

MOMENTS WITH MATHEMATICA*

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Mathematica, an interactive software system that does computer algebra and other mathematical computations, is a valuable tool for solving large problems involving symbol manipulation. Mathematica symbolically performs algebraic and calculus operations such as factorization, substitution, linear algebra, solution of polynomial equations, limits, and evaluation of integrals and derivatives. Numerical computations and visualization of advanced functions by two- or three-dimensional contour plots are also attractive features of the system. Although more efficient packages (e.g., Matlab) are available for large-scale numerical tasks such as matrix inversion, Mathematica can algebraically perform manipulations of this type. Many potential applications of computer algebra systems in chemical engineering research and education are possible to imagine, and in this article we discuss some examples.

The developer of Mathematica, Stephen Wolfram, is the author of a helpful manual called *Mathematica: A System for Doing Mathematics by Computer* (Addison-Wesley Publishing Company, 1988). The book is readable and readily understood by those with a general familiarity of mathematics and computers. Our experience is that studying the manual with the software at hand to work the numerous illustrations is helpful in learning the system. Operations with Mathematica can also be programmed (e.g., do-loops for iterative computations); see, for example, *Programming in Mathematica*.^[1]

Several computer algebra systems are available on the market and promise to automate mathematical computations. Mathematica is particularly attractive because it can be installed in a desktop computer, although speed is compromised. In its workstation configuration, however, Mathematica is fast and user-friendly. Computer algebra systems probably will radically change problem solving in applied mathematics; tedious mathematical compu-

tations will be much less important than the fundamental problem formulation.

Opportunities are plentiful in chemical engineering research and teaching for the application of computerized symbolic manipulation. As an example of its use, we have applied Mathematica to the computation of moment expressions for several problems in separations and chemical reaction engineering.

MOMENTS IN CHEMICAL ENGINEERING

The computation of moments is useful for (1) interpreting experimental concentration profiles, (2) determining mass transport parameters from experimental data, (3) predicting concentration histories, and (4) designing and scaling-up separation processes.

The temporal moments are given by

$$m_n(z) = (-1)^n \lim_{s \rightarrow 0} d^n \bar{c} / ds^n = \int_0^\infty t^n c(t, z) dt \quad (1)$$

where the Laplace transform of the concentration is defined by

$$\bar{c}(s, z) = \int_0^\infty c(t, z) e^{-st} dt \quad (2)$$

Numerical or analytical integration provides values or expressions for the moments when $c(t, z)$ is known or when $\bar{c}(s, z)$ can be derived from a model of the



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process. Thus, we avoid inverting \bar{c} , a task that often is not feasible. The algebraic manipulations to obtain the moments from a mathematical model are:

1. solution of differential equations to determine \bar{c}
2. derivatives with respect to the Laplace transform parameter s
3. limits as $s \rightarrow 0$

The development of \bar{c} in a series provides an easy way to find the lower-order moments. Expanding e^{-st} in Eq. (2) leads to

$$\bar{c}(s, z) = \sum_{n=0}^{\infty} s^n (-1)^n m_n(z) / n! \quad (3)$$

The reduced moments are defined as

$$\mu'_n(z) = m_n / m_0 \quad (4)$$

and the central moments are given by

$$\mu_n(z) = (1/m_0) \int_0^{\infty} (t - \mu'_1)^n c(t, z) dt \quad (5)$$

The binomial expansion of Eq. (5), written in terms of the binomial coefficients, yields

$$\mu_n(z) = \left((1/m_0) \sum_{i=0}^n \binom{n}{i} m_{n-i} (-\mu'_1)^i \right) \quad (6)$$

The first four moments have an important physical significance. The zeroth moment, m_0 , is the area under the concentration plot $c(t)$ and is proportional to the mass of the species. The mass balance ensures that $m_0(z) = m_0(z=0)$ for species that do not react. The first reduced moment μ'_1 , is the position of the peak and gives the average position of the species. The second reduced central moment, μ_2 , measures the spread of the peak. The third reduced central

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moment, μ_3 , is a measure of the skewness of the peak.

For many cases, mathematical models provide the moment expressions in terms of mass transport parameters and geometric properties. From experimental methods, we obtain the concentration $c(t)$. Then the moments can be obtained by numerical integration using Eq. (1). Equating the experimentally determined moments to the moment expressions based on a model of the process represents a method for obtaining equations where the mass transport parameters are the unknowns. Schneider and Smith^[2] obtained estimates for the intraparticle diffusion, axial dispersion, and adsorption coefficients using this method. Mitchell^[3] used probabilistic arguments to obtain the spatial distribution, mean position, and variance about the mean of macromolecules moving in an external field and undergoing reversible isomerization. By comparing these results to experiments, the author was able to provide values for the forward and backward switching rates. The same problem was treated by Killalea and McCoy,^[4] who derived expressions of spatial moments.

The concentration profiles can be constructed using the moments in a Gram-Charlier expansion^[5] *i.e.*,

$$c(t, z) = m_0 e^{-x^2} \sum_{n=0}^{\infty} a_n H_n(x) \quad (7)$$

where

$$x = (t - \mu'_1) / \sqrt{2\mu_2}$$

Expressions of a_0 , a_1 , a_2 , a_3 , and a_4 are depicted in Table 1. The coefficients of the series, a_j , depend on the reduced central moments and are obtained using the orthogonality condition satisfied by the Hermite polynomials, H_n ,

$$\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{nm} \quad (8)$$

where e^{-x^2} is the weighting function. The first five Hermite polynomials are given in Table 1. This procedure is useful for predicting concentration profiles when values of the model parameters are known. Breakthrough curves for fixed-bed adsorbents and reactors can be represented using moments of the impulse response.^[6] As an alternative to Hermite polynomials, the Laguerre polynomials

TABLE 1
Hermite Polynomials and Coefficients of
Gram-Charlier Expansion, Eq. (12)

$H_0(x) = 1$	(1-1)
$H_1(x) = 2x$	(1-2)
$H_2(x) = 4x^2 - 2$	(1-3)
$H_3(x) = 8x^3 - 12x$	(1-4)
$H_4(x) = 16x^4 - 48x^2 + 12$	(1-5)
$a_0 = 1/\sqrt{2\pi\mu_2}$	(1-6)
$a_1 = 0$	(1-7)
$a_2 = 0$	(1-8)
$a_3 = \mu_3 / (3! 2^2 \sqrt{\pi\mu_2^2})$	(1-9)
$a_4 = (\mu_4 / \mu_2^2 - 3) / (4! 4 \sqrt{2\pi\mu_2})$	(1-10)

are frequently used.^[7]

Mehta, *et al.*,^[8] were able to obtain agreement between experimental elution curves and Hermite polynomial series representation. In addition, fitting the two results provided a criterion for the trimming of tails and leading edges. Thus, it is possible to account for phenomena such as end effects. Elution curves in chromatographic columns are nearly Gaussian when dispersion is small relative to convection. For such cases, the first term in the series, the Gaussian approximation, will provide an accurate representation of the pulse.

Chromatography, a widely used separation process, utilizes differences in species behavior, *e.g.*, solid-fluid adsorption, to effect the separation. Reliable ways that make use of the moment theory to analyze and optimize chromatographic separations have been developed. For two solutes A and B, separation is usually satisfactory when

$$R_s = (\mu'_{1A} - \mu'_{1B}) / (\sqrt{\mu'_{2A}} + \sqrt{\mu'_{2B}}) \geq 2 \quad (9)$$

The resolution, R_s , provides a criterion for separation of two species when narrow pulses are injected. We can define the Height Equivalent to a Theoretical Plate concept by

$$\text{HETP} = L\mu_2 / \mu_1'^2 \quad (10)$$

Contrary to R_s , HETP depends only on one input sample size and is an important characteristic for evaluating chromatographic processes.

EXAMPLE PROBLEMS

To illustrate how Mathematics can be used to assist in finding moment expressions for problems of interest to chemical engineers, we discuss three examples. A list of essential commands to solve these problems is available from the authors.

Fluid-Solid Adsorption and Reaction in a CSTR

We consider a continuous-flow stirred tank reactor (CSTR) fed with an input pulse of adsorbable species. As a representation of a catalytic reac-

tion, the adsorbed molecules undergo a reaction that is assumed first-order in the adsorbate concentration. The Laplace transform of $c(t)$, $\bar{c}(s)$, is readily found from the governing equations listed below.

- Mass balance in the fluid

$$\varepsilon \partial c / \partial t = \theta(c_0 - c) - A_p k_p (c - c_i(R)) \quad (11)$$

- Mass balance on an individual particle

$$\beta \partial c_i / \partial t = (D_i / r^2) \partial (r^2 \partial c_i / \partial r) / \partial r - k_{ads} c_i + k_d c_a \quad (12)$$

- Reversible adsorption with first-order surface reaction

$$\partial c_a / \partial t = k_{ads} c_i - k_d c_a - k_r c_a \quad (13)$$

- Initial conditions

$$c = c_i = c_a = 0 \quad \text{for } t = 0 \quad (14)$$

- Boundary conditions

$$(\partial c_i / \partial r)_{r=0} = 0 \quad \text{and} \quad D_i (\partial c_i / \partial r)_{r=R} = k_r (c - c_i)_{r=R} \quad (15)$$

- The inlet concentration is considered an impulse

TABLE 2
The Laplace Transform and Temporal Moments for Fluid-Solid Adsorption and Reaction in a CSTR

$$\bar{c}(s) = \frac{\theta c_0}{\varepsilon s + \theta + A_p k_p - RA_p k_p^2 / (D_i [bR \coth(bR) + k_p R / D_i - 1])} \quad (2-1)$$

$$b = \sqrt{\frac{\beta s + k_{ads} - k_{ads} k_d / (s + k_r + k_d)}{D_i}} \quad (2-2)$$

$$m_0 = \frac{\theta c_0}{\psi} \quad (2-3)$$

$$b_0 = \sqrt{\frac{k_{ads} - k_{ads} k_d / (k_r + k_d)}{D_i}} \quad (2-4)$$

$$v = [b_0 R \coth(b_0 R) + k_p R / D_i - 1] \quad (2-5)$$

$$\psi = \theta + A_p k_p - RA_p k_p^2 / (D_i v) \quad (2-6)$$

$$m_1 = \frac{\theta c_0 \left(\varepsilon + RA_p k_p^2 \left(\frac{R \xi \coth(b_0 R)}{2D_i b_0} + \frac{R^2 \xi (1 - \coth^2(b_0 R))}{2D_i} \right) \right)}{\psi^2} \quad (2-7)$$

$$\xi = (\beta + k_{ads} k_d / (k_r + k_d))^2 \quad (2-8)$$

$$m_2 = \frac{2\theta c_0}{\psi^3} \left(\varepsilon + RA_p k_p \left(\frac{R \xi \coth(b_0 R)}{2D_i b_0} + \frac{R^2 \xi (1 - \coth^2(b_0 R))}{2D_i} \right) \right)^2 / (D_i v^2) + \frac{2\theta c_0 RA_p k_p^2}{\psi^2 D_i v^3} \left(\frac{R \xi \coth(b_0 R)}{2D_i b_0} + \frac{R^2 \xi (1 - \coth^2(b_0 R))}{2D_i} \right)^2 - \frac{\theta c_0 RA_p k_p^2}{\psi^2 D_i v^2} \left(\frac{R \xi^2 \coth(b_0 R)}{4D_i^2 b_0^3} + \frac{R^2 \xi^2 (1 - \coth^2(b_0 R))}{4D_i^2 b_0^2} - \frac{2R^3 \xi^2 \coth(b_0 R) (1 - \coth^2(b_0 R))}{4D_i^2 b_0} \right) - \frac{\theta c_0 RA_p k_p^2}{\psi^2 D_i v^2} \left(\frac{Rk_{ads} k_d \coth(b_0 R)}{(D_i b_0 (k_r + k_d))^3} - \frac{R^2 k_{ads} k_d (1 - \coth^2(b_0 R))}{(D_i (k_r + k_d))^3} \right) \quad (2-9)$$

$$c_0(t) = c_0 \delta(t) \quad (16)$$

The complex nature of the expression for $\bar{c}(s)$, determined from the Laplace transformed solution of Eqs. (11) to (16), makes using Mathematica to compute m_0 , μ'_1 , μ_2 very attractive. We provide expressions for $\bar{c}(s)$, and for m_0 , m_1 , and m_2 in Table 2.

Chromatographic Separation Based on Fluid-Solid Adsorption

Let us consider separation processes based on fluid-solid adsorption such as the adsorption of hydrocarbons on silica gel in a chromatographic column.^[2] The concentration of adsorbing gas, $c(z,t)$, is the solution of the following equations:

- Mass balance of adsorbable component in the gas phase

$$(E_A/\alpha) \partial^2 c / \partial z^2 - v \partial c / \partial z - \partial c / \partial t - 3D_i(1-\alpha)/(R\alpha) \left(\frac{\partial c_i}{\partial r} \right)_{r=R} = 0 \quad (17)$$

- Mass balance of adsorbable component in the particle

$$(D_i/\beta) (\partial^2 c_i / \partial r^2 + 2/r \partial c_i / \partial r) - \partial c_i / \partial t - (\rho_p/\beta) \partial c_{ads} / \partial t = 0 \quad (18)$$

- Linear rate of adsorption

$$\partial c_{ads} / \partial t = k_{ads} (c_i - c_{ads} / K_A) \quad (19)$$

- Boundary conditions

$$\begin{aligned} D_i (\partial c_i / \partial r)_{r=R} &= k_f (c - c_i) \\ (\partial c_i / \partial r)_{r=0} &= 0 \quad \text{for } t > 0 \end{aligned} \quad (20)$$

- Initial conditions

$$\begin{aligned} c &= 0 & \text{at } z > 0 & \text{for } t = 0 \\ c_i &= 0 & \text{at } r \geq 0 & \text{for } t = 0 \end{aligned} \quad (21)$$

- Bed-inlet condition

$$\begin{aligned} c &= c_0(t) & \text{at } z = 0 & \text{for } 0 \leq t \leq t_{0A} \\ c &= 0 & \text{at } z = 0 & \text{for } t > t_{0A} \end{aligned} \quad (22)$$

Kubin^[9] and Kucera^[10] solved this system of equations and obtained $\bar{c}(s,z)$, the Laplace transform of $c(t,z)$, given by Eq. (3-1) in Table 3. Expressions for m_0 , μ'_1 , and μ_2 were also presented by Schneider and Smith^[21] (see Table 3). The computations done by hand require many hours of tedious labor. Simple and fast computations with Mathematica provide an identical result. The procedure is straightforward when a few special techniques are applied. Instead of λ defined by Eq. (3-4) in Table 3, we use its development in series around the point $s = 0$ to order s^7 . Around the point $\lambda = 0$, we apply the series

$$\sqrt{\lambda} \tanh(R\sqrt{\lambda}) = R\lambda - (R^3\lambda^2)/3 + 2(R^5\lambda^3)/15 + 0(\lambda^3) \quad (23)$$

To avoid taking the derivatives of $\lambda^{1/2}$ around $\lambda = 0$, which presents some problems, we substitute the left-hand side of Eq. (23) into the definition of $h(s)$, Eq. (3-3) in Table 3. This allows one to obtain a development in series of $h(s)$ around the point $s = 0$ to order s^4 , which is used in Eq. (3-2) to develop the series for γ .

Finally, we are able to compute the derivatives of $\bar{c}(s,z)$ and obtain μ'_1 , and μ_2 . Unfortunately, rearranging the result into a neat form requires human judgement and is not convenient with Mathematica. However, this task is readily performed by hand.

Spatial Moments of Moving and Interchanging Isomers

We are interested in finding the spatial moments of two isomers A_1 and A_2 , which are moving, and switching back and forth between the two isometric states as a first-order reaction. This system describes electrophoresis, gel filtration, or sedimentation if the species are moving respectively in an electrostatic, velocity, or centrifugal field. The system is a type of chromatographic reactor.

The governing equations of the concentration are

TABLE 3
The Laplace Transform and Temporal Moments for Chromatographic Separation Based on Fluid-Solid Adsorption

$$\bar{c}(s,z) = (c_0/s) (1 - e^{-st_{0A}}) e^{-\gamma z} \quad (3-1)$$

$$\gamma = -(v\alpha/2E_A) + \sqrt{(v\alpha/2E_A)^2 + (s\alpha/E_A)(1+h(s))} \quad (3-2)$$

$$h(s) = (3k_f/R) \left[\frac{1/s - 1/((sD_i/k_f)\sqrt{\lambda} \coth(R\sqrt{\lambda}) + s(1 - (D_i/Rk_f)))}{1/((sD_i/k_f)\sqrt{\lambda} \coth(R\sqrt{\lambda}) + s(1 - (D_i/Rk_f)))} \right] \quad (3-3)$$

$$\lambda = (s\beta/D_i) \left(1 + \rho_p K_A k_{ads} / (\beta(K_A s + k_{ads})) \right) \quad (3-4)$$

$$m_0 = m_0(z=0) \quad (3-5)$$

$$\mu'_1 = (z/v)(1 + \delta_0) + \mu'_1(z=0) \quad (3-6)$$

$$\mu_2 = (2z/v) \left[\delta_1 + (E_A/\alpha)(1 + \delta_0)^2 (1/v^2) \right] + \mu_2(z=0) \quad (3-7)$$

$$\delta_0 = ((1-\alpha)\beta/\alpha) \left(1 + (K_A \rho_p/\beta) \right) \quad (3-8)$$

$$\delta_1 = ((1-\alpha)\beta/\alpha) \left[\frac{K_A^2 \rho_p / (\beta k_{ads}) + (R^2 \beta / 15) \left(1 + (\rho_p K_A / \beta) \right)^2 (1/D_i - 5/(Rk_f))}{(R^2 \beta / 15) \left(1 + (\rho_p K_A / \beta) \right)^2 (1/D_i - 5/(Rk_f))} \right] \quad (3-9)$$

When $c_0(t=0) = c_0$ for $0 \leq t \leq t_{0A}$ we have the following results:

$$m_0 = c_0 t_{0A} \quad \mu'_1(z=0) = t_{0A}/2 \quad \mu_2(z=0) = t_{0A}^2/12 \quad (3-10)$$

$$\begin{cases} \frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2} - v_1 \frac{\partial c_1}{\partial x} - k_1 c_1 + k_2 c_2 \\ \frac{\partial c_2}{\partial t} = D_2 \frac{\partial^2 c_2}{\partial x^2} - v_2 \frac{\partial c_2}{\partial x} - k_2 c_2 + k_1 c_1 \end{cases} \quad (24)$$

where D_j is the diffusion of axial dispersion coefficient, v_j is the species velocity, and k_j is the rate constant for isomerization.

- The boundary conditions are

$$c_j(t, x \rightarrow \pm\infty) = 0 \quad \text{for } j=1 \text{ and } 2 \quad (25)$$

- The initial conditions are infinitesimally narrow distributions

$$c_j(t=0, x) = f_j \delta(x) \quad \text{for } j=1 \text{ and } 2 \quad (26)$$

with the total initial concentration given by $f_1 + f_2 = 1$.

Mathematica provides (a) the Fourier transform of $c_j(x, t)$ defined by

$$\bar{c}_j(k, t) = \int_{-\infty}^{+\infty} c_j(x, t) e^{-ikx} dx \quad (27)$$

and (b) the limits of the successive derivatives of \bar{c}_j .

In terms of $c_j(x, t)$ and $\bar{c}_j(k, t)$, the n^{th} spatial moment of species A_j is given by

$$m_{nj}(t) = \int_{-\infty}^{+\infty} c_j(x, t) x^n dx = (i)^n \lim_{k \rightarrow 0} d^n \bar{c}_j(k, t) / dk^n \quad (28)$$

Thus we are able to compute expressions for m_{0j} , m_{1j} , and m_{2j} (see Table 4). Similar results were presented by Killalea and McCoy^[4] and can be used to construct the concentration profiles as explained in section I.3. Mathematica can handle readily such algebraic calculations.

Isomerization in a Countercurrent Chromatographic Reactor

Based on the movement in opposite directions of a sorbent and a fluid, a countercurrent chromatographic reactor can carry out separation and reaction simultaneously. This can push to completion a reaction limited by equilibrium. Thus, such a device can enhance the conversion of the product in reversible reactions of type $A_1 \leftrightarrow A_2$. Experimental investigation of such a system was provided by Takeuchi, *et al.*,^[11] who studied xylene isomerization.

The governing equations are given by a special form of Eq. (24)

$$\begin{cases} -u_1 \frac{dc_1}{dx} - k_1 c_1 + k_2 c_2 = 0 \\ -u_2 \frac{dc_2}{dx} + k_1 c_1 - k_2 c_2 = 0 \end{cases} \quad (29)$$

TABLE 4

Spatial Moments for Moving and Interchanging Isomers

$$m_{01} = (k_2/k_+) (f_1 - f_2/k_+) e^{-k_+ t} \quad (4-1)$$

$$m_{11} = \Delta v k_2 (k_1 - k_2 + f_1 k_+) (1 - e^{-k_+ t}) / k_+^3 - t [(k_2 - f_1 k_+) (v_1 k_1 + v_2 k_2) e^{-k_+ t} - k_2 (v_1 k_2 + v_2 k_1)] / k_+^2 \quad (4-2)$$

$$m_{21} = (2k_2/k_+) (D_1 - D_2) [k_2(1-f_1) - k_1(1+f_1)] (e^{-k_+ t} - 1) - (2k_2(\Delta v)^2/k_+^5) [k_2^2(1-f_1)(e^{-k_+ t} - 1) + k_1^2(1+2f_1)(e^{-k_+ t} - 1) + k_1 k_2(4-f_1)(1 - e^{-k_+ t})] + (2t/k_+^2) [D_1 k_2^2 + D_2 k_1 k_2 (1+f_1 e^{-k_+ t}) + D_1 k_1^2 f_1 e^{-k_+ t} - k_2^2(1-f_1) e^{-k_+ t} (D_1 k_1 + D_2 k_2)] - (2t(\Delta v)^2/k_+^4) k_1 k_2 [k_1 f_1 e^{-k_+ t} - k_2 (1 + (1-f_1) e^{-k_+ t})] - (2t(\Delta v)/k_+^4) (v_1 k_1 + v_2 k_2) [2k_1^2 f_1 + k_2(1-f_1)(k_2 - k_1)] e^{-k_+ t} - (t^2 e^{-k_+ t}/k_+^2) (f_1 - k_2/k_+) (v_1 k_1 + v_2 k_2)^2 - (t^2 k_2/k_+^3) (v_1 k_2 + v_2 k_1)^2 \quad (4-3)$$

where

$$\Delta v = v_1 - v_2 \quad (4-4)$$

$$k_+ = k_1 + k_2 \quad (4-5)$$

To find m_{02} , m_{12} , and m_{22} , interchange subscripts 1 and 2.

TABLE 5

Concentration Profiles for Isomerization in a Countercurrent Chromatographic Reactor

$$c_1 = A e^{-rx} + B \quad (5-1)$$

$$c_2 = -(u_1/u_2) A e^{-rx} + (k_1/k_2) B \quad (5-2)$$

where

$$A = (c_{10} k_1 u_2 e^{rL}) / (k_2 u_1 + k_1 u_2 e^{rL}) \quad (5-3)$$

$$B = (c_{10} k_1 u_1 + c_{20} u_2 k_1) / (k_1 u_2 + k_2 u_1) \quad (5-4)$$

$$c_{20} = (c_{10} k_1 u_1 (1 - e^{rL})) / (k_2 u_1 + k_1 u_2 e^{rL}) \quad (5-5)$$

$$r = k_1/u_1 + k_2/u_2 \quad (5-6)$$

where

$$u_1 = u - u_s K_1 \quad \text{and} \quad u_2 = u - u_s K_2$$

We have made the following assumptions: (1) steady state, (2) adsorption equilibrium, (3) no axial dispersion, (4) linear adsorption isotherm, (5) isothermal operation, (6) first-order reversible reactions, and (7) constant linear velocities.

The solid adsorbent, moving countercurrently to the fluid at velocity u_s carries the adsorbates A_1 and A_2 , which have adsorption equilibrium K_1 and K_2 . We select the feed, sorbent, and species velocities in such a way that (1) A_1 is continuously fed at the bottom of the reactor, (2) sorbent is supplied at the top of the reactor, (3) A_1 is less strongly adsorbed than A_2 , (4) A_1 is moving upward with the fluid and A_2 is transported downward by the sorbent, and (5) A_1 is completely converted in the reactor and the exiting stream is free of A_2 . Thus, the boundary conditions are

$$\begin{cases} c_1(0^+) = c_{10} \\ c_2(L^-) = 0 \end{cases} \quad (30)$$

The concentrations present discontinuities at the inlet and outlet of the reactor. The flux conservation equations provide values for these jumps.

$$\begin{cases} c_1(L^+) = c_1(L^-)u_1/u \\ c_2(0^-) = -c_2(0^+)u_2/u_s \end{cases} \quad (31)$$

Expressions for the concentrations c_1 and c_2 are depicted in Table 5. With Mathematica, one can first find these expressions, then perform numerical simulations, and finally plot the results.

CONCLUSIONS

We have described the computation of expressions of moments using Mathematica for chemical reaction or separation processes. These computations are exceedingly tedious to perform and to confirm when done by hand. Mathematica is an interesting tool for solving problems with algebraic manipulations because it is user-friendly, powerful, and fast. This is particularly true when the software is run on a Unix machine rather than a smaller, slower personal computer. It should be clear that Mathematica has limitations, some of which can be overcome by skillful organizing of the computational steps. The numerical, graphic, and programming capabilities of Mathematica are exciting potentials that can be applied in multiple areas of chemical engineering.

NOMENCLATURE

- α = interparticle void fraction in the adsorbent bed
- $A_p = 3 n_p / R \rho_p$
- β = interparticle void fraction (internal porosity) of the adsorbent
- c = concentration of the adsorbable fluid in the interparticle space
- c_0 = input concentration of the adsorbable fluid
- c_1, c_2 = concentration of species A_1, A_2
- c_{ads} = concentration of the adsorbed fluid
- c_i = concentration of the adsorbable fluid in the pore space
- δ_0, δ_1 = defined by Eqs. (3-8) and (3-9)
- D_1, D_2 = diffusion or axial dispersion coefficient of species A_1, A_2
- D_i = effective intraparticle diffusion coefficient

- $\varepsilon = 1 - n_p / \rho_p$
- E_A = effective axial dispersion coefficient
- f_1, f_2 = rate constant of species A_1, A_2
- γ = defined by Eq. (3-2)
- $h(p)$ = function given by Eq. (3-3)
- K_1, K_2 = adsorption equilibrium constant
- k_1, k_2 = rate constant of species A_1, A_2
- K_A = adsorption equilibrium constant
- k_{ads} = adsorption rate constant
- k_d = desorption rate parameter
- k_f = mass transfer coefficient in column
- k_p = mass transfer coefficient in the CSTR
- k_r = surface reaction rate
- L = length of chromatographic reactor
- λ = defined by Eq. (3-4)
- m_n = n^{th} moment
- m_{nj} = n^{th} moment of species A_j where $j = 1$ or 2
- n_p = number of particles (grams/vol. of reactor)
- θ = ratio of volumetric flow rate to CSTR volume
- R = radius of the spherical particle of adsorbent
- ρ_p = apparent particle density
- s = variable in the Laplace transformation
- t = time
- t_{0A} = time of duration of the injection of adsorbate
- u = superficial fluid velocity
- u_1, u_2 = velocities of species A_1, A_2 in the countercurrent column
- u_s = superficial solid velocity
- v = linear velocity of the carrier gas in the interparticle space
- v_1, v_2 = velocities of species A_1, A_2
- x = axial coordinate in the countercurrent column
- z = length coordinate of the bed of adsorbent

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