

An improved linear formula for cyclic adsorption, diffusion and reaction in a catalyst

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Abstract—Simple linear models including the linear driving force (LDF) model for approximating unsteady-state diffusion, adsorption in an adsorbent under cyclic operating environments have been proposed to reduce the computational load of the exact partial differential equations. The models are in the form of a first-order ordinary differential equation and consist of a term with the external concentration surrounding the adsorbent particle and another term with the average adsorbate concentration in the adsorbent. Although very simple to use, the approximation models are first-order approximations of the pore diffusion model, and hence their accuracy is not high enough to compute fine details of fast responses. By incorporating the time derivative of the external concentration into the approximation, an improved linear formula for cyclic adsorption is developed in this study. As the time derivative is usually computed simultaneously with the external concentration, the improved formula has little additional complexity over the previous approximations in its applications, and yet it is considerably more accurate than the previous first-order approximations for cyclic adsorption.

Keywords: Cyclic Adsorption, Pore Diffusion Model, Approximation, Linear Formula for Cyclic Operation, Linear Driving Force Model

INTRODUCTION

An accurate mathematical description of the dynamic mass transfer in a spherical catalyst in which a first-order reaction takes place is the pore diffusion model represented by the parabolic partial differential equation [1].

$$\frac{\partial c}{\partial t} = \frac{D_e}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c}{\partial r} \right) - kc \quad (1)$$

$$c(R, t) = h(c_f(t)), \quad \frac{\partial c}{\partial r} \Big|_{r=0} = 0$$

At $r=R$, the catalyst is in contact with the external fluid phase, of which the concentration is c_f . Because of the adsorption in the catalyst, $c(R, t)$ is a function of c_f which we denote as $h(c_f)$. For example, if the adsorption isotherm is linear, $h(c_f)=Kc_f$. The equation is rarely used alone and usually coupled with a mass balance equation for the flowing phase external to the particle, such as

$$\varepsilon_b \frac{\partial c_f}{\partial t} = - \frac{\partial(Uc_f)}{\partial z} - (1 - \varepsilon_b) A_e D_e \frac{\partial c}{\partial r} \Big|_{r=R} \quad (2)$$

The last term in Eq. (2) is the mass exchange rate between the particle and the external fluid phase. In principle, Eqs. (1) and (2) are solved simultaneously, but the solution process is extremely complicated and difficult.

It can be shown that

$$A_e D_e \frac{\partial c}{\partial r} \Big|_{r=R} = \frac{\partial \bar{c}}{\partial t} + k \bar{c} \quad (3)$$

where \bar{c} is the average concentration in the particle. Hence, for estimation of the mass exchange rate, it is sufficient to determine $\bar{c}(t)$ rather than $c(r, t)$ at every point in the particle as in Eq. (1). Although the exact \bar{c} can only be obtained from $c(r, t)$ by solving Eq. (1) with Eq. (2), a number of approximations for \bar{c} have been proposed to simplify the solution.

In the absence of reaction ($k=0$), the first and well-known approximation of \bar{c} is the linear driving force (LDF) formula [2].

$$\frac{\partial \bar{c}}{\partial t} = \frac{15}{\tau_0} (h(c_f) - \bar{c}) \quad (4)$$

where $\tau_0 (=R^2/D_e)$ is the diffusion time constant. As Eq. (4) had been obtained as a first-order approximation for a unit step response of Eq. (1), it has a limited accuracy and is valid for slowly varying c_f . An improved LDF formula has been developed for better accuracy in the approximation [3].

$$\frac{\partial \bar{c}}{\partial t} = \frac{21}{2 \tau_0} (h(c_f) - \bar{c}) + \frac{3}{10} \frac{\partial h}{\partial t} \quad (5)$$

As Eq. (5) is coupled with Eq. (2), $\partial c_f / \partial t$ is always computed and available. Thus, compared to Eq. (4), the additional term $\partial h / \partial t (= \partial h / \partial c_f)(\partial c_f / \partial t)$ in Eq. (5) does not add complexity to the solution but improves the approximation accuracy considerably [3].

Eqs. (4) and (5) were developed for noncyclic adsorption, but are also applicable for slow cyclic adsorptions [3]. Eq. (4) has been used in simulations of cyclic adsorption [4-6]. As the frequency of the cyclic operation increases, however, the LDF models with the constant coefficients become poor in their approximation accuracy [3,7,8]. To improve the accuracy and to retain the simple structure of approximation, the LDF model, Eq. (4), has been modified by substituting the constant 15 in the equation with an empirical factor as a function of period of the cycle [7,8].

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$$\frac{\partial \bar{c}}{\partial t} = \frac{7.27}{\sqrt{P} \tau_0} (h(c_f) - \bar{c}) \quad (6)$$

where P is the period of the cyclic adsorption. The empirical LDF for cyclic adsorption has been experimentally shown to be inadequate in simulation of a pressure swing adsorption [9]. A theoretical linear formula for cyclic adsorption (LFC), similar to the LDF model, has been developed [10].

$$\frac{\partial \bar{c}}{\partial t} = \frac{1}{\tau_0} [\alpha(h(c_f) - A_0) - \beta(\bar{c} - A_0)] \quad (7)$$

where

$$\alpha = \omega^2 \mu + \frac{\psi^2}{\mu}, \quad \beta = \frac{\psi}{\mu}, \quad \omega = \frac{2\pi}{P/\tau_0} \quad (8)$$

$$\mu = \sum_{n=1}^{\infty} \frac{6}{n^4 \pi^4 + \omega^2}, \quad \psi = \sum_{n=1}^{\infty} \frac{6n^2 \pi^2}{n^4 \pi^4 + \omega^2}$$

A_0 is the time average of $h(c_f)$ over a cycle

$$A_0 = \frac{1}{P} \int_0^P h(c_f(t)) dt \quad (9)$$

It can be shown that as $\omega \rightarrow 0$, the coefficients $\alpha \rightarrow 15$ and $\beta \rightarrow 15$, and Eq. (7) becomes identical to the LDF equation, Eq. (4) [10].

Higher accuracy than that of Eq. (7) can be obtained by using high-order approximations [11-14]. The high-order approximations are usually expressed in the form of simultaneous first-order differential equations and the number of the equations increases with the approximation order. Although easier to calculate than the pore diffusion model Eq. (1), the high-order approximations become more complicated and thus numerically more intensive when compared to the single, first-order approximation.

As $\partial c_f / \partial t$ is computed and available during computation of the solution, the information has been incorporated into the formula to approximate \bar{c} more accurately for noncyclic adsorption as represented by Eq. (5), but such a formula has not been explicitly given in the literature for the case of cyclic adsorption. We have developed an approximation for cyclic operations that is more accurate than the previous first-order approximation but, like the previous ones, can be represented by a single first-order differential equation.

CYCLIC DIFFUSION, ADSORPTION AND REACTION IN A PARTICLE

In addition to a spherical catalyst, we also consider catalysts in the form of infinite slab and infinite cylinder. The dimensionless pore diffusion model for the three geometries can be written as

$$\frac{\partial q}{\partial \tau} = \frac{1}{x^{\zeta}} \frac{\partial}{\partial x} \left(x^{\zeta} \frac{\partial q}{\partial x} \right) - \phi^2 q = \frac{\zeta \partial q}{x \partial x} + \frac{\partial^2 q}{\partial x^2} - \phi^2 q \quad (10)$$

$$\left. \frac{\partial q(x, \tau)}{\partial x} \right|_{x=0} = 0, \quad q(1, \tau) = f(\tau)$$

ζ is the shape factor for the three geometries ($\zeta=0$ for an infinite slab, $\zeta=1$ for an infinite cylinder and $\zeta=2$ for a sphere). The volume-average concentration is

$$\bar{q}(\tau) = (\zeta+1) \int_0^1 x^{\zeta} q(x, \tau) dx \quad (11)$$

The volume-average concentration $\bar{q}(t)$ is of main interest because the mass exchange rate between the adsorbent and its surrounding can be conveniently expressed in terms of \bar{q} as in Eq. (3).

Applying the Laplace transformation to Eq. (10), we obtain [12]

$$\bar{Q}(s) = G_{\zeta}(s + \phi^2) F(s) \quad (12)$$

$$G_{\zeta}(s + \phi^2) = \frac{(\zeta+1) I_{(\zeta+1)/2}(\sqrt{s + \phi^2})}{\sqrt{s + \phi^2} I_{\zeta/2}(\sqrt{s + \phi^2})} = \begin{cases} \frac{\tanh \sqrt{s + \phi^2}}{\sqrt{s + \phi^2}} & \zeta=0 \\ \frac{2 I_1(\sqrt{s + \phi^2})}{\sqrt{s + \phi^2} I_0(\sqrt{s + \phi^2})} & \zeta=1 \\ 3 \left(\frac{\coth \sqrt{s + \phi^2}}{\sqrt{s + \phi^2}} - \frac{1}{s + \phi^2} \right) & \zeta=2 \end{cases}$$

where $\bar{Q}(s)$ and $F(s)$ are Laplace transforms of $\bar{q}(\tau)$ and $f(\tau)$, respectively, and $G_{\zeta}(s + \phi^2)$ is the transfer function relating the volume-average concentration $\bar{q}(\tau)$ and the surface concentration $f(\tau)$. The function I_{α} in Eq. (12) is the modified Bessel function.

A first-order approximation of the transfer function would be in the form of

$$G_a(s) = \frac{\alpha}{s + \beta} \quad (13)$$

For noncyclic operations, the two coefficients of approximation, α and β , can be obtained by the method of Pade [11]. In this method, the power series of $G_a(s)$ agrees with the power series of $G_{\zeta}(s + \phi^2)$ to the highest possible order. For the approximation Eq. (13), the agreement is

$$G_{\zeta}(\phi^2) = G_a(0) \text{ and } G'_{\zeta}(\phi^2) = G'_a(0) \quad (14)$$

From these two equations in Eq. (14), α and β are determined. For example, the Pade approximation for $\zeta=2$ and $\phi=0$ is $G_a(s) = 15/(s+15)$, which is equivalent to the LDF model of Eq. (4). For cyclic operations, however, the two coefficients are tuned to the angular speed of the cycle, which is defined in Eq. (8). Substituting s with $j\omega$ in Eqs. (12) and (13), we obtain

$$\text{Re}(G_{\zeta}(j\omega + \phi^2)) = \text{Re}(G_a(j\omega)) \quad (15)$$

$$\text{Im}(G_{\zeta}(j\omega + \phi^2)) = \text{Im}(G_a(j\omega)), \quad \text{where } j = \sqrt{-1}$$

Here Re and Im stand for the real and imaginary part of the complex number, respectively. If we let $A = \text{Re}(G_{\zeta}(j\omega + \phi^2))$, $B = \text{Im}(G_{\zeta}(j\omega + \phi^2))$, Solving Eq. (15) for α and β we have

$$\alpha = -\frac{(A^2 + B^2)\omega}{B}, \quad \beta = -\frac{A}{B}\omega \quad (16)$$

The time-domain equation for Eq. (13) is

$$\frac{d\bar{q}}{d\tau} = \alpha f(\tau) - \beta \bar{q} \quad (17)$$

Unlike the Pade approximation, $G_a(s)$ with the two coefficients of Eq. (16) is not equal to $G_{\zeta}(s + \phi^2)$ at $s=0$, i.e., $G_{\zeta}(\phi^2) \neq G_a(0)$. This difference between the approximate and the exact transfer func-

tions at $s=0$ requires a correction of p by a constant to obtain \bar{q} . It has been shown that [11]

$$\bar{q} = p + \frac{A_0}{C_0} [G_\zeta(\phi^2) - G_a(0)] \quad (18)$$

In Pade approximations, such correction is unnecessary since $G_\zeta(\phi^2) = G_a(0)$. It can be shown that α and β in Eq. (8) and those in Eq. (16) are identical when $\zeta=2$ and $\phi=0$ [11]. Therefore Eqs. (16-18) are an extension of Eqs. (7) and (8) to cases where $\phi>0$ and its shape is an infinite slab or cylinder. It is noted that for $\zeta=2$ and $\phi=0$, $\alpha \rightarrow 15$ and $\beta \rightarrow 15$ as $\omega \rightarrow 0$, and Eq. (17) becomes identical to the LDF formula for noncyclic adsorption, Eq. (4).

In simulation of adsorbers, the concentration around an adsorbent particle, c_p , as well as the time rate of the concentration $\partial c_p / \partial t$ is computed simultaneously along the adsorbent bed. As has been shown with Eq. (5) for noncyclic adsorption [3], a considerably more accurate approximation similar to Eq. (5) can also be obtained for cyclic adsorption incorporating $\partial c_p / \partial t$ or equivalently $\partial f / \partial \tau$ into the approximation formula. The transfer function for such an approximation is

$$G_b(s) = \frac{\alpha_0 + \alpha_1 s}{\beta_0 + s} \quad (19)$$

For cyclic operations, the three coefficients α_0 , α_1 and β_0 are to be tuned to the cycle frequency. Matching $G_b(s)$ and $G_\zeta(s + \phi^2)$ at $s=j\omega$ gives two conditions as in Eq. (15).

$$\text{Re}(G_\zeta(j\omega + \phi^2)) = \text{Re}(G_a(j\omega)) \quad (20)$$

$$\text{Im}(G_\zeta(j\omega + \phi^2)) = \text{Im}(G_a(j\omega))$$

We need another condition to determine the three coefficients. As the third condition, we use

$$G_\zeta(2\omega + \phi^2) = G_a(2\omega) \quad (21)$$

Solving Eqs. (20) and (21) simultaneously for the three coefficients, we obtain

$$\begin{aligned} \alpha_0 &= \frac{-\omega(2A^2 - 2AC + 2B^2 - BC)}{A + 2B - C} \\ \alpha_1 &= \frac{A^2 - AC + B^2 + 2BC}{A + 2B - C} \\ \beta_0 &= \frac{-\omega(2A - V - 2C)}{A + 2B - C} \end{aligned} \quad (22)$$

where

$$\begin{aligned} A &= \text{Re}(G_\zeta(j\omega + \phi^2)), \\ B &= \text{Im}(G_\zeta(j\omega + \phi^2)), \\ C &= G_\zeta(2\omega + \phi^2) \end{aligned} \quad (23)$$

The proposed approximation is an improved linear formula for cyclic operation (ILFC).

$$\frac{dp}{d\tau} = \alpha_0 f(\tau) - \beta_0 p + \alpha_1 \frac{df}{d\tau} \quad (24)$$

and a constant correction as in Eq. (18) to obtain \bar{q} is

$$\bar{q} = p + \frac{A_0}{C_0} [G_\zeta(\phi^2) - G_b(0)] \quad (25)$$

When $\zeta=2$ (sphere) and $\phi=0$, the coefficients can be calculated by

$$\begin{aligned} \beta_0 &= \begin{cases} 10.5 + 0.0806\omega + 0.0113\omega^2 & \text{when } 0 \leq \omega \leq 20 \\ \frac{\omega\sqrt{2\omega}}{2\sqrt{2\omega}-5} & \omega > 20 \end{cases} \\ \alpha_0 &= \begin{cases} 10.5 + 0.0946\omega + 0.00528\omega^2 & \text{when } 0 \leq \omega \leq 20 \\ \frac{18\omega - 27\sqrt{2\omega} + 30}{2\sqrt{2\omega}-5} & \omega > 20 \end{cases} \\ \alpha_1 &= \begin{cases} 0.3 - 6.42 \times 10^{-3}\omega + 8.7 \times 10^{-5}\omega^2 & \text{when } 0 \leq \omega \leq 20 \\ \frac{3 - 9/\sqrt{2\omega}}{2\sqrt{2\omega}-5} & \omega > 20 \end{cases} \end{aligned} \quad (26)$$

The second-order polynomials in Eq. (26) for the coefficients when $\omega < 20$ were obtained from least square fittings of the exact values of the coefficients and the fitting errors were less than 1%. The functions of ω for the coefficients when $\omega > 20$, were obtained from the asymptotes of the coefficient functions. For noncyclic adsorption or very slow cyclic adsorption, $\omega \rightarrow 0$, the approximation becomes

$$\frac{d\bar{q}}{d\tau} = 10.5(f(\tau) - \bar{q}(\tau)) + 0.3 \frac{df}{d\tau} \quad (27)$$

Eq. (27) is identical to the improved LDF approximation Eq. (5) in dimensionless form for noncyclic adsorption [3]. Thus the proposed formula, Eqs. (22)-(25), is an extension of the improved LDF to cyclic adsorption processes.

DISCUSSION

We compared the approximations of the past and the proposed one for various predefined forcing functions to examine their approximation accuracies. For this purpose, we needed the exact responses as a reference for comparison, which can be obtained from the solution for a spherical catalyst [3].

$$\bar{q}(\tau) = 6 \sum_{n=1}^{\infty} \exp(-\lambda_n \tau) \int_0^{\tau} \exp(\lambda_n \xi) f(\xi) d\xi, \quad \lambda_n = \phi^2 + n^2 \pi^2 \quad (28)$$

We considered a rectangular wave concentration forcing

$$f(\tau) = \begin{cases} 1, & 0 \leq \tau < h \\ 0, & h \leq \tau < T \end{cases} \quad f(\tau + T) = f(\tau) \quad (29)$$

As the cycle repeats, the response of each successive cycle becomes identical. Such a response is called the cyclic steady state. For the forcing of Eq. (29), the cyclic steady state by Eq. (28) is

$$\bar{q}(\tau) = \begin{cases} 6 \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \left(1 + \exp(-\lambda_n \tau) \left[\frac{\exp(-\lambda_n(T-h)) - \exp(-\lambda_n T)}{1 - \exp(-\lambda_n T)} - 1 \right] \right), & 0 \leq \tau \leq h \\ 6 \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \frac{\exp(-\lambda_n(\tau-h)) - \exp(-\lambda_n T)}{1 - \exp(-\lambda_n T)}, & h < \tau < T \end{cases} \quad (30)$$

To compare the approximations in numbers, we used an error scale defined by

$$Er = \frac{\int_0^T (\bar{q}_{\text{exact}} - \bar{q}_{\text{approx}})^2 d\tau}{\int_0^T \bar{q}_{\text{exact}}^2 d\tau} \quad (31)$$

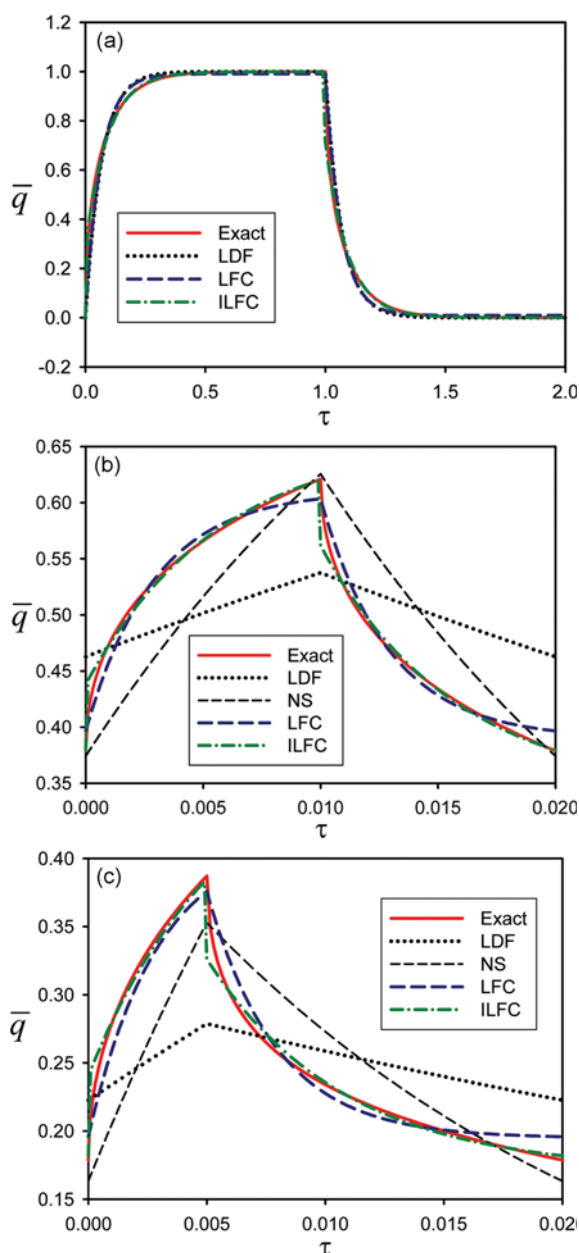


Fig. 1. Comparison of approximations of the responses of a spherical adsorbent under a rectangular wave concentration forcing. Approximation formulas are linear driving force formula (LDF), Eq. (4), the formula by Nakao and Suzuki (NS), Eq. (6), the linear formula for cyclic adsorption (LFC), Eqs. (16)–(18), and the improved linear formula for cyclic adsorption (ILFC), Eqs. (22)–(25). The period and the time of adsorption are (a) $T=2$ and $h=T/2$, (b) $T=0.02$ and $h=T/2$, and (c) $T=0.02$ and $h=T/4$.

We first considered the case of no reaction ($\phi=0$) and a sphere adsorbent ($\zeta=2$). Fig. 1(a)–(b) is the responses of two square wave concentration forcing of $T=2$ and $T=0.02$. For $T=2$ ($\omega=\pi$), the linear formula for cyclic operation (LFC), Eq. (17) with Eq. (18), becomes

$$\frac{dp}{d\tau} = 15.186f(\tau) - 15.4656p, \quad \bar{q} = p + 0.009 \quad (32)$$

Eq. (32) is very close to the LDF, Eq. (4), and hence the responses of LDF and LFC are virtually identical in Fig. 1(a). Er of LDF and LFC are 0.0514 and 0.0471, respectively. The improved linear formula for cyclic operation (ILFC), Eqs. (24) and (25), becomes

$$\frac{dp}{d\tau} = 10.85f(\tau) - 10.86p + 0.2806\frac{df}{d\tau}, \quad \bar{q} = p + 0.0008 \quad (33)$$

This is similar to Eq. (27) for noncyclic operations. Although the response by LFC closely approximates the exact response, the response by Eq. (33) is more accurate with $Er=0.0224$.

For a faster cycle, $T=0.02$ ($\omega=100\pi$), LFC and ILFC are

$$\frac{dp}{d\tau} = 75.46f(\tau) - 341.4p, \quad \bar{q} = p + 0.3895 \quad (34)$$

$$\frac{dp}{d\tau} = 55.48f(\tau) - 174.48p + 0.0585\frac{df}{d\tau}, \quad \bar{q} = p + 0.3410 \quad (35)$$

The empirical formula by Nakao and Suzuki [7], Eq. (6), was developed for fast cycles of $T<0.2$ and hence applicable for $T=0.02$. Eq. (6) for this case is

$$\frac{d\bar{q}}{d\tau} = 51.4(f(\tau) - \bar{q}(\tau)) \quad (36)$$

For the fast cyclic operation, the coefficients in LFC and ILFC are vastly different from the constant coefficients for noncyclic operations. As shown in Fig. 1(b), the LDF and Eq. (36) show considerable errors in the responses. Er of LDF and Eq. (36) are 0.1201 and 0.0950, respectively. The coefficient in Nakao and Suzuki formula has been fitted to the amount of adsorption at the end of the adsorption phase for a square wave concentration forcing with equal time of adsorption and desorption ($h=T/2$), and thus Eq. (36) was able to correctly predict the peak amount of adsorption. Fig. 1(b) also shows that LFC (Eq. (34)) and ILFC (Eq. (35)), on the other hand, yield accurate responses with $Er=0.0168$ (LFC) and $Er=0.0129$ (ILFC).

Fig. 1(c) shows the responses for a rectangular wave forcing of unequal adsorption and desorption phases ($f(\tau)=1$ for $0 \leq \tau < 0.005$, $f(\tau)=0$ for $0.005 \leq \tau < 0.02$, $T=0.002$). As the period of the cycle is the same, Eqs. (34)–(36) are used to obtain the responses. Eq. (36) by Nakao and Suzuki, although better than LDF, results in a poorly accurate response and is unable to predict the peak adsorption amount because the rectangular wave forcing of $h=T/4$ is different from the specific forcing function it has been based on. Er of each approximation was 0.1894 (LDF), 0.1487 (Nakao and Suzuki, Eq. (36)), 0.0403 (LFC) and 0.0261 (ILFC). Here again ILFC gives the best accuracy.

In the presence of reaction ($\phi>0$), only LFC, Eqs. (17) and (18), and ILFC, Eqs. (24) and (25), are valid. Fig. 2 shows the responses

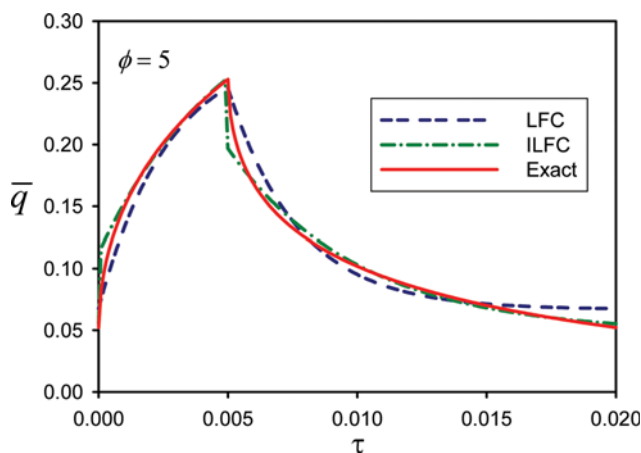


Fig. 2. Comparison of approximations of the responses of a spherical catalyst in the presence of a reaction ($\phi=5$) under a rectangular wave reactant concentration forcing. Approximation formulas are the linear formula for cyclic adsorption (LFC), Eqs. (16)-(18), and the improved linear formula for cyclic adsorption (ILFC), Eqs. (22)-(25). The period and the time of adsorption are $T=0.02$ and $h=T/4$.

of LFC and ILFC for $\phi=5$ and the same $f(\tau)$ of Fig. 1(c) (Eq. (29) with $T=0.02$ and $h=T/4$). When compared to Fig. 1(c), the responses of LFC and ILFC similarly approximate the exact response except the decrease in the peak height of the adsorption due to the presence of the reaction ($\phi=5$). Er of LFC and ILFC are 0.0749 and 0.0475, respectively.

Indeed, more accurate high-order models have been proposed for the approximation [10,12,13]. These models, however, involve multiple first-order differential equations, and the computational load largely depends on the number of equations. The proposed model can be regarded as the most accurate approximate formula for cyclic operations in the form of a single first-order differential equation.

CONCLUSION

An improved linear formula for cyclic adsorption and reaction (ILFC) has been developed. The approximation is a first-order ordinary differential equation, Eq. (24), with coefficients determined by Eqs. (22) and (23) and a constant correction by Eq. (25). In addition to the shape of the sphere, the approximation is also applicable to cylindrical and slab shapes. When compared to the previous first-order approximations, the proposed first-order approximation has significantly better accuracy.

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NOMENCLATURE

A : real part of $G_c(j\omega+\phi)$

A_e : external area of adsorbent particle per volume of the bed [m^{-1}]
 A_0 : time-average concentration of over a period [$mol\ m^{-3}$]
 B : imaginary part of $G_c(j\omega+\phi)$
 C : $G_c(2\omega+\phi^2)$
 C_0 : reference concentration [$mol\ m^{-3}$]
 c : concentration in adsorbent [$mol\ m^{-3}$]
 \bar{c} : average concentration in adsorbent [$mol\ m^{-3}$]
 c_f : concentration in flow phase [$mol\ m^{-3}$]
 D_e : effective diffusivity [$m^2\ s^{-1}$]
 Er : error of approximation defined by Eq. (31)
 $f(\tau)$: dimensionless concentration forcing function ($=h(c_f)/C_0$)
 G_a : approximate transfer function, Eq. (13)
 G_b : approximate transfer function, Eq. (19)
 G_c : exact transfer function defined in Eq. (12)
 h : dimensionless time of adsorption in a cycle, Eq. (29)
 $h(c_f)$: concentration in adsorbent at $r=R$, a function of c_f [$mol\ m^{-3}$]
 j : imaginary number ($=\sqrt{-1}$)
 k : reaction rate constant [s^{-1}]
 P : period of cyclic operation [s]
 q : dimensionless concentration in adsorbent ($=c/C_0$)
 \bar{q} : dimensionless average concentration in adsorbent ($=\bar{c}/C_0$)
 r : radial position in adsorbent [m]
 R : radius of adsorbent [m]
 s : Laplace variable
 t : time [s]
 T : dimensionless period of cyclic adsorption ($=P/\tau_0$)
 U : superficial velocity of the flow through the bed [$m\ s^{-1}$]
 z : axial position in the bed [m]

Greek Letters

α : coefficient defined in Eq. (16)
 α_0 : coefficient defined in Eq. (22)
 α_1 : coefficient defined in Eq. (22)
 β : coefficient defined in Eq. (16)
 β_0 : coefficient defined in Eq. (22)
 ε_b : adsorbent or catalyst bed void fraction
 ζ : shape factor of adsorbent: 0 for an infinite slab, 1 for an infinite cylinder and 2 for a sphere
 ϕ : thiele modulus
 ω : angular velocity of cyclic operation ($=2\pi/T$)
 τ : dimensionless time ($=t/\tau_0$)
 τ_0 : diffusion time constant ($=R^2/De$) [s]

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