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Research Article

Analytical Solution of Non-Isothermal Diffusion-Reaction Processes and Effectiveness Factors

Vembu Ananthaswamy and Lakshmanan Rajendran

Department of Mathematics, The Madura College, TamilNadu, Madurai 625011, India

Correspondence should be addressed to Lakshmanan Rajendran; raj_sms@rediffmail.com

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The mathematical modeling of nonlinear boundary value problems in catalytically chemical reactor is discussed. In this paper, we obtain the approximate analytical solution and the effectiveness factors for the evolution of single-step transformations under non-isothermal conditions using homotopy perturbation method. We have applied it to many reaction models and obtained very simple analytical expressions for the shape of the corresponding transformation rate peaks. These analytical solutions represent a significant simplification of the system's description allowing easy curve fitting to experiment. The accuracy achieved with our method is checked against several reaction models and numerical results. A satisfactory agreement is noted.

1. Introduction

Non-isothermal systems, where reaction and diffusion take place, are typical in the chemical process industry [1] and also in biological systems [2–4]. The chemical reaction is always central in these systems, because the rate of the reaction often will determine how fast chemicals can be produced. A high rate can be realized when the reaction is far from equilibrium. But an operation far from equilibrium is also an operation in which the energy dissipation is large. With the present interest to save valuable resources, chemical reactors should be studied also from the perspective of obtaining a more energy-efficient operation, in addition to maintaining the production of chemicals. In biological systems, one may expect that energy efficiency is an issue of survival, especially under harsh conditions [5]. In such cases and probably many others, a thermodynamic description will be important to understand the transport phenomena involved [4, 6]. Studies of minimum energy dissipation start with an expression for the entropy production [7–9].

Chemical reactions are inherently non-linear processes, and are most successfully described in the field of reaction kinetics by the law of mass action [10, 11]. The reaction rate is not commonly expressed as a function of the reaction Gibbs energy. This is not surprising, because classical non-equilibrium thermodynamics [12, 13] assumes a linear relation between these two variables, and experimental evidence indicates that this is only correct very close to chemical equilibrium. The first to address this problem successfully was Kramers [14] who described the reaction as a diffusion process along a reaction coordinate.

The extension in the context of non-equilibrium thermodynamics was first proposed by Prigogine and Mazur [15–17]. By integrating over these variables to obtain the thermodynamic level, one can describe several phenomena, which are non-linear on the macroscopic level, and which retain a linear force-flux relation on the mesocopic level. This applies not only to chemical reactions [18], but for instance also to adsorption [19], nucleation [20], electrode over potentials [21] and active transport in biology [4]. The number of cases studied is now growing fast. The coupling of chemical reactions to other processes is then important [8, 18, 22–25]. Non-equilibrium thermodynamics is not only a theory for transport processes, it is also a theory for fluctuations. It has been demonstrated that the fluctuating contributions to the thermodynamic fluxes in a non-equilibrium system satisfy the fluctuation-dissipation theorem just like they do in equilibrium [26].

The theory of non-equilibrium thermodynamics is based on the assumption of local thermodynamic equilibrium. The validity of this assumption has been established by molecular dynamics simulations in several cases [27–29]. Fluctuations and the resulting correlation functions away from equilibrium were then not considered. One of the major findings has been that although local equilibrium is valid for the description of the mean values of thermodynamic fields, it is no longer valid for the description of the fluctuations around their average non-equilibrium values [26]. Recently Vergara et al. [30] developed the multicomponent diffusion system including cross-term diffusion coefficients relating to flux of the component i to concentration gradients of component j. But in our problem the cross-diffusion is neglected. Ikeda et al. [31] analyzed this problem for a reaction-diffusion problem with a temperature gradient using a linear approximation for the description of the reaction. For the reaction-diffusion problem the assumption of local equilibrium has to be extended to be valid also along the reaction coordinate. However, to the best of our knowledge, till date no general analytical expressions of mass concentrations and effectiveness factors have been reported. The purpose of this communication is to derive the approximate analytical expression of mass concentration for planar particles by solving the non-linear differential equations using He's homotopy perturbation method [32–35].

2. Mathematical Formulation of the Problem and Analysis

The mathematical description of a catalytic chemical reactor $(m, q) : mA + qB \rightarrow P$ is given by [1]

$$\frac{d^2u}{dx^2} - \phi^2 f(u) = 0 \quad \text{for } 0 < x < L,$$
$$u = 1 \quad \text{at } x = L, \qquad \frac{du}{dx} = 0 \quad \text{at } x = 0, \tag{1}$$

where x is the spatial coordinate, $f(u)$ is the reaction rate function (which is non-linear), and L is the half thickness of porous slab (m). The mass concentration u is defined as the following function:

$$u = \frac{C_A}{C_{\mathrm{AS}}}, \tag{2}$$

where C_A is the volumetric molar concentration of the key component A, C_{AS} is the surface value of the key component A, and ϕ is the corresponding Thiele modulus which is defined as follows:

$$\phi = \sqrt{\frac{L^2 k_S C_{\mathrm{AS}}^{m-1} C_{\mathrm{BS}}^{p}}{D_A}}. \tag{3}$$

Here k_S, D_A, and C_{BS} are the specific kinetic constant, effective diffusivity coefficient, and the dimensionless concentration of the component B, respectively. Also the temperature T and the mass concentration u are no longer independent, which satisfies the following relation:

$$T = d(1 - u) + 1, \tag{4}$$

where d is the thermicity of the reaction and is defined as follows:

$$d = \frac{D_A C_{\mathrm{AS}} (-\Delta H)}{k T_S}. \tag{5}$$

Here $-\Delta H$ is the reaction heat; k is the effective thermal conductivity inside the porous slab; and T_S is the dimensional temperature at the external pellet surface. $\Delta H/T_S$ represents the entropy change "ΔS" of a system under this process. Entropy increases in all spontaneous processes. Hence entropy may be regarded as a measure of disorder or randomness of the molecules of the system. For isothermal process, the entropy changes of the universe during a reversible process are zero. The entropy of the universe increases in an irreversible process. The parameter d represents the deviation from isothermal conditions, being $d < 0$ and $d > 0$ for endothermic and exothermic reactions, respectively. Now the dimensionless reaction rate function $f(u)$ including (1) is given by

$$f(u) = u^{m+q} \exp\left[\frac{c(1-u)}{d(1-u)+1}\right], \tag{6}$$

where the parameter c is defined as follows:

$$c = \gamma \cdot d, \tag{7}$$

where γ is the Arrhenius group and is defined as

$$\gamma = \frac{E}{R T_S}. \tag{8}$$

Here E denotes the activation energy; R is the universal gas constant. Hence the corresponding non-linear boundary value problem is given by

$$\frac{d^2u}{dx^2} - \phi^2 u^{m+q} \exp\left[\frac{c(1-u)}{d(1-u)+1}\right] = 0 \quad \text{for } 0 < x < L,$$
$$u = 1 \quad \text{for } x = L, \qquad \frac{du}{dx} = 0 \quad \text{for } x = 0. \tag{9}$$

Using the following dimensionless variables:

$$z = 1 - \frac{x}{L}, \qquad y = 1 - u. \tag{10}$$

Now (9) becomes in dimensionless form as follows:

$$\frac{d^2y}{dz^2} - \phi^2 (1-y)^{m+q} \exp\left[\frac{cy}{dy+1}\right] = 0 \quad \text{for } 0 < z < 1, \tag{11}$$

$$y = 0 \quad \text{for } z = 0, \qquad \frac{dy}{dz} = 0 \quad \text{for } z = 1. \tag{12}$$

The internal effectiveness factor (η) is a measure of the relative importance of diffusion to reaction limitations. That is,

$$\eta \equiv \frac{\text{actual overall reaction rate}}{\text{rate if entire surface were exposed to } C_{\mathrm{AS}}, T_S}. \tag{13}$$

The effectiveness factor for the heterogeneous chemical reaction is [22–26]

$$\eta = \frac{1}{\phi^2}\left[\frac{dy}{dz}\right]_{z=0}. \tag{14}$$

3. Solution of Boundary Value Problem Using HPM

Recently, many authors have applied the homotopy perturbation method (HPM) to solve the non-linear problems in physics and engineering sciences [36–39]. Recently this method is also used to solve some of the non-linear problem in physical sciences [32–34]. This method is a combination of homotopy in topology and classic perturbation techniques. He used to solve the Lighthill equation [32], the Diffusion equation [33], and the Blasius equation [34, 35]. The HPM is unique in its applicability, accuracy and efficiency. The HPM uses the imbedding parameter p as a small parameter, and only a few iterations are needed to search for an asymptotic solution. Using this method, we can obtain the following solution to (11) and (12) for the following three cases (see Appendices A–C):

Case 1. When the reaction orders $q = 0$ and $m = 0$, the analytical solution of (11) to (12) using homotopy perturbation method [35, 40–44] is

$$\begin{aligned} y(z) = {} & \left[\frac{d\left(3+\tan^2(k)\right)}{2c^2} - \frac{1}{c}\right] + \left[\frac{1}{c} + k_1\right]\cos(kz) \\ & + \left[\frac{\tan(k)}{c} + k_2\right](\sin(kz)) \\ & - \left[\frac{\phi^2 d\left(\left(1-\tan^2(k)\right)\cos(2kz) + 2\tan(k)\sin(2kz)\right)}{6ck^2}\right] \\ & + \left[\frac{\phi^2 d\left(\tan(k)\, z\cos(kz) - z\sin(kz)\right)}{kc}\right], \end{aligned} \tag{15}$$

where

$$k = \phi\sqrt{c}, \tag{16}$$

$$k_1 = \left[\frac{\phi^2 d\left(1-\tan^2(k)\right)}{6ck^2}\right] - \left[\frac{d\left(3+\tan^2(k)\right)}{2c^2}\right], \tag{17}$$

$$\begin{aligned} k_2 = {} & \frac{1}{k\cos(k)}\left\{\left[kk_1\sin(k)\right] - \left(\frac{\phi^2 d}{3ck}\right)\right. \\ & \times\left[\left(1-\tan^2(k)\right)\sin(2k)\right. \\ & \left.\left. -2\tan(k)\cos(2k)\right] \right. \\ & - \left(\frac{\phi^2 d}{kc}\right)\left[\tan(k)\left(\cos(k) - k\sin(k)\right)\right. \\ & \left.\left. -\left(\sin(k) + k\cos(k)\right)\right]\right\}, \end{aligned} \tag{18}$$

provided $c \neq 0$. Using (14), the effectiveness factor η is given by

$$\begin{aligned} \eta = {} & \left[\frac{\sin\left(a\sqrt{c}\right)}{a\sqrt{c}\cos\left(a\sqrt{c}\right)}\right] - \left[\frac{d\sin\left(a\sqrt{c}\right)}{ac^{3/2}\cos\left(a\sqrt{c}\right)}\right] \\ & - \left[\frac{2d\sin\left(a\sqrt{c}\right)}{3ac^{3/2}\cos^3\left(a\sqrt{c}\right)}\right] + \left[\frac{d}{a\cos^2\left(a\sqrt{c}\right)}\right]. \end{aligned} \tag{19}$$

Case 2. When the reaction orders $q = 0$ and $m = 1$, we can obtain the analytical solution of (11) to (12) using homotopy perturbation method as follows:

$$\begin{aligned} y(z) = {} & \left[\frac{(c+cd)\left(3+\tan^2(a)\right)}{2(c-1)^3} - \frac{1}{(c-1)}\right] \\ & + \left[\frac{1}{(c-1)} + a_1\right](\cos(az)) + \left[\frac{\tan(a)}{(c-1)} + a_2\right](\sin(az)) \\ & - \left[\frac{\phi^2(c+cd)\left(\left(1-\tan^2(a)\right)\cos(2az) + 2\tan(a)\sin(2az)\right)}{6a^2(c-1)^2}\right] \\ & + \left[\frac{\phi^2(c+cd)\left(\tan(a)\, z\cos(az) - z\sin(az)\right)}{a(c-1)^2}\right], \end{aligned} \tag{20}$$

where

$$a = \phi\sqrt{c-1}, \tag{21}$$

$$\begin{aligned} a_1 = {} & \left[\frac{\phi^2(c+cd)\left(1-\tan^2(a)\right)}{6a^2(c-1)^2}\right] \\ & - \left[\frac{(c+cd)\left(3+\tan^2(a)\right)}{2(c-1)^3}\right], \end{aligned} \tag{22}$$

$$\begin{aligned} a_2 = {} & \frac{1}{a\cos(a)}\left\{\left(aa_1\sin(a)\right) - \left(\frac{\phi^2(c+cd)}{3a(c-1)^2}\right)\right. \\ & \times\left[\left(1-\tan^2(a)\right)\sin(2a) - 2\tan(a)\cos(2a)\right] \\ & + \left(\frac{\phi^2(c+cd)}{a(c-1)^2}\right)\left[\tan(a)\left(\cos(a) - a\sin(a)\right)\right. \\ & \left.\left. -\left(\sin(a) + a\cos(a)\right)\right]\right\}, \end{aligned} \tag{23}$$

provided $c \neq 1$. Using (14), the effectiveness factor η is given by

$$\begin{aligned} \eta = {} & \left[\frac{c^2\sin\left(a\sqrt{c-1}\right)}{a\cos\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right] \\ & + \left[\frac{cd\sin\left(a\sqrt{c}\right)}{(c-1)^2\cos^2\left(a\sqrt{c-1}\right)}\right] \\ & - \left[\frac{2cd\sin\left(a\sqrt{c-1}\right)}{3a(c-1)^{5/2}\cos^3\left(a\sqrt{c-1}\right)}\right] \end{aligned}$$

$$
\begin{aligned}
&- \left[\frac{2c\sin\left(a\sqrt{c-1}\right)}{3a\cos^3\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right] \\
&- \left[\frac{cd\sin\left(a\sqrt{c-1}\right)}{3a\cos\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right] \\
&- \left[\frac{7c\sin\left(a\sqrt{c-1}\right)}{3a\cos\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right] \\
&+ \left[\frac{c}{\cos^2\left(a\sqrt{c-1}\right)(c-1)^2}\right] \\
&+ \left[\frac{\sin\left(a\sqrt{c-1}\right)}{a\cos\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right].
\end{aligned} \tag{24}
$$

Case 3. When the reaction orders $q = 1$ and $m = 1$, the analytical solution of (11) to (12) using the homotopy perturbation method is given by

$$
\begin{aligned}
y(z) = &\left[\frac{(cd+2c-1)\left(3+\tan^2(b)\right)}{2(c-2)^3} - \frac{1}{(c-2)}\right] \\
&+ \left[\frac{1}{(c-2)} + b_1\right](\cos(bz)) \\
&- \left[\frac{\phi^2(cd+2c-1)\left(\left(1-\tan^2(b)\right)\cos(2bz)+2\tan(b)\sin(2bz)\right)}{6b^2(c-2)^2}\right] \\
&+ \left[\frac{\phi^2(cd+2c-1)(\tan(b)\,z\cos(bz)-z\sin(bz))}{b(c-2)^2}\right] \\
&+ \left[\frac{\tan(b)}{(c-2)} + b_2\right](\sin(bz)),
\end{aligned} \tag{25}
$$

$$
b = \phi\sqrt{c-2}, \tag{26}
$$

$$
\begin{aligned}
b_1 = &\left[\frac{\phi^2(cd+2c-1)\left(1-\tan^2(b)\right)}{6b^2(c-2)^2}\right] \\
&- \left[\frac{(cd+2c-1)\left(3+\tan^2(b)\right)}{2(c-2)^3}\right],
\end{aligned} \tag{27}
$$

$$
\begin{aligned}
b_2 = &\left(\frac{1}{b\cos(b)}\right)\left\{bb_1\sin(b) - \left[\frac{\phi^2(cd+2c-1)}{3b(c-2)^2}\right]\right. \\
&\times\left(\left(1-\tan^2(b)\right)\sin(2b)\right. \\
&\left.-2\tan(b)\cos(2b)\right) \\
&+ \left[\frac{\phi^2(cd+2c-1)}{b(c-2)^2}\right] \\
&\times(\tan(b)(\cos(b) - b\sin(b)) \\
&\left.-(\sin(b)+b\cos(b)))\right\}.
\end{aligned} \tag{28}
$$

The above expression is valid only if $c \neq 2$. Using (14), the effectiveness factor η is given by

$$
\begin{aligned}
\eta = &\left[\frac{c^2\sin\left(a\sqrt{c-2}\right)}{a\cos\left(a\sqrt{c-2}\right)(c-2)^{5/2}}\right] \\
&+ \left[\frac{cd\sin\left(a\sqrt{c}\right)}{(c-2)^2\cos^2\left(a\sqrt{c-2}\right)}\right] \\
&- \left[\frac{2cd\sin\left(a\sqrt{c-2}\right)}{3a(c-2)^{5/2}\cos^3\left(a\sqrt{c-2}\right)}\right] \\
&- \left[\frac{4c\sin\left(a\sqrt{c-2}\right)}{3a\cos^3\left(a\sqrt{c-2}\right)(c-2)^{5/2}}\right] \\
&- \left[\frac{cd\sin\left(a\sqrt{c-2}\right)}{3a\cos\left(a\sqrt{c-2}\right)(c-2)^{5/2}}\right] \\
&- \left[\frac{14c\sin\left(a\sqrt{c-2}\right)}{3a\cos\left(a\sqrt{c-2}\right)(c-2)^{5/2}}\right] \\
&+ \left[\frac{2c}{\cos^2\left(a\sqrt{c-2}\right)(c-2)^2}\right] \\
&+ \left[\frac{13\sin\left(a\sqrt{c-2}\right)}{3a\cos\left(a\sqrt{c-1}\right)(c-1)^{5/2}}\right] \\
&+ \left[\frac{2\sin\left(a\sqrt{c-2}\right)}{3a\cos\left(a\sqrt{c-2}\right)(c-2)^{5/2}}\right] \\
&- \left[\frac{1}{\cos^2\left(a\sqrt{c-2}\right)(c-2)^2}\right].
\end{aligned} \tag{29}
$$

4. Numerical Simulation

The non-linear equations (11) to (12) for the five cases are solved by numerical methods. The function pdex4, in Matlab software, is used to solve two-point boundary value problems (BVPs) for ordinary differential equations which are given in Appendices D–H. In Tables 1, 2, 3, 4, and 5, the numerical results are also compared with the obtained analytical expressions (see (15), (20), and (25)) and Villa et al. [1] results for some fixed value of $\phi = 0.5$.

5. Results and Discussions

Tables 1–5 represent the dimensionless mass concentration $y(z)$ versus the dimensionless spatial coordinate z for the following different values of the dimensionless parameters c and d:

(i) when $m = 0$, $q = 0$, $\phi = 0.5$, $c > 0$, and $d > 0$.

(ii) when $m = 0$, $q = 0$, $\phi = 0.5$, $c < 0$, and $d < 0$.

Table 1: Comparison of our analytical expression of concentration profiles $y(z)$ with numerical results and Villa et al. [1] results corresponding to Case 1, for $m = 0$, $q = 0$, and $\phi = 0.5$, when $c > 0$ and $d > 0$.

c	d			Dimensionless spatial coordinate z				
				0.0	0.25	0.5	0.75	1.00
2.5	0.5	$y(z)$	Numerical	0.000000	0.073340	0.128200	0.162200	0.173700
			Analytical (15)	0.000000	0.070005	0.121817	0.153614	0.164329
			Villa et al. [1]	0.000000	0.074132	0.129628	0.164013	0.175663
2	0.4	$y(z)$	Numerical	0.000000	0.068130	0.118500	0.149500	0.160000
			Analytical (15)	0.000000	0.066522	0.115447	0.145359	0.155421
			Villa et al. [1]	0.000000	0.068637	0.119455	0.150699	0.161243
1	0.2	$y(z)$	Numerical	0.000000	0.060340	0.104200	0.130700	0.139700
			Analytical (15)	0.000000	0.060165	0.103798	0.130241	0.139099
			Villa et al. [1]	0.000000	0.060524	0.104481	0.131152	0.140093
0.5	0.1	$y(z)$	Numerical	0.000000	0.057310	0.098580	0.123500	0.131804
			Analytical (15)	0.000000	0.057319	0.098578	0.123460	0.131775
			Villa et al. [1]	0.000000	0.057394	0.098722	0.123652	0.131985
0.25	0.05	$y(z)$	Numerical	0.000000	0.055960	0.096080	0.120200	0.128300
			Analytical (15)	0.000000	0.055977	0.096116	0.120262	0.128321
			Villa et al. [1]	0.000000	0.055994	0.096149	0.120306	0.128369

Table 2: Comparison of our analytical expression of concentration profiles $y(z)$ with numerical results and Villa et al. [1] results corresponding to Case 1, for $m = 0$, $q = 0$, and $\phi = 0.5$, when $c < 0$ and $d < 0$.

c	d			Dimensionless spatial coordinate z				
				0.0	0.25	0.5	0.75	1.00
−2.5	−0.5	$y(z)$	Numerical	0.000000	0.044356	0.074890	0.092878	0.098564
			Analytical (15)	0.000000	0.044254	0.074608	0.092320	0.098140
			Villa et al. [1]	0.000000	0.045077	0.076180	0.094425	0.100440
−5	−0.5	$y(z)$	Numerical	0.000000	0.037821	0.062402	0.076523	0.080991
			Analytical (15)	0.000000	0.037461	0.062200	0.076257	0.080814
			Villa et al. [1]	0.000000	0.039354	0.065829	0.081121	0.086125
−7.5	−0.5	$y(z)$	Numerical	0.000000	0.032841	0.053973	0.068000	0.070002
			Analytical (15)	0.000000	0.032651	0.053454	0.067831	0.069662
			Villa et al. [1]	0.000000	0.035385	0.058706	0.072018	0.076351
−4	−0.2	$y(z)$	Numerical	0.000000	0.040345	0.067145	0.083100	0.087989
			Analytical (15)	0.000000	0.040097	0.067028	0.082520	0.087574
			Villa et al. [1]	0.000000	0.041559	0.069825	0.086265	0.091662
−5	−0.2	$y(z)$	Numerical	0.000000	0.038110	0.062899	0.077121	0.081987
			Analytical (15)	0.000000	0.037684	0.062628	0.076831	0.081440
			Villa et al. [1]	0.000000	0.039551	0.066203	0.081619	0.086668

(iii) when $m = 1$, $q = 0$, $\phi = 0.5$, $c > 0$, and $d > 0$.

(iv) when $m = 1$, $q = 0$, $\phi = 0.5$, $c < 0$, and $d < 0$.

(v) when $m = 1$, $q = 1$, $\phi = 0.5$, $c > 0$, and $d > 0$.

From these tables it is evident that the values of the dimensionless mass concentration $y(z)$ decrease, when dimensionless parameters c and d decrease. In Tables 1–5, our analytical results for the mass concentrations $y(z)$ are compared with the numerical results and Villa et al. results [1]. Villa et al. [1] obtained the analytical solution of this problem only for taking the parametric restrictions.

In Tables 1–4, our analytical results are compared with the numerical results and Villa et al. [1] results. A good agreement between them is noted. In Table 5 for the Case 3,

Table 3: Comparison of our analytical expression of concentration profiles $y(z)$ with numerical results and Villa et al. [1] results corresponding to Case 2, for $m = 1$, $q = 0$, and $\phi = 0.5$, when $c > 0$ and $d > 0$.

c	d			Dimensionless spatial coordinate z				
				0.0	0.25	0.5	0.75	1.00
2	0.4	$y(z)$	Numerical	0.000000	0.059510	0.102600	0.128600	0.137400
			Analytical (20)	0.000000	0.058307	0.100271	0.125535	0.133966
			Villa et al. [1]	0.000000	0.059654	0.102825	0.128938	0.137675
1.01	0.2	$y(z)$	Numerical	0.000000	0.054380	0.093160	0.116400	0.124100
			Analytical (20)	0.000000	0.055077	0.093182	0.116617	0.123772
			Villa et al. [1] ($c = 1$)	0.000000	0.054316	0.093042	0.116241	0.123967
0.5	0.1	$y(z)$	Numerical	0.000000	0.052160	0.089100	0.111100	0.118400
			Analytical (20)	0.000000	0.052036	0.88869	0.110829	0.118125
			Villa et al. [1]	0.000000	0.052090	0.088971	0.110966	0.118275
0.25	0.05	$y(z)$	Numerical	0.000000	0.051160	0.087260	0.108700	0.115900
			Analytical (20)	0.000000	0.051052	0.087075	0.108510	0.115625
			Villa et al. [1]	0.000000	0.051065	0.087099	0.108542	0.115660
0.1	0.02	$y(z)$	Numerical	0.000000	0.050590	0.086210	0.107400	0.114400
			Analytical (20)	0.000000	0.050474	0.086019	0.107144	0.114151
			Villa et al. [1]	0.000000	0.050476	0.086023	0.107149	0.114157
0.01	0.002	$y(z)$	Numerical	0.000000	0.050250	0.085590	0.106600	0.113500
			Analytical (20)	0.000000	0.050130	0.085393	0.106333	0.113278
			Villa et al. [1]	0.000000	0.050130	0.085393	0.106333	0.113278
0.001	0.0002	$y(z)$	Numerical	0.000000	0.050220	0.085530	0.106500	0.113500
			Analytical (20)	0.000000	0.050096	0.085330	0.106253	0.113191
			Villa et al. [1]	0.000000	0.050096	0.085330	0.106253	0.113191

Table 4: Comparison of our analytical expression of concentration profiles $y(z)$ with numerical results and Villa et al. [1] results corresponding to Case 2, for $m = 1$, $q = 0$, and $\phi = 0.5$, when $c < 0$ and $d < 0$.

c	d			Dimensionless spatial coordinate z				
				0.0	0.25	0.5	0.75	1.00
−0.3	−0.1	$y(z)$	Numerical	0.000000	0.048975	0.083298	0.103610	0.110432
			Analytical (20)	0.000000	0.048969	0.083271	0.103588	0.110316
			Villa et al. [1]	0.000000	0.048985	0.083302	0.103629	0.110361
−0.5	−0.1	$y(z)$	Numerical	0.000000	0.048943	0.082101	0.102105	0.108924
			Analytical (20)	0.000000	0.048246	0.081952	0.101881	0.108475
			Villa et al. [1]	0.000000	0.048288	0.082031	0.101987	0.108591
−1.0	−0.1	$y(z)$	Numerical	0.000000	0.046786	0.078998	0.097997	0.104789
			Analytical (20)	0.000000	0.046530	0.078818	0.097825	0.104101
			Villa et al. [1]	0.000000	0.046673	0.079091	0.098191	0.104500
−1.5	−0.1	$y(z)$	Numerical	0.000000	0.045001	0.076001	0.094255	0.100213
			Analytical (20)	0.000000	0.044931	0.075901	0.094050	0.100030
			Villa et al. [1]	0.000000	0.045214	0.076442	0.094775	0.100821
−2.0	−0.1	$y(z)$	Numerical	0.000000	0.043678	0.073356	0.090611	0.096987
			Analytical (20)	0.000000	0.043438	0.073179	0.090530	0.096234
			Villa et al. [1]	0.000000	0.043888	0.074037	0.091678	0.097487

Table 5: Comparison of our analytical expression of concentration profiles $y(z)$ with numerical results and Villa et al. [1] results corresponding to Case 3, for $m = 1$, $q = 1$, and $\phi = 0.5$, when $c > 0$ and $d > 0$.

c	d			Dimensionless spatial coordinate z				
				0.0	0.25	0.5	0.75	1.00
1.99	0.4	$y(z)$	Numerical	0.000000	0.053770	0.092021	0.114923	0.122500
			Analytical (25)	0.000000	0.053168	0.090154	0.110179	0.119763
			(error %)	(0.0000)	(1.1195)	(2.0288)	(4.0102)	(2.2342)
			Villa et al. [1] ($c = 2$)	0.000000	0.013657	0.023410	0.029260	0.031210
			(error %)	(0.0000)	(74.6010)	(74.5601)	(74.5394)	(74.5224)
1.0	0.2	$y(z)$	Numerical	0.000000	0.049970	0.085070	0.105900	0.112800
			Analytical (25)	0.000000	0.049630	0.084442	0.105065	0.108007
			(error %)	(0.0000)	(0.6804)	(0.7640)	(0.7884)	(4.2491)
			Villa et al. [1]	0.000000	0.013358	0.022862	0.028549	0.030442
			(error %)	(0.0000)	(73.2679)	(73.1256)	(73.0415)	(73.0124)
0.5	0.1	$y(z)$	Numerical	0.000000	0.048300	0.082010	0.101900	0.108500
			Analytical (25)	0.000000	0.048078	0.081632	0.101452	0.108007
			(error %)	(0.0000)	(0.4596)	(0.4609)	(0.4396)	(0.4543)
			Villa et al. [1]	0.000000	0.013216	0.022601	0.028210	0.030076
			(error %)	(0.0000)	(72.6376)	(72.7766)	(72.3159)	(72.2801)
0.25	0.05	$y(z)$	Numerical	0.000000	0.047510	0.080580	0.100100	0.106500
			Analytical (25)	0.000000	0.046859	0.079420	0.098604	0.104941
			(error %)	(0.0000)	(1.3702)	(1.4395)	(1.4945)	(1.4638)
			Villa et al. [1]	0.000000	0.013146	0.022473	0.028044	0.029897
			(error %)	(0.0000)	(72.3300)	(72.1109)	(71.9840)	(71.9276)
0.1	0.02	$y(z)$	Numerical	0.000000	0.047060	0.079750	0.099010	0.105400
			Analytical (25)	0.000000	0.046859	0.079420	0.098604	0.104941
			(error %)	(0.0000)	(0.4271)	(0.4137)	(0.4100)	(0.4354)
			Villa et al. [1]	0.000000	0.013104	0.022397	0.027946	0.029791
			(error %)	(0.0000)	(72.1546)	(71.9159)	(71.7745)	(72.3531)
0.01	0.002	$y(z)$	Numerical	0.000000	0.046790	0.079260	0.098380	0.104700
			Analytical (25)	0.000000	0.046588	0.078929	0.097971	0.104259
			(error %)	(0.0000)	(0.4317)	(0.41756)	(0.4157)	(0.4212)
			Villa et al. [1]	0.000000	0.013080	0.022352	0.027887	0.029727
				(0.0000)	(72.0453)	(71.7991)	(71.6537)	(71.6074)
0.001	0.0002	$y(z)$	Numerical	0.000000	0.046760	0.079210	0.098320	0.104600
			Analytical (25)	0.000000	0.046561	0.078880	0.097907	0.104191
			(error %)	(0.0000)	(0.4255)	(0.4166)	(0.4200)	(0.3910)
			Villa et al. [1]	0.000000	0.013077	0.022347	0.027881	0.029721
			(error %)	(0.0000)	(72.0337)	(71.7876)	(71.6425)	(71.5860)

our analytical results and Villa et al. [1] results are compared with the numerical results. Our analytical result gives good agreement with the numerical results. In Table 6, the effectiveness factors for the Cases 1 and 2, a satisfactory agreement between our results and Villa et al. [1] results is noted.

6. Conclusion

The steady state non-linear reaction-diffusion equation has been solved analytically and numerically. A simple and approximate dimensionless mass concentrations $y(z)$ are derived by using the HPM for all values of dimensionless parameters c, d, and ϕ. The HPM is an extremely simple method and it is also a promising method to solve other non-linear equations. This method can be easily extended to find the solution of all other non-linear equations. The proposed formulas are used to find the thiele module range, in which multiple values of the effectiveness factor should be searched. The present method is quick and efficient and is able to reduce

Table 6: Comparison of our effectiveness factors ((19), (24), and (29)), and Villa et al. [1] when $\phi = 0.5$.

Cases	c	d	Effectiveness factors (η)	
			Villa et al. [1]	Our results
Case 1 ($m = 0,\ q = 0$)	2.5	0.5	1.3195	1.2526
	2	0.4	1.2294	1.1952
	1	0.2	1.0961	1.0903
	0.5	0.1	1.0446	1.0434
	0.25	0.05	1.0215	1.0213
	−2.5	−0.5	0.8142	0.8280
	−5	−0.5	0.7461	0.7157
	−7.5	−0.5	0.6797	0.6360
	−4	−0.2	0.7827	0.7592
	−5	−0.2	0.7493	0.7193
Case 2 ($m = 1,\ q = 0$)	2.0	0.4	1.0820	1.0603
	1.01	0.2	($c = 1$) 0.9940	0.9890
	0.5	0.1	0.9572	0.9564
	0.25	0.05	0.9403	0.9401
	0.1	0.02	0.9306	0.9305
	0.01	0.002	0.9249	0.9249
	0.001	0.0002	0.9243	0.9242
	−0.3	−0.5	0.9059	0.9057
	−0.5	−0.5	0.8944	0.8937
	−1.0	−0.5	0.8676	0.8653
	−1.5	−0.2	0.8435	0.8389
	−2.0	−0.2	0.8214	0.8142
Case 3 ($m = 1,\ q = 1$)	1.99	0.4	($c = 2$) 0.9991	0.9678
	1.0	0.2	0.9793	0.9168
	0.5	0.1	0.9699	0.8910
	0.25	0.05	0.9653	0.8783
	0.1	0.02	0.9626	0.8708
	0.01	0.002	0.9609	0.8663
	0.001	0.0002	0.9608	0.8658

significantly the amount of computations in simulations of the catalytic chemical reactors.

Appendices

A. Solution of Nonlinear Equations (11) and (12) Using HPM

In this Appendix, we indicate how (15) in this paper is derived. To find the solution of (11) and (12), when $q = 0$ and $m = 0$. When $cy/(dy + 1)$ small, then (11) reduces to

$$\frac{d^2y}{dz^2} + \phi^2\left[1 + cy - cdy^2\right] = 0. \tag{A.1}$$

We construct the homotopy as follows:

$$(1-p)\left[\frac{d^2y}{dz^2} + \phi^2 cy + \phi^2\right] + p\left[\frac{d^2y}{dz^2} + \phi^2 cy - \phi^2 cdy^2 + \phi^2\right] = 0. \tag{A.2}$$

The analytical solution of (A.1) is

$$y = y_0 + py_1 + p^2y_2 + \cdots. \tag{A.3}$$

Substituting (A.3) into (A.2), we get

$$(1-p)\left[\frac{d^2\left(y_0+py_1+p^2y_2+\cdots\right)}{dz^2} +\phi^2 c\left(y_0+py_1+p^2y_2+\cdots\right)+\phi^2\right] + p\left[\frac{d^2\left(y_0+py_1+p^2y_2+\cdots\right)}{dz^2} +\phi^2 c\left(y_0+py_1+p^2y_2+\cdots\right) -\phi^2 cd\left(y_0+py_1+p^2y_2+\cdots\right)^2+\phi^2\right]=0. \tag{A.4}$$

Comparing the coefficients of like powers of p in (A.4) we get

$$p^0:\frac{d^2y_0}{dz^2}+\phi^2cy_0+\phi^2=0,$$
$$p^1:\frac{d^2y_1}{dz^2}+\phi^2cy_1-\phi^2cdy_0^2=0. \tag{A.5}$$

The initial approximations are as follows:

$$y_0(0)=0,\qquad y_0'(1)=0,$$
$$y_i(0)=y_i'(1)=0,\quad i=1,2,3\ldots. \tag{A.6}$$

Solving (A.5) and using the boundary conditions (A.6) we obtain the following results:

$$y_0=\frac{1}{c}\left[\cos(kz)+\tan(k)\sin(kz)-1\right],$$
$$y_1=k_1\cos(kz)+k_2\sin(kz)+\left[\frac{d\left(3+\tan^2(k)\right)}{2c^2}\right] -\left[\frac{\phi^2 d\left(1-\tan^2(k)\right)\cos(2kz)}{6ck^2}\right] -\left[\frac{\phi^2 d\tan(k)\sin(2kz)}{3ck^2}\right] +\left[\frac{\phi^2 d\tan(k)\,z\cos(kz)}{ck}\right]-\left[\frac{\phi^2 dz\sin(kz)}{ck}\right], \tag{A.7}$$

where k, k_1, and k_2 are defined in the text (16), (17), and (18), respectively.

According to the HPM, we can conclude that

$$y=\lim_{p\to 1}y(t)=y_0+y_1. \tag{A.8}$$

After putting (A.7) into (A.8) we obtain the solution in the text (15).

B. Solution of Nonlinear Equations (11) and (12) Using HPM

In this Appendix, we indicate how (20) in this paper is derived. To find the solution of (11) and (12), when $q=0$ and $m=1$. When $cy/(dy+1)$ small, then (11) reduces to

$$\frac{d^2y}{dz^2}+\phi^2\left[1+(c-1)y-(c+cd)y^2\right]=0. \tag{B.1}$$

We construct the homotopy as follows:

$$(1-p)\left[\frac{d^2y}{dz^2}+\phi^2(c-1)y+\phi^2\right] +p\left[\frac{d^2y}{dz^2}+\phi^2(c-1)y-\phi^2(c+cd)y^2+\phi^2\right]=0. \tag{B.2}$$

The analytical solution of (B.1) is

$$y=y_0+py_1+p^2y_2+\cdots. \tag{B.3}$$

Substituting (B.3) into (B.2), we get

$$(1-p)\left[\frac{d^2\left(y_0+py_1+p^2y_2+\cdots\right)}{dz^2} +\phi^2(c-1)\left(y_0+py_1+p^2y_2+\cdots\right)+\phi^2\right] +p\left[\frac{d^2\left(y_0+py_1+p^2y_2+\cdots\right)}{dz^2}+\phi^2(c-1) \times\left(y_0+py_1+p^2y_2+\cdots\right)-\phi^2(c+cd) \times\left(y_0+py_1+p^2y_2+\cdots\right)^2+\phi^2\right]=0. \tag{B.4}$$

Comparing the coefficients of like powers of p in (B.4) we get

$$p^0:\frac{d^2y_0}{dz^2}+\phi^2(c-1)y_0+\phi^2=0,$$
$$p^1:\frac{d^2y_1}{dz^2}+\phi^2(c-1)y_1+\phi^2(c+cd)y_0^2=0. \tag{B.5}$$

The initial approximations are as follows:

$$y_0(0)=0,\quad y_0'(1)=0,$$
$$y_i(0)=y_i'(1)=0,\quad i=1,2,3\ldots. \tag{B.6}$$

Solving (B.5) and using the boundary conditions (B.6) we obtain the following results:

$$y_0 = \left(\frac{1}{(c-1)}\right)[\cos(az) + \tan(a)\sin(az) - 1],$$

$$\begin{aligned} y_1 = {} & [a_1\cos(az) + a_2\sin(az)] + \left[\frac{(c+cd)\left(3+\tan^2(a)\right)}{2(c-1)^3}\right] \\ & - \left[\frac{\phi^2(c+cd)\left(1-\tan^2(a)\right)\cos(2az)}{6(c-1)^2a^2}\right] \\ & - \left[\frac{\phi^2(c+cd)\tan(a)\sin(2az)}{3(c-1)^2a^2}\right] \\ & + \left[\frac{\phi^2(c+cd)\tan(a)\,z\cos(az)}{(c-1)^2a}\right] \\ & - \left[\frac{\phi^2(c+cd)\,z\sin(az)}{(c-1)^2a}\right], \end{aligned} \tag{B.7}$$

where a, a_1, and a_2 are defined in the text (21), (22), and (23) respectively.

According to the HPM, we can conclude that

$$y = \lim_{p\to 1} y(t) = y_0 + y_1. \tag{B.8}$$

After putting (B.7) into (B.8) we obtain the solution in the text (20).

C. Solution of Nonlinear Equations (11) and (12) Using HPM

In this Appendix, we indicate how (25) in this paper is derived. To find the solution of (11) and (12), when $q = 1$ and $m = 1$.

When $cy/(dy+1)$ small, then (11) reduces to

$$\frac{d^2y}{dz^2} + \phi^2\left[1 + (c-2)y - (cd+2c-1)y^2\right] = 0. \tag{C.1}$$

We construct the homotopy as follows:

$$\begin{aligned} & (1-p)\left[\frac{d^2y}{dz^2} + \phi^2(c-2)y + \phi^2\right] \\ & + p\left[\frac{d^2y}{dz^2} + \phi^2(c-2)y - \phi^2(cd+2c-1)y^2 + \phi^2\right] = 0. \end{aligned} \tag{C.2}$$

The analytical solution of (C.1) is

$$y = y_0 + py_1 + p^2y_2 + \cdots. \tag{C.3}$$

Substituting (C.3) into (C.2), we get

$$\begin{aligned} & (1-p)\left[\frac{d^2\left(y_0 + py_1 + p^2y_2 + \cdots\right)}{dz^2}\right. \\ & \qquad \left. + \phi^2(c-2)\left(y_0 + py_1 + p^2y_2 + \cdots\right) + \phi^2\right] \\ & + p\left[\frac{d^2\left(y_0 + py_1 + p^2y_2 + \cdots\right)}{dz^2} + \phi^2(c-2)\right. \\ & \qquad \times \left(y_0 + py_1 + p^2y_2 + \cdots\right) - \phi^2(cd+2c-1) \\ & \qquad \left. \times\left(y_0 + py_1 + p^2y_2 + \cdots\right)^2 + \phi^2\right] = 0. \end{aligned} \tag{C.4}$$

Comparing the coefficients of like powers of p in (C.4) we get

$$\begin{aligned} p^0 &: \frac{d^2y_0}{dz^2} + \phi^2(c-2)y_0 + \phi^2 = 0, \\ p^1 &: \frac{d^2y_1}{dz^2} + \phi^2(c-2)y_1 - \phi^2(cd+2c-1)y_0^2 = 0. \end{aligned} \tag{C.5}$$

The initial approximations is as follows:

$$\begin{aligned} & y_0(0) = 0, \quad y_0'(1) = 0, \\ & y_i(0) = y_i'(1) = 0, \quad i = 1, 2, 3\ldots. \end{aligned} \tag{C.6}$$

Solving (C.5) and using the boundary conditions (C.6) we obtain the following results:

$$\begin{aligned} y_0 = {} & \frac{1}{(c-2)}[\cos(bz) + \tan(b)\sin(bz) - 1], \\ y_1 = {} & [b_1\cos(bz) + b_2\sin(bz)] \\ & + \left[\frac{(cd+2c-1)\left(3+\tan^2(b)\right)}{2(c-2)^3}\right] \\ & - \left[\frac{\phi^2(cd+2c-1)\left(1-\tan^2(b)\right)\cos(2bz)}{6(c-2)^2b^2}\right] \\ & - \left[\frac{\phi^2(cd+2c-1)\tan(b)\sin(2bz)}{3(c-2)^2b^2}\right] \\ & + \left[\frac{\phi^2(cd+2c-1)\tan(b)\,z\cos(bz)}{(c-2)^2b}\right] \\ & - \left[\frac{\phi^2(cd+2c-1)\,z\sin(bz)}{(c-2)^2b}\right], \end{aligned} \tag{C.7}$$

where b, b_1, and b_2 are defined in the text (26), (27), and (28), respectively.

According to the HPM, we can conclude that

$$y = \lim_{p\to 1} y(t) = y_0 + y_1. \tag{C.8}$$

After putting (C.7) into (C.8) we obtain the solution in the text (25).

D. MATLAB Program to Find the Numerical Solution of Nonlinear Equations (11) and (12)

```
function pdex4
m = 0;
x =[0 0.25 0.5 0.75 1];
t=linspace(0,10000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
xlabel ('Distance x')
ylabel ('u(x,t)')
%-------------------------------------------------------
--------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
a=0.5;
c=1;
d=0.2;
m=0;
p=0;
F =a^2*(1-u)^(m+p)*exp(c*u/(1+d*u))
s = F;
%-------------------------------------------------------
--------
function u0 = pdex4ic(x); %create initial conditions
u0 = 1;
%-------------------------------------------------------
--------
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)  %create
boundary conditions
pl = ul;
ql = 0;
pr = 0;
qr = 1.
```

E. MATLAB Program to Find the Numerical Solution of Nonlinear Equations (11) and (12)

```
function pdex4
m = 0;
x =[0 0.25 0.5 0.75 1];
t=linspace(0,10000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
xlabel('Distance x')
ylabel('u(x,t)')
%-------------------------------------------------------
--------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
a=0.5;
c=−7.5;
d=−0.5;
m=0;
p=0;
F =a^2*(1-u)^(m+p)*exp(c*u/(1+d*u))
s = F;
%-------------------------------------------------------
--------
function u0 = pdex4ic(x); %create initial conditions
u0 = 1;
%-------------------------------------------------------
--------
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)  %create
boundary conditions
pl = ul;
ql = 0;
pr = 0;
qr = 1.
```

F. MATLAB Program to Find the Numerical Solution of Non-Linear Equations (11) and (12)

```
function pdex4
m = 0;
x =[0 0.25 0.5 0.75 1];
t=linspace(0,10000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
```

```
xlabel('Distance x')
ylabel('u(x,t)')
%-------------------------------------------------------
--------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
a=0.5;
c=2;
d=0.4;
m=1;
p=0;
F =a^2*(1-u)^(m+p)*exp(c*u/(1+d*u));
s = F;
%-------------------------------------------------------
--------
function u0 = pdex4ic(x); %create initial conditions
u0 = 1;
%-------------------------------------------------------
--------
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)  %create
boundary conditions
pl = ul;
ql = 0;
pr = 0;
qr = 1.
```

G. MATLAB Program to Find the Numerical Solution of Non-Linear Equations (11) and (12)

```
function pdex4
m = 0;
x =[0 0.25 0.5 0.75 1];
t=linspace(0,10000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
xlabel('Distance x')
ylabel('u(x,t)')
%-------------------------------------------------------
--------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
a=0.5;
c=−1.5;
d=−0.1;
m=1;
p=0;
F =a^2*(1-u)^(m+p)*exp(c*u/(1+d*u))
s = F;
%-------------------------------------------------------
--------
function u0 = pdex4ic(x); %create initial conditions
u0 = 1;
%-------------------------------------------------------
--------
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)  %create
boundary conditions
pl = ul;
ql = 0;
pr = 0;
qr = 1.
```

H. MATLAB Program to Find the Numerical Solution of Non-Linear Equations (11) and (12)

```
function pdex4
m = 0;
x =[0 0.25 0.5 0.75 1];
t=linspace(0,10000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
xlabel('Distance x')
ylabel('u(x,t)')
%-------------------------------------------------------
--------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
a=0.5;
c=1;
d=0.2;
m=1;
p=1;
```

```
F =a^2*(1-u)^(m+p)*exp(c*u/(1+d*u))

s = F;

%-------------------------------------------------------------

function u0 = pdex4ic(x); %create initial conditions

u0 = 1;

%-------------------------------------------------------------

function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)  %create boundary conditions

pl = ul;

ql = 0;

pr = 0;

qr = 1.
```

Nomenclature

x:	Spatial coordinate (m)
z:	Dimensionless spatial coordinate
u, y:	Dimensionless mass concentration of reactive component A
$f(u)$:	Dimensionless reaction rate
v, w:	Dimensionless functions
L:	Half thickness of porous slab (m)
m, q:	Whole numbers which denote the reaction order
P:	Product chemical component in a chemical reaction
R:	Universal gas constant
T:	Functions which represent temperature profile in the porous slab ($^\circ$K)
C_A:	Volumetric molar concentration of the key component A
C_{AS}:	Surface value of the key component A
D_A:	Effective diffusivity coefficient
k_S	Specific kinetic constant
C_{BS}:	Dimensionless concentration of component B
d:	Thermicity of the reaction
γ:	Arrhenius group
$c = \gamma \cdot d$:	Dimensionless parameter
ϕ:	Thiele modulus
η:	Effectiveness factor for the heterogeneous chemical reaction.

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