

CALCULATING THE CROSS-SECTIONAL TEMPERATURE
PROFILE OF A TUBULAR REACTOR WITH RADIATIVE HEATING

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The cross-sectional temperature profile of a tubular reactor with radiative heating is calculated analytically.

The design of high-temperature chemical reactors is a difficult problem and has not yet been definitively solved to this very day. Essential for calculating the diameter of a reactor tube is the knowledge of the temperature profile across the tube.

Under conditions of variable thermal conductivity and uniform irradiation of the lateral surface, the authors attempt here to establish the relation between temperature and tube radius in the case of hydrocarbons undergoing pyrolysis. Hydrocarbons undergo pyrolysis at high values of the Reynolds number, i.e., under turbulence conditions. In view of this, determining the temperature-dependence is closely involved with selecting the proper coefficient of turbulent viscosity. We have made the choice on the basis of published data [1-10] and assume a radial viscosity profile most closely corresponding to the given process.

An analytical solution to the problem is found by dividing the total stream into a laminar sublayer and a mainstream region, both transfer mechanisms being operative in the latter. The two solutions, separate for each region, and then smoothly coupled at the edge of the laminar sublayer into a single solution for the entire tube.

The cross-sectional temperature profile of a tube is defined by the equation

$$\frac{1}{r} \cdot \frac{d}{dr} \left(\lambda(r) r \frac{dT}{dr} \right) + q_p k f(c) = 0. \quad (1)$$

The process of hydrocarbon pyrolysis is essentially a first-order reaction [11-15] with heat absorption, i.e., here

$$q_p = -|q_p|, \quad k f(c) = kv. \quad (2)$$

The temperature-dependence of the coefficient of the reaction rate is determined according to the Arrhenius equation

$$k = k_0 \exp(-E/RT), \quad k_0 = \text{const.} \quad (3)$$

We factorize the exponent as in [16], i.e.,

$$\exp(-E/RT) \approx \exp(-E/RT_0) \exp(E(T - T_0)/RT_0^2), \quad (4)$$

with T_0 denoting the temperature near which the reaction occurs. We then change to dimensionless variables

$$\Theta = E(T - T_0)/RT_0^2, \quad x = r/R_{TP}, \quad \lambda_1 = \lambda/\lambda_0, \quad (5)$$

and then, with the aid of (2)-(5), Eq. (1) yields

$$\frac{1}{x} \cdot \frac{d}{dx} \left(\lambda_1(x) x \frac{d\Theta}{dx} \right) = \frac{\delta}{\lambda_0} \exp \Theta, \quad (6)$$

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where

$$\delta = |q_p| c k_0 R_t^2 E \exp(-E/RT_0)/RT_0^2.$$

We next formulate the boundary conditions. Assuming a linear temperature profile in the tube wall* and considering that the reactant mixture is heated radiatively, we have

$$\frac{\lambda_0 RT_0^2}{E} \cdot \frac{d\Theta}{dx} \Big|_{x=1} = -\alpha R_t \left\{ \left[\frac{RT_0^2}{E} \left(\frac{\lambda_0 \delta_w}{\lambda_w R_t} \cdot \frac{d\Theta}{dx} \Big|_{x=1} + \Theta \Big|_{x=1} \right) + T_0 \right]^4 - T_\infty^4 \right\}. \quad (7)$$

The other boundary condition is the condition of a finite Θ at the tube axis.

The thermal conductivity $\lambda_1(x)$ consists of the molecular component and the turbulent component, the latter being calculated from the coefficient of turbulent viscosity according to [2, 3]. In dimensionless form $\lambda_1(x)$ is

$$\lambda_1(x) = \begin{cases} 1 + a_1 x(\alpha - x), & 0 \leq x \leq \alpha, \\ 1, & \alpha \leq x \leq 1, \end{cases}$$

where $\alpha = 1 - \delta_0/R_t$, δ_0 denotes the thickness of the laminar sublayer, and constant a_1 depends on the process characteristics.

Since this is the form of function $\lambda_1(x)$, it is logical to solve the problem for two regions: the laminar sublayer (I) and the remaining region (II) where both transfer mechanisms are operative, whereupon to couple both solutions smoothly at the edge of the laminar sublayer.

I. $\alpha \leq x \leq 1$, $\lambda_1(x) \approx 1$ and Eq. (6) becomes

$$\frac{1}{x} \cdot \frac{d}{dx} \left(x \frac{d\Theta}{dx} \right) = \frac{\delta}{\lambda_0} \exp \Theta. \quad (8)$$

For (8) we find two solutions, by a substitution proposed in [16], but one of them can be shown not to yield a smooth overall solution for the entire tube and, therefore, must be discarded. Finally, for the dimensionless temperature Θ in the laminar sublayer we have the following expression

$$\Theta = \ln \frac{4c_1^{(n)} x \sqrt{\frac{2\delta c_1^{(n)}}{\lambda_0}}^{-2} \exp(c_2^{(n)} \sqrt{c_1^{(n)}})}{\left[1 - x \sqrt{\frac{2\delta c_1^{(n)}}{\lambda_0}} \exp(c_2^{(n)} \sqrt{c_1^{(n)}}) \right]^2}, \quad (9)$$

where constants $c_1^{(n)}$ and $c_2^{(n)}$ are yet to be defined.

II. $0 \leq x \leq \alpha$. Within this region we must solve Eq. (6). The solution can be found by the method of successive approximations. The right-hand side of the first approximation is assumed equal to zero, equivalent to the absence of any reaction. For this case, considering that Θ must be finite at the axis, we have

$$\Theta_1 = c_4^{(1)} = \text{const.} \quad (10)$$

We next smoothly couple Θ_1 with (9), which together with the boundary condition at the tube wall (7) yields a system of equations for determining the constants $c_1^{(1)}$, $c_2^{(1)}$, and $c_4^{(1)}$. Proving the existence of a solution to this system reduces to proving the existence of a solution to a transcendental equation which, as has turned out, is of the form in every approximation:

$$\begin{aligned} & -\frac{\lambda_0 RT_0^2}{E \alpha R_t} \left[\frac{\alpha^{x_n} (b_n + x_n) (x_n - 2) + (b_n - x_n) (x_n + 2)}{\alpha^{x_n} (b_n + x_n) + (x_n - b_n)} \right] + T_\infty^4 = \left[\frac{RT_0^2}{E} \left(\frac{\lambda_0 \delta_w}{\lambda_w R_t} \right. \right. \\ & \times \left. \frac{\alpha^{x_n} (b_n + x_n) (x_n - 2) + (b_n - x_n) (x_n + 2)}{\alpha^{x_n} (b_n + x_n) + (x_n - b_n)} + \ln \left(\frac{2\lambda_0}{\delta} \frac{x_n^2 \alpha^{x_n} (b_n^2 - x_n^2)}{[\alpha^{x_n} (b_n + x_n) + (x_n - b_n)]^2} \right) \right) + T_0 \left. \right]^4, \quad (11) \end{aligned}$$

where

$$x_n = \sqrt{\frac{2\delta c_1^{(n)}}{\lambda_0}}, \quad b_n = 2 + \alpha \frac{d\Theta_n}{dx} \Big|_{x=\alpha}, \quad (12)$$

* This is permissible, because the curvature of the tube wall may be disregarded.



Fig. 1. Radial temperature profile of a reactor tube: obtained analytically (solid curve) and in an electrolytic trough (dashed curve).

and n is the order of the approximation. This equation is solved graphically. It apparently always has a solution, if the condition

$$\frac{RT_0^2}{E\kappa R_t} \left[\frac{2(b_n - 2) + 2b_n |\ln \alpha|}{2 - b_n |\ln \alpha|} \right] + T_\infty^4 > 0 \quad (13)$$

is satisfied.

This criterion is valid for the given process. An evaluation of x_n leads to absurd results. For further calculations, therefore, we let $x_n = 0$ and thus obtain the closest approximation solution to Eq. (11). Such a choice of x_n is justified by the feasibility of following it up with an exact solution to this equation and with a smooth overall solution for the entire tube.

The second approximation yields a logarithmic temperature profile:

$$\Theta_2 = \alpha_1 \ln |x - p_1| + \alpha_2 \ln |x - p_2| + c_4^{(2)},$$

where constants α_1 , α_2 , p_1 , and p_2 characterize the process.

For the succeeding approximations we take into account the smallness of the coefficients in the logarithmic terms (α_1 and α_2). The calculation here is analogous, only the values of α_1 and α_2 are different.

The feasibility of an exact solution to Eq. (11) depends on the value of parameter b_n , which in fact characterizes the gradient $d\Theta_n/dx$ at the edge of the laminar sublayer. Considering the recurrence relation between b_n , b_{n-1} , b_{n-2} as well as the relation between these parameters and the coefficients in the expression for Θ_{n-1} , we find that the solution will be exact for b_7 . Knowing b_7 , we find x_7 from (11) and with it all other constants, i.e., we obtain the following temperature profile of the mainstream:

$$\Theta = \alpha_1 \ln |x - p_1| + \alpha_2 \ln |x - p_2| + \alpha_3 x + c_4^{(7)},$$

where α_1 is the determining coefficient. The calculation cannot be continued further by this method, since α_1 becomes now sufficiently large (as a result of a sudden jump in b_n).

The analytical solution obtained here implies an appreciable temperature drop along the radius of a reactor tube (about 75°C), which agrees with the result obtained in an electrolytic trough [18], but this temperature drop is not uniform: about 25-30°C across the thermal sublayer, although the latter is only approximately $2 \cdot 10^{-4}$ m thick in a tube of radius $R_t = 6.2 \cdot 10^{-2}$ m.

It is to be noted that four fifths of the total temperature drop (about 60°C) occurs along one tenth of the radius, while the remaining temperature drop (about 15°C) occurs along the rest of the radius.

Temperature profiles obtained analytically and in an electrolytic trough are shown in Fig. 1.

Evidently, the electrolytic trough yielded a value for the temperature difference within the mainstream which was too high, because the thermal conductivity there had been simulated [18] on the basis of its mean values.

NOTATION

r	is the radius of any point from the center;
T	is the temperature;
q_p	is the total molar heat of reaction;
E	is the activation energy;
T_∞	is the temperature of the heating gases;
δ_w	is the thickness of the tube wall;
R_t	is the tube radius;
λ_0	is the molecular component of thermal conductivity;
λ_w	is the thermal conductivity of the wall material;
R	is the universal gas constant;
κ	is the Stefan-Boltzmann constant.

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