÁK

Department of Chemical Engineering
Technical University of Budapest
H-1521 Budapest, Hungary

Abstract

An analytical solution was given to predict the exit concentration of a tubular reactor with completely segregated flow for second-order reaction using the axial dispersion model. The calculated exit concentrations agree with the numerical solution published by LINDFORS (1974).

Keywords: axial dispersion, tubular reactor, second-order reaction, segregated flow.

The conversion in case of reactions with non-linear kinetics in a continuous flow isothermal reactor is influenced by macro- and micromixing in the system. The macromixing is characterised by the residence time distribution (RTD). The mixing on molecular scale (micromixing) may range from one extreme of maximum mixedness to the other extreme of completely segregated flow. In case of complete segregation the fluid travels through the reactor in discrete packets and no mass exchange occurs between them, so the packets behave as small batch reactors. When the packets of fluid move at velocities differing randomly from the mean velocity the RTD can be described by the axial dispersion model. The cumulative RTD function $F(\vartheta)$ for this model was derived by HIBY and SCHÜMMER (see paper of WESTERTERP and LANDSMAN, 1962).

The RTD density function $E(\vartheta)$ can be obtained by the differentiation of $F(\vartheta)$:

$$E(\vartheta) = \frac{2}{Pe} \exp\left(\frac{Pe}{2}\right) \sum_{j=1}^{\infty} N_j \cdot \exp(-m_j \vartheta), \quad (1)$$

where

$$N_j = (-1)^{j+1} \cdot \frac{\gamma_j^2}{1 + m_j}; \quad m_j = \frac{\gamma_j^2}{Pe} + \frac{Pe}{4}$$

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and γ_j are the positive roots of the equation

$$\operatorname{ctg}\gamma_j = \frac{\gamma_j}{Pe} + \frac{Pe}{4\gamma_j}.$$

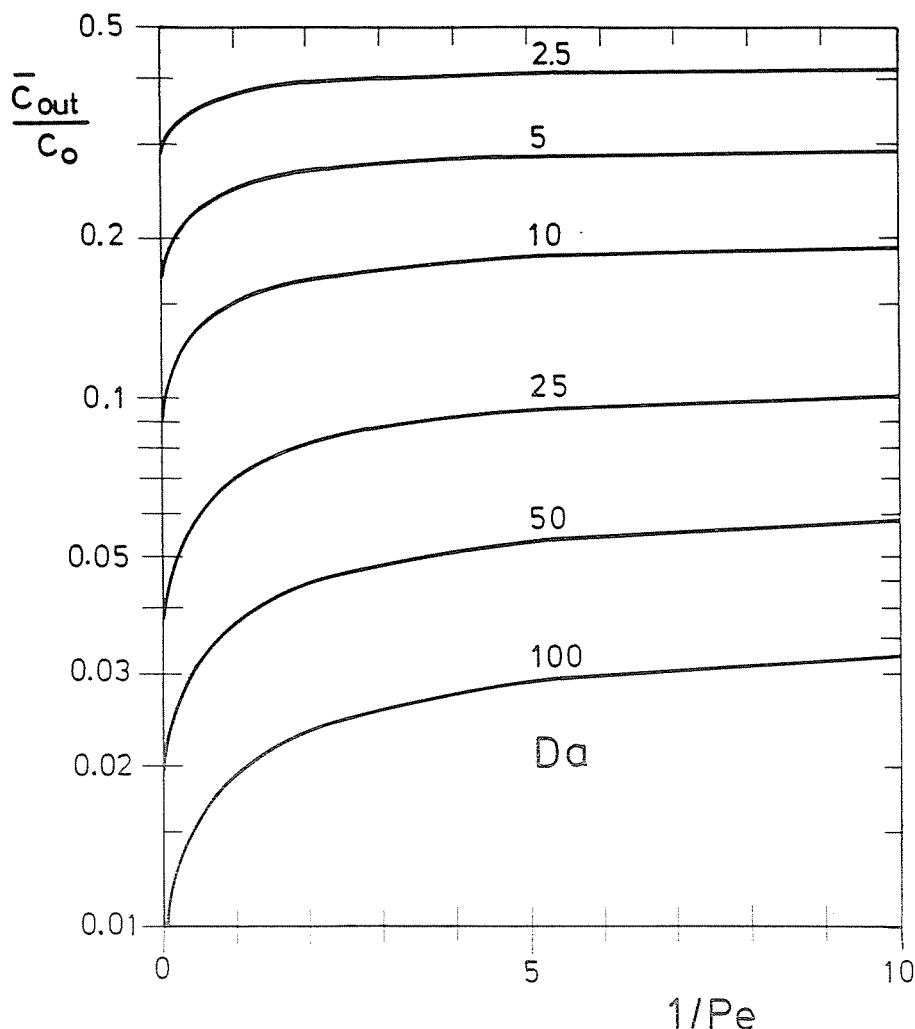


Fig. 1. Exit concentration for second-order reaction in a tubular reactor with segregated flow.

Consider a packet of fluid that spends time t in the reactor. The concentration in it when leaving the system is c_{out} . This can be calculated from batch reactor data. For second-order irreversible reaction c_{out} is

$$c_{out} = c_{batch} = \frac{c_0}{1 + ktc_0}. \quad (2)$$

If the reactor operates steady-state the average exit concentration can be predicted using the following equation (DANCKWERTS, 1958):

$$\bar{c}_{\text{out}} = \int_0^{\infty} c_{\text{batch}} - E(\vartheta) d\vartheta, \quad (3)$$

Substituting *Eqs.* (1) and (2) in the above equation gives:

$$\frac{\bar{c}_{\text{out}}}{c_0} = \frac{2}{Da - Pe} \exp\left(\frac{Pe}{2}\right) \sum_{j=1}^{\infty} N_j - \exp(z_j) - E_1(z_j), \quad (4)$$

where $z_j = m_j/Da$ and $E_1(z)$ is the exponential integral

$$E_1(z) = \int_z^{\infty} \frac{e^{-x}}{x} dx.$$

Fig. 1 shows the ratio of the average exit concentration \bar{c}_{out} to the initial concentration c_0 . For computing $E_1(z)$, and $E_1(z) - \exp(z)$ in case of $z > 4$, we used rational Chebyshev approximation (CODY and THACHER, 1969). LINDFORS (1974) calculated the exit concentration numerically by using *Eqs.* (1), (2) and (3). His results show very good agreement with our solution.

Notation

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|----------------------|--|
| c | concentration of reactant, mol/m ³ |
| D | axial dispersion coefficient, m ² /s |
| $E(\vartheta)$ | residence time distribution density function |
| $E_1(z)$ | exponential integral |
| $F(\vartheta)$ | cumulative residence time distribution function |
| k | reaction rate coefficient, m ³ /(mol s) |
| L | length of the reactor, m |
| t | time, s |
| v | linear velocity, m/s |
| $Da = k\tau c_0$ | Damköhler number |
| $Pe = vL/D$ | Peclet number |
| <i>Greek letters</i> | |
| $\tau = L/v$ | mean residence time, s |
| ϑ | dimensionless time defined as t/τ |
| <i>Subscripts</i> | |
| 0 | refers to initial condition |
| out | outlet |

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