INFLUENCE OF LONGITUDINAL MIXING ON THE DEGREE OF REACTANT CONVERSION IN A CHEMICAL FLOW REACTOR

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The method of small perturbations in the approximation of a "weak" chemical reaction (low dimensionless reaction rate) is used to obtain, to terms of third order, an approximate analytic solution to the problem of the concentration distribution in a one-dimensional chemical flow reactor. This solution makes it possible to analyze the dependence of the degree of conversion of the original reactant on the longitudinal diffusion and other factors. An autocatalytic reaction, in which the degree of conversion depends nonmonotonically on the Péclet number, is considered as an example. The investigation shows that for different values of the parameters of the problem longitudinal mixing can both increase and decrease the degree of conversion. The results make it possible to identify ranges of variation of the parameters which characterize the operation of the reactor in which longitudinal mixing has different influences on the degree of chemical conversion and find the degree of longitudinal mixing which ensures optimal operation of the chemical reactor.

Longitudinal mixing in chemical flow reactors has a strong influence on the degree of conversion, the selectivity, and other characteristics [1]. Variation of the intensity of longitudinal mixing is one of the means of influencing the yield of such reactors [2, 3]. The theoretical prerequisite for choosing the optimal level of longitudinal mixing in a reactor is knowledge of the functional connection between the degree of conversion of the original reactant, the selectivity, and the other characteristics which govern the efficiency of the reactor, on the one hand, and the coefficient of longitudinal diffusion (the Péclet number), on the other. The dependence of the efficiency of a chemical reactor on the intensity of longitudinal mixing has been discussed on many occasions (see,
for example, [1-13]). Mathematically, the finding of this dependence reduces to analyzing the solution of a nonlinear two-point boundary-value problem, which usually does not have an analytic solution. Various approaches are used.

Until recently, a restriction was made to analyzing nearly limiting cases — the model of an ideal displacement reactor and the model of an ideal mixing reactor — with subsequent extrapolation of the results to intermediate values of the coefficient of longitudinal diffusion [1-7]. However, as is shown by a deeper analysis, the conclusions obtained in such an approach are valid only for the simplest systems, and are incorrect in more complicated cases [13]. Attempts to extend these results by approximate solution of the boundary-value problems by the method of asymptotic expansions at small and large Péclet numbers also fail to yield the solution for intermediate values of the mixing intensity.

In a number of papers (see, for example, [8-10]), the dependence of the degree of conversion in the reactor on the coefficient of longitudinal diffusion has been analyzed under the assumption of an analogy between a flow reactor with longitudinal mixing and a reactor with recycling, since the solution to the problem for the latter is much simpler. However, it has not been established to what extent the results obtained for a reactor with recycling correspond to a reactor with longitudinal mixing.

The papers [11-12] give the results of numerical calculations of the concentration profiles for definite models of chemical reactors for various special values of the Péclet number; in [12], the influence of longitudinal mixing on the degree of conversion was investigated numerically for the case of an autocatalytic reaction. It was found that if an intermediate mixing level ensures a maximum conversion, then the optimal Péclet number corresponding to this level is in the interval (0, 2). These results indicate that the degree of conversion depends in a complicated manner on the coefficient of longitudinal diffusion, but they do not permit the determination of sufficiently general laws.

1. Formulation of the Problem and Approximate Solution

In dimensionless variables, the equations and boundary conditions for the reactant concentration in a one-dimensional isothermal chemical flow reactor, and also in an adiabatic reactor in which the coefficients of diffusion and thermal diffusivity are equal, can be written in the case of a single-stage chemical reaction in the form

\[ \frac{1}{P} \frac{d^2 c}{dx^2} - \frac{dc}{dx} = f(c), \quad x=0, \quad -\frac{1}{P} \frac{dc}{dx} + c = c_f; \quad x=1, \quad \frac{dc}{dx} = 0 \]

(1.1)

\[ c = \frac{C}{C_f}, \quad x = \frac{X}{L}, \quad P = \frac{UL}{D}, \quad f(c) = \frac{LF(C)}{UC_f}, \quad c_f = \frac{C_f}{C_o} \]

Here, \( X \) is the spatial coordinate \((0 \leq X \leq L)\), \( L \) is the length of the reactor, \( C \) is the reactant concentration in the reactor, \( C_f \) is the reactant concentration at the entrance to the reactor, \( C_0 \) is the characteristic value of the concentration \( C_f \), \( U \) is the rate at which the reactant is supplied, \( D \) is the effective diffusion coefficient, \( F(C) \) is the dependence of the reaction rate on the reactant concentration, and \( P \) is the Péclet number. We also introduce \( \xi = (C_f - C)/C_f \), the degree of reactant conversion.

We shall assume that the dimensionless reaction rate is low, i.e., \( f(c) = \epsilon f_1(c) = O(\epsilon), \epsilon \ll 1 \) (weak chemical reaction), and seek an approximate solution to the problem (1.1) in the form of an expansion in powers of \( \epsilon \):

\[ c(x) = \sum_{n=0}^{\infty} \epsilon^n c_n(x) \]

(1.2)

Substituting the expansion (1.2) in (1.1), representing the function \( f_1(c) \) as a series in powers of \( \epsilon \), and equating the coefficients of equal powers of \( \epsilon \), we obtain the equations and boundary conditions for the functions \( c_n(x) \) for \( n = 0, 1, 2, 3 \):

\[ n=0, \quad \frac{1}{P} \frac{d^2 c_0}{dx^2} - \frac{dc_0}{dx} = 0 \]