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EXACT SOLUTION OF A NONLINEAR BOUNDARY VALUE PROBLEM OF THE THEORY OF CHEMICAL REACTORS*

V.S. BERMAN and V.V. VOSTOKOV

An exact solution is obtained for a nonlinear boundary value model problem of stationary concentration distribution in a one-dimensional tubular isothermal chemical reactor with longitudinal stirring, in which a single chemical reaction takes place. It is show that depending on the values of the problem parameters there are either no stationary modes, a single or two different stationary modes. Regular and singular perturbation methods are used to construct the asymptotic solutions of the problem, and the latter are compared with the exact solutions.

1. Formulation and general solution of the problem. We consider a model nonlinear boundary value problem arising in the course of studying the stationary modes of performance of a one-dimensional tubular isothermal chemical reactor with longitudinal stirring. We write the problem in the following dimensionless form:

$$\frac{1}{P}\frac{d^2c}{dx^2}-\frac{dc}{dx}=\frac{1}{2\Gamma^2c},\quad 0\leqslant x\leqslant 1,\quad \Gamma=\frac{c_0}{\sqrt{2k}} \tag{1.1}$$

$$\frac{1}{P}\frac{dc}{dx}=c-1,\quad x=0;\quad \frac{dc}{dx}=0,\quad x=1$$

where $c(x)$ is the stationary distribution of concentrations along the reactor length, $c_0>0$ is the concentration of the reagent entering the reactor, $k>0$ is the kinetic constant and $P>0$ is the Peclet number. The right-hand side of (1.1) should contain a kinetic function describing the dependence of the chemical reaction rate on the concentration /1,2/. One of the characteristic features of this function is, that it vanishes at $c=0$. In the present case the right-hand side of (1.1) contains a function proportional to $1/c$. This function has a singularity at zero, but at large concentrations it approximates sufficiently well the kinetic function of the autocatalytic reaction /3,4/ on the segment of its monotonous decrease.

Below we obtain an exact solution for the problem (1.1) and draw a number of important conclusions concerning the existence and number of the solutions. Equation (1.1) is an Emden–Fowler type equation, which was already studied analytically in /5–7/. The exact solution of this equation obtained here has not, as far as we know, been obtained before.

Let us introduce a new independent variable and new unknown function

$$s=\frac{1+2\alpha}{2\alpha}[1-\exp(-Px)],\quad v=\sqrt{2}\,\gamma\frac{1+2\alpha(1-s)}{2\alpha}c$$

$$\alpha=[\exp(P)-1]/2,\ \gamma=\Gamma\sqrt{P}$$

In the v and s variables the problem (1.1) assumes the form

$$\frac{d^2v}{ds^2}=\frac{1}{v},\quad 0\leqslant s\leqslant 1;\quad \frac{dv}{ds}=-\sqrt{2}\,\gamma,\quad s=0;\quad \frac{dv}{ds}=-2\alpha v,\quad s=1 \tag{1.2}$$

Equation (1.2) allows lowering of the order. Assuming that the derivatives dc/dx and dv/ds cannot be positive (reagent concentration within the reactor cannot increase) and integrating the corresponding first order equation from 1 to s, we write the general solution of (1.2) in the form of the following quadrature:

$$\int\limits_{v(1)}^{v(s)}\frac{du}{\sqrt{\ln u+A}}=\sqrt{2}\,(1-s),\quad 0\leqslant s\leqslant 1 \tag{1.3}$$

where A and $v(1)$ are undetermined constants. Using the boundary conditions (1.2), we obtain

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$$A = \gamma^2 - \ln v(0) = 2\alpha^2 v^2(1) - \ln v(1) \tag{1.4}$$

The second equation of (1.4) gives the relation connecting constants A and $v(1)$. To find the constant $v(1)$ we put in (1.3) $s = 0$, and consider the first equation of (1.4). This yields

$$I(\gamma) - I(y) - \alpha \exp(y^2) / y = 0, \quad y = \sqrt{2}\alpha\, v(1) = \gamma c(1) \tag{1.5}$$

$$I(z) = \int_0^z \exp(u^2)\, du; \qquad I(z) = \frac{\exp(z^2)}{2z}(1 + o(1)), \quad z \to \infty$$

Solving simultaneously (1.3) and (1.5), we obtain the exact solution of problem (1.2), and the problem of existence and number of solutions reduces to that of analysing the transcendental equation (1.5).

2. Existence and number of solutions. Let us investigate the transcendental algebraic equation (1.5). Depending on the value of the parameters α and γ the equation either has no roots, or has two different roots on the interval $(0, \gamma)$, or has a single root

$$y = a, \quad a^2 = \alpha / (2\alpha + 1) \tag{2.1}$$

The latter follows from the condition that the derivative of the left-hand side of (1.5) vanishes. When $y = a$, equation (1.5) becomes

$$I(\Gamma\sqrt{P}) = I(a) + \alpha \exp(a^2) / a \tag{2.2}$$

Equation (2.2) determines single-valued the function $\Gamma = \Gamma^*(P)$. Its graph on the ΓP plane represents a critical curve separating the regions $\Gamma > \Gamma^*(P)$ in which two solutions of (1.5) exist (and hence two solutions of (1.2)) from $\Gamma < \Gamma^*(P)$ where there are no solutions at all. When $\Gamma = \Gamma^*(P)$, a solution of (1.5) and of (1.2) exists and is unique. We can obtain the asymptotic expressions for function $\Gamma^*(P)$. The computations yield

$$\Gamma^*(P) = \sqrt{2} - \frac{\sqrt{2}}{12} P + o(P), \quad P \to 0 \tag{2.3}$$

$$\Gamma^*(P) = 1 + \frac{1}{4}\frac{\ln P}{P} - \frac{1}{32}\frac{\ln^2 P}{P^2} + o\left(\frac{\ln^2 P}{P^2}\right), \quad P \to \infty$$

Equation (2.2) was solved numerically by expanding the integral $I(z)$ in terms of the Chebyshev polynomials /8/. The critical curve represents a smooth function decreasing monotonously from $\sqrt{2}$ at $P \to 0$ to 1 at $P \to \infty$. Next we obtain the asymptotic expressions for the roots of (1.5). In the case of a single root its exact value is given by (2.1). Let us consider the domain of existence of two solutions. Taking into account the fact that $c(1) = y / \gamma$, we obtain the following expressions at fixed Γ:

$$c_{1,2}(1) = \frac{1}{2\Gamma}(\Gamma \pm \sqrt{\Gamma^2 - 2}) + o(1), \quad P \to 0 \tag{2.4}$$

$$c_1(1) = \frac{\sqrt{\Gamma^2 - 1}}{\Gamma} + o(1), \quad c_2(1) = \exp[-P(\Gamma^2 - 1)](1 + o(1)), \quad P \to \infty \tag{2.5}$$

The expressions obtained are all meaningful, since by virtue of (2.3) the domain of existence of two solutions is $\Gamma > \sqrt{2}$ when $P \to 0$ and $\Gamma > 1$ when $P \to \infty$. From (1.4) we obtain the following expressions for $c(0)$ and $c(1)$: $c(0) = c(1)\exp\{P\Gamma^2[1 - c^2(1)] - P\}$. This yields the asymptotic expressions for $c(0)$, and computations yield

$$c_{1,2}(0) = c_{1,2}(1)(1 + o(1)), \quad P \to 0; \quad c_{1,2}(0) = 1 + o(1), \quad P \to \infty \tag{2.6}$$

The first expression in (2.6) means that the reagent concentration, in zero approximation with respect to P, remains constant throughout the reactor length (complete stirring). This fully agrees with the result of direct application of the method of regular expansions over the parameter $P \to 0$ /1,9/ to systems of the type (1.1). The second expression in (2.6) means that when $P \to \infty$ then we have $c(0) = 1$ (perfect displacement) in the reactor with longitudinal stirring.

The stationary modes obtained must be checked for stability. When $P \to 0$, we can show /1,2,10/ that the solution corresponding to $c_1(0)$ and $c_1(1)$ is stable, while the solution corresponding to $c_2(0)$ and $c_2(1)$ is unstable. It can be assumed that a similar situation obtains at any value of the Peclet number.

Fig.1 depicts the dependence of the concentration at the reactor entry and exit on the Peclet number for both modes, at various values of the parameter Γ. The solid curves represent the concentration at the reactor entry, and the dashed lines at the exit, for $\Gamma = 1.5$ (curves *1* correspond to the first mode, i.e. $c_1(0)$ and $c_1(1)$ and curves 2 to the second mode, i.e. to $c_2(0)$ and $c_2(1)$). The dot-dash line represents the concentation at the exit for $\Gamma = 1.25$. We see that at large P two different stationary modes exist (corresponding to the region lying above the critical curve). When $P \approx 2$, both modes merge into a single mode (point on the critical curve) and vanish altogether at smaller values of P (region below the critical curve). We can also obtain asymptotic expressions for the roots of (1.5) for the case $\Gamma \to \infty$ with fixed P. The computations yield

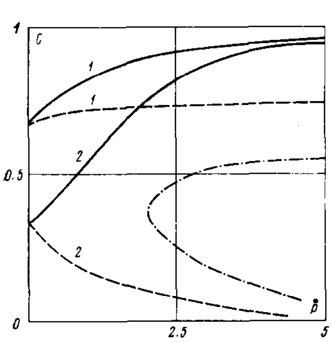

Fig.1

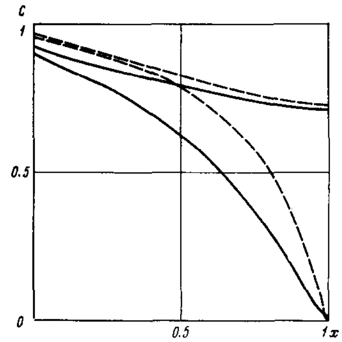

Fig.2

$$c_1(1) = 1 - \frac{1}{2\Gamma^2} + o\left(\frac{1}{\Gamma^2}\right), \quad \Gamma \to \infty \tag{2.7}$$

$$c_2(1) = [\exp(P) - 1] \exp(-\Gamma^2 P)(1 + o(1)),$$

$$\Gamma \to \infty$$

With the roots of equation(1.5) known and constant A obtained from (1.4), we can use the quadrature (1.3) to calculate the function $v(s)$ and hence obtain the stationary distribution of the concentration $c(x)$ along the reactor length.

Fig.2 depicts the results of numerical solution of the equations (1.5) and (1.3). Solid curves represent two stationary modes at $P = 3$, and the dashed lines at $P = 6$ (curves *1* correspond to the first mode, i.e. to $c_1(0)$ and $c_1(1)$ and curves *2* to the second mode, i.e. to $c_2(0)$ and $c_2(1)$). From (2.5) we see that when $P \to \infty$ (perfect displacement), two different stationary modes exist. However, if we pass to the limit as $P \to \infty$ in the initial problem (1.1), we lose one of the modes. This is caused by the fact that in this case such a passage is not always correct since the right-hand side of (1.1) has a singularity at the zero and one of the solutions obtained becomes discontinuous at the limit as $P \to \infty$. The function appearing in the right-hand side of (1.1) is proportional to $1/c$. We note that the substitution $c \to c + \beta$ leads to a more general case, with all results obtained above still valid.

3. Asymptotic analysis. Below we use the regular and singular perturbation methods to construct the asymptotic solutions of the problem (1.1) for the case of $P \to \infty$ at fixed Γ and of $\Gamma \to \infty$ at fixed P. The validity of these methods in the present case can be established by comparing the asymptotic solutions obtained, with the exact solutions obtained above. First we consider the case of $\Gamma \to \infty$ (P fixed). One of the solutions can be constructed using the method of direct (regular) expansions /11/ assuming that the right-hand side of (1.1) is always small. Writing the solution sought in the form of a power series in small parameter $1/\Gamma$, substituting this expansion into (1.1) and passing to the appropriate limit, we obtain the coefficients of the expansion. At $x = 1$ the solution obtained coincides with the first root of (2.7). In the case when the right-hand side of (1.1) cannot be neglected, we can use the expansion method of asymptotic matching /11,12/ to construct the second solution of (1.1). In the outer region $0 \leqslant x < 1$ we neglect the reaction. Taking into account the left boundary condition and replacing the right condition by $c(x) \to 0$ we obtain, as $x \to 1$ (near the reactor exit the reaction must play a significant part)

$$c(x) = 1 - \exp[P(x-1)] \tag{3.1}$$

In the inner region $1 - \delta < x \leqslant 1$ we introduce, near the reactor exit, a new variable $z = (1-x)/\delta$, where $\delta = \delta(\Gamma)$ is a small parameter to be defined later. We seek the solution in the form

$$c(z) = f(\Gamma) u(z)(1 + o(1)) \tag{3.2}$$

Let us now pass in (1.1) from the variable x to the variable z. Substituting into it the expansion (3.2) we obtain $f(\Gamma) = \delta(\Gamma)/\Gamma$, and for $u(z)$ we have the problem

$$\frac{d^2u}{dz^2} = \frac{P}{2u}; \quad \frac{du}{dz}(0) = 0 \tag{3.3}$$

solution of this problem with $z \to \infty$ has the form

$$u(z) = \sqrt{P}\, z \left[\sqrt{\ln z} + \frac{1}{4} \frac{\ln \ln z}{\sqrt{\ln z}} (1 + o(1))\right]$$

Substituting $f(\Gamma)$ and $u(z)$ obtained into the expansion (3.2) and matching it at $z \to \infty$ with the expansion (3.1) where $x \to 1$, we obtain the following equation for $\delta(\Gamma)$:

$$\Gamma \sqrt{P} = \rho(\delta); \quad \rho(\delta) = \sqrt{\omega} + \frac{1}{4} \frac{\ln \omega}{\sqrt{\omega}} (1 + o(1)), \quad \omega = -\ln \delta \tag{3.4}$$

Its solution yields $\delta(\Gamma) = \Gamma(\exp(-P\Gamma^2)$ which agrees with the second root of (2.7).

Let us now construct asymptotic solutions of the problem (1.1) with $P \to \infty$ and Γ fixed. In this case we have a singular problem for both solutions /12/ and the method of regular expansions cannot be used. We shall use therefore once again the method of matching asymptotic expansions. We seek the solution in the outer region $0 \leqslant x < 1$ in the form of a series $c(x) = y_0(x) + y_1(x)/P + o(1/P)$. Computing the functions y_0 and y_1 we obtain a solution, which does not satisfy the right boundary condition. To satisfy this condition we consider the boundary layer $1-1/P < x \leqslant 1$, near the point $x = 1$, introducing a new variable $\xi = P(1-x)$ and seeking the solution in the form $c(\xi) = c_0(\xi) + c_1(\xi)/P + o(1/P)$. Calculating the function c_0 and matching $c_0(\xi)$ at $\xi \to \infty$ with $y_0(x)$ at $x \to 1$, we obtain at the reactor exit a value coinciding with the first root of (2.5).

Let us construct a solution corresponding to the second root. The solution corresponds to the case in which the chemical reaction cannot be neglected. Instead of the right boundary condition we impose on $c_0(\xi)$ the condition that $c_0(\xi) \to 0$ as $\xi \to 0$. Computations and matching with $y_0(x)$ yield

$$c_0(\xi) = \sqrt{1 - \frac{1}{\Gamma^2}}\,[1 - \exp(-\xi)] \tag{3.5}$$

To satisfy the right boundary condition we introduce another boundary layer $1 - \varepsilon < x \leqslant 1$ lying inside the first boundary layer near the point $x = 1$. Here $\varepsilon = \varepsilon(P)$ is a small parameter to be defined below. We introduce a new variable $\tau = (1-x)/\varepsilon$ within the second layer and seek the solution in the form

$$c(\tau) = g(P)\omega(\tau)(1 + o(1)) \tag{3.6}$$

Now we pass in problem (1.1) from the variable x to the variable τ and substitute into the resulting expression the expansion(3.6). This yields $g(P) = \varepsilon(P)\sqrt{P}$ and for $\omega(\tau)$ we have the following problem:

$$\frac{d^2w}{d\tau^2} = \frac{1}{2\Gamma^2 w}, \qquad \frac{dw}{d\tau}(0) = 0 \tag{3.7}$$

Solution of the problem with $\tau \to \infty$ is analogous to the solution of (3.3) with $z \to \infty$. Substituting this solution and function $g(P)$ obtained,into the expansion (3.6) and matching it at $\tau \to \infty$ with the expansion (3.5) we obtain, as $\xi \to 0$, for $\varepsilon(P)$ the equation $\sqrt{P(\Gamma^2 - 1)} = \rho(\varepsilon)$ where ρ is a function of a small parameter defined by (3.4). Solving this equation we obtain

$$\varepsilon(P) = \frac{1}{\sqrt{P}} \exp[-P(\Gamma^2 - 1)]$$

which agrees with the second root of (2.5).

Thus the asymptotic solutions of (1.1) constructed here agree with the exact solutions. This confirms the applicability of the asymptotic methods discussed here to solving approximately nonlinear boundary value problems in the case when the exact solution is not known.

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REFERENCES

1. ARIS R., Analysis of the Processes in Chemical Reactors. Moscow, Khimiia, 1967.
2. PERLMUTTER D.D., Stability of Chemical Reactors. New York, Prentice Hall, 1972.
3. EMANUEL' N.M. and KNOPPE D.T., Course in Chemical Kinetics. Moscow, Vysshaia shkola, 1974.
4. MATSUURA T. and KATO M., Concentration stability of the isothermal reactor. Chem. Engng. Sci. Vol.22, 1967.
5. BELLMAN R., Stability Theory of Differential Equations Solution.New York, McGraw-Hill,1953.
6. SANSONE G., Ordinary Differential Equations. Moscow, Izd-vo inostr. lit. 1954.(translated from Italian).
7. KAMKE E., Differentialgleichungen, Leipzig, 1959.
8. LUKE Y.L., The Special Functions and their Approximation. New York, Academic Press, 1969.
9. COHEN D., Multiple solutions and periodic oscillations in nonlinear diffusion processes. J. SIAM Appl. Math. Vol.25, No.4, 1973.
10. VOL'TER B.V. and SAL'NIKOV I.V., Stability of the Modes of Chemical Reactor Performance. Moscow, KHIMIIA, 1981.
11. NAYFEH A.H., Perturbation Methods. New York, London, Wiley, 1973.
12. COLE J.D., Perturbation Methods in Applied Mathematics. Waltham, Mass. Blaisdell Publ. Co. 1968.

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