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Manuscript received February 23, 1982; revision received August 25, and accepted September 3, 1982.

Curve-Fitting Monotonic Functions

K. VISWANATHAN

Department of Chemical Engineering
Indian Institute of Technology,
Hauz Khas, New Delhi 110016, India

INTRODUCTION

The identification of the form of the functional relationship between variables is generally approached by trial and error. Some standard forms of functions are tried for a particular shape, and the one that deviates least from the actual values, experimentally obtained, is chosen (Davies, 1962). Or, a least square polynomial is fitted. Once the form of the function is known, the problem at hand can be solved analytically.

The method given in this paper can be used to avoid excessive trial and error in arriving at a functional form. The method is developed for functions known to be monotonic which is often the case in engineering examples. In such cases polynomials are not suitable as they may not everywhere have a positive (or negative) slope. The analysis described here can be applied when theoretical expressions are not available. In the present study, only one independant variable and one dependant variable are considered.

THEORETICAL DEVELOPMENT

A new variable Z is defined as

$$Z = \frac{x}{y}\frac{dy}{dx} = \frac{xy'}{y} \tag{1}$$

Z is the ratio of fractional change in y to that of x. It will be called the monotonic transform of y with respect to x and will be written as $\text{mon}_x\, y$ (to be read as mon y to the base x) or simply mon y. Some standard forms of monotonically increasing functions, Table 1, are considered. Table 1 also gives the monotonic transforms of the various functions.

Our aim is to calculate Z from experimentally-obtained x and y values. For this, the following finite difference approximation which follows from Eq. 1 is used.

$$Z\Bigg|_{x = \frac{x_i + x_{i+1}}{2}} = \frac{ln(y_{i+1}/y_i)}{ln(x_{i+1}/x_i)} \tag{2}$$

It can be shown that Eq. 2 would be exact for

$$ln\, y = a(ln\, x)^2 + m\, ln\, x + ln\, C$$

or

$$y = Cx^{m + a\, ln\, x}$$

TABLE 1. SOME FREQUENTLY OCCURING MONOTONICALLY INCREASING FUNCTIONS AND THEIR MONOTONIC TRANSFORMS

Name	Function	Monotonic Transform
Basic 1	$y = Cx^m$	$Z = m$
Basic 2	$y^* = C\exp(bx^n)$	$Z = nbx^n$
Basic 3	$y = C\exp(bx^{-n})$	$Z = nbx^{-n}$
Basic 4	$y = \left(\frac{1}{b}\, ln\, \frac{x}{C}\right)^{1/n}$	$Z = \frac{1}{n ln(x/C)}$
Basic 5	$y = \left(-\frac{1}{b}\, ln\, \frac{x}{C}\right)^{-1/n}$	$Z = \frac{-1}{n ln(x/C)}$
Nonbasic 1	$y = Cx^m \exp(bx^n)$	$Z = m + nbx^n$
Nonbasic 2	$y = Cx^m \exp(-bx^{-n})$	$Z = m + nbx^{-n}$
Nonbasic 3	$y = Cx^m (lnbx)^{1/n}$	$Z = m + \frac{C^n x^{mn}}{ny^n}$
Nonbasic 4	$y = Cx^m (-lnbx)^{-1/n}$	$Z = m + \frac{C^{-n} x^{-mn}}{ny^{-n}}$

* The general form $CK^{b'x^n}$ is included here where b equals $b' lnK$.

As a particular case, the method is exact for $y = Cx^m$ (for any m) whereas the corresponding existing finite difference equation for the derivative is exact only for m equal to 0, 1 and 2.

The error in the numerical estimation of the monotonic transform from Eq. 2 for any other functional form is given by:

$$E = \frac{Z_{\text{calc. from Eq. 2}} - Z_{\text{actual at } x = (x_i + x_{i+1})/2}}{Z_{\text{actual at } x = (x_i x_{i+1})/2}} \qquad (3)$$

For basic form 2, Eq. 3 becomes:

$$E = \frac{ln(\exp(bx_{i+1}^n - bx_i^n))/ln(x_{i+1}/x_i)}{nb((x_i + x_{i+1})/2)^n} - 1 \qquad (4)$$

which can be simplified to:

$$E = \left(\frac{(1 - f^n)}{ln(1/f)}\right) \Big/ \left(\frac{n(1 + f)^n}{2^n}\right) - 1 \qquad (5)$$

where f equals (x_i/x_{i+1}).

For basic form 3, the error can be shown to be given by Eq. 5 with n replaced by $-n$.

It can be seen from Eq. 5 that the error in the estimation of Z is a function only of the ratio of the consecutive values of the independant variable, f. Further, it can be shown (by applying L'Hospital rule) that this error approaches zero as f approaches unity. Hence the method tends to exactness as x increases if Δx between observations is constant whereas error in the existing finite difference formulae for derivative is a function of Δx. The error analysis allows us to reject certain experimental points for which error in calculating Z may be unacceptable.

From Eqs. 2 and 3 and the fact that monotonic transform of the product of two functions equals the sum of the monotonic transforms of the two functions (that is, mon(fg) = mon f + mon g) it follows that:

$$E_{fg} = (Z_f E_f + Z_g E_g)/(Z_f + Z_g) \qquad (6)$$

Thus E_{fg} is in between E_f and E_g. Hence, the error in calculating Z for the nonbasic forms 1 to 4 in Table 1 is less than the error for basic forms 2 to 5 respectively as it was shown before that the error for basic 1 is zero.

PROCEDURE

The results obtained above are used here to develop a procedure to arrive at the functional relationship. Physical considerations of the problem will often eliminate certain forms of the functions. For example,

1. If $y = 0$ at $x = 0$, the forms like $C \exp(bx^n)$ and $C(ln\, bx)^{1/n}$ are eliminated.
2. If y' is also known to be monotonically increasing then only $C \exp(bx^n)(n > 1)$ and $Cx^m \exp(bx^n)(m > 1)$ are possible.

From experimental x,y data, Z is to be calculated according to Eq. 2. From the nature of variation of Z, the possible functional forms can be obtained as follows.

Increasing Z	Decreasing Z
$Z = m + nb\,x^n$	$Z = m + nb\,x^{-n}$
$Z = m + \dfrac{y^n}{nC^n x^{mn}}$	$Z = m + \dfrac{y^{-n}}{nC^{-n} x^{-mn}}$

Then any one of the following steps shall be followed by the function.

Step 1. If Z is nearly a constant, $y = Cx^m$ where the constant $Z = m$. The C values are evaluated at all experimental x,y values as $C = yx^{-m}$. An average value of C may be taken.

Step 2. If Z is monotonically increasing, from calculated Z values find Z at $x = 0$ and equate it to m.

2.1. A linear plot of $ln(Z - m)$ vs. $ln\, x$ means $y = Cx^m \exp(bx^n)$. From the slope and intercept n and b can be calculated. Then C values are calculated at all x,y points and an average C is taken.

2.2. A linear plot of $ln(Z - m)$ vs. $ln(y/x^m)$ means $y = Cx^m(-ln\, bx)^{-1/n}$. From the slope and intercept n and C can be calculated. Then b values are calculated at all x,y points and an average b is taken.

Step 3. If Z is monotonically decreasing, from calculated Z values find Z at $x = \infty$ and equate it to m.

3.1. A linear plot of $ln(Z - m)$ vs. $ln\, x$ means $y = Cx^m \exp(-bx^{-n})$.

3.2. A linear plot of $ln(Z - m)$ vs. $ln(y/x^m)$ means $y = Cx^m(ln\, b\, x)^{1/n}$.

The constants n, b and C are evaluated in exactly the same manner as that explained in Step 2.

If no step explained above is followed by the data to reasonable accuracy, it means that none of the functional forms considered here is adequate to represent the data.

With conventional approach direct fitting of only two-parameter equation is possible. Since mon C = 0 the multiplication constant attached to any function gets eliminated in the monotonic transform thereby enabling two parameters to be found first from $Z - x$ relationship and then C is found from experimental x,y data; this is completely different from conventional methods. For example, if $y = \exp(bx^n)$, a plot of $ln(ln\, y)$ vs. $ln\, x$ can yield n and b. But if $y = C \exp(bx^n)$, the conventional method fails totally. Initial elimination of the constant C from the scene enables *three-parameter equation to be fit using monotonic transform.* In four-parameter NONBASIC forms, determination of m as proposed may not yield the best value. Still, the error in $y - x$ relationship would not differ much from the lowest value (corre-

TABLE 2. SUMMARY OF CALCULATIONS FOR THE EXAMPLE

1 x	2 y	3 Z	4 lnx_{av}	5 $ln(Z - 0.12)$	6 C
0	0				—
0.149	0.314	—	−2.60	—	0.378
0.297	0.346	0.143	−1.50	−3.78	0.375
0.841	0.408	0.159	−0.56	−3.24	0.368
1.68	0.482	0.241	−0.08	−2.1	0.376
2.38	0.530	0.273	0.71	−1.88	0.379
3.36	0.584	0.281	1.05	−1.83	0.380
6.73	0.768	0.394	1.62	−1.3	0.397
9.42	0.882	0.42	2.10	−1.2	0.398
15.85	0.984	0.21	2.54	−2.4	0.345

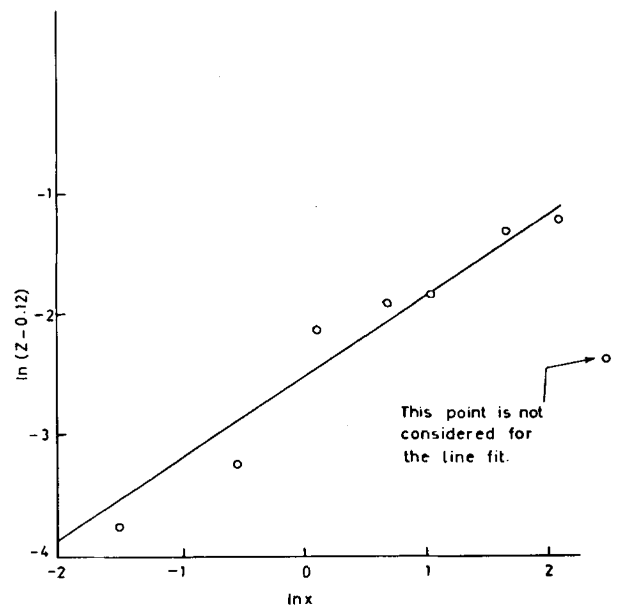

Figure 1. Plot of $ln(Z - 0.12)$ vs. $ln\, x$ to obtain the Parameters n and b for the considered example.

TABLE 3. SUMMARY OF EQUATIONS FOR PARTICLE SIZE DISTRIBUTION

Reference	Material	Parameters of NONBASIC 2 in Table 1				Range of x 'mm'	Average absolute error, %
		C	m	b	n		
Smith (1960)	Cement kiln feed	1.0	0	0.0005	2.56	0–0.297	3
	Taconite tailings	0.88	0.25	0	—	0–0.84	2.6
		1.44	0.0	0.5000	0.50	0.84–1.68	
	Phosphate concentrate	1.0	0	0.0008	3.05	0–0.297	2
	Borax tailings	0.377	0.12	−0.1368	−0.60	0–15.85	4
	Magnetite	0.05	−1.3	0.0024	1.94	0–0.044	3
	Crude anhydride	1.0	0	0.1730	0.84	0–3.36	5
	Red mud Slurry	1.0	0	0.0700	0.71	0–1.68	4
Shook et al. (1973)	Sand	1.0	0	0.0868	1.85	0–1.19	3
	Sand	1.0	0	0.0828	1.06	0–2.38	2
	Sand	1.0	0	0.0004	4.40	0–1.6	5
Govindan (1979)	Sand	1.0	0	0.0003	4.77	0–0.5	5

sponding to the best relationship) as there are three other parameters which would automatically get adjusted in the best possible manner for the corresponding m-value. This is shown to be true later in examples where such forms are encountered.

Example

The particle-size distribution data of Borax refining tailings (Smith, 1970) is given in Table 2, Columns 1 and 2. Calculations up to column 4 are straightforward. Z is seen to be monotonically increasing. Hence Z at $x = 0$ is to be found (Step 2). It can be seen from column 3 that Z at $x = 0$ might be 0.12. Hence according to step 2.1 $ln(Z - 0.12)$ is plotted against $ln\ x$ in Figure 1. Without including the last point the slope is 0.6.

$$\text{Slope} = n = 0.6$$
$$\text{Intercept} = ln\ nb = -2.5$$
$$\therefore b = \exp(-2.5/0.6) = 0.1368$$

Hence the equation is

$$y = Cx^{0.12} \exp(0.1368x^{0.6}) \quad (7)$$

From experimental x,y values C is calculated and given in column 6. The average of all C values is 0.377. Hence Eq. 7 becomes

$$y = 0.377x^{0.12} \exp(0.1368\ x^{0.6}) \quad (8)$$

The maximum error involved in the numerical estimation of monotonic transform from Eqs. 5 and 6 is (for minimum f = 0.297/0.841)0.0086 or 0.86%. This means that the numerical approximation (Eq. 2) used here to calculate monotonic transform is very powerful and this fact can be used in a number of other ways too.

Eleven more sets of particle-size distributions reported by Shook et al. (1973), Smith (1970), and Govindan (1979) were tested with the method developed. Excepting one all the sets could be correlated by the present method. The equations thus obtained are summarized in Table 3 along with the error values. An interesting point which can be observed from Table 3 is that most of the data are well represented by

$$y = \exp(-bx^{-n}) \quad (9)$$

This is different from all the distributions generally considered to be standard (Viswanathan et al., 1982). Equation 9 can also be considered as a standard particle size distribution.

CONCLUDING REMARKS

The method developed in this paper has been successfully used to find compact functional relationships in many other applications such as compression ratios of R114 (working fluid in heat pumps), centrifugal efficiency of a cyclone etc. The described monotonic transform can be effectively used in eliminating trial and error to find standard functional relationships also (Viswanathan and Mani, 1980). The low error in the numerical estimation of the monotonic transform from Eq. 2 can also be effectively put to use for numerical estimation of derivative.

The nine forms of relationships considered in this paper (Table 1) are for monotonically increasing functions. Similar methods can be developed for monotonically decreasing functions.

NOTATION

a = a constant
b = a constant
C = a constant
E = relative error involved in the numerical estimation of monotonic transform, given by Eq. 3
f = ratio of consecutive values of the independent variable, x_i/x_{i+1}
m an exponent
n = an exponent
x = independant variable
y = dependant variable
Z = monotonic transform defined as $\frac{x}{y}\frac{dy}{dx}$

Subscript

i = refers to data point

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Manuscript received January 12, 1982; revision received March 29, and accepted April 19, 1982.

Analytical Solution for a First-Order Reaction in a Packed Bed with Diffusion

J. C. HUANG, D. ROTHSTEIN,
and R. MADEY

Department of Physics
Kent State University
Kent, OH 44242

An analytical solution for a packed bed reactor with a first-order reaction is important in reactor analysis. Transient-state solutions for a reactive adsorbate in a packed bed relate closely to the solutions for nonreactive adsorbates. Rosen (1952) derived a solution for the breakthrough curve for a nonreactive adsorbate with both interfacial and intraparticle diffusional resistances. Rasmuson and Neretnieks (1980) extended the model of Rosen to include longitudinal dispersion; however, they chose the first Bromwich path of integration for inverting the Laplace transform of a function with branch points. In this paper, we choose the second Bromwich path in order to derive the transient solution for a gas sample flowing through a packed bed where a first-order reaction takes place in the solid phase. The solution for a radioactive gas can be generalized from our solution, and the solution for a nonreactive gas is a simplification of our solution.

The differential equations, which describe the gas-phase concentration C and the solid-phase concentration q, are written as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial z} - D_L\frac{\partial^2 C}{\partial z^2} = -\frac{1-\epsilon}{\epsilon}\frac{\partial \overset{\Delta}{q}}{\partial t} - \frac{1-\epsilon}{\epsilon}\lambda\overset{\Delta}{q} \quad (1)$$

and

$$\frac{\partial q}{\partial t} = D_s\left(\frac{\partial^2 q}{\partial r^2} + \frac{2}{r}\frac{\partial q}{\partial r}\right) - \lambda q \quad (2)$$

Here we assumed that the gas-phase concentration does not change significantly over a distance equal to a diameter of the catalyst pellets. This assumption was discussed by Babcock et al. (1966). The average solid-phase concentration $\overset{\Delta}{q}$ for spherical pellets is given by

$$\overset{\Delta}{q} = \frac{3}{R^3}\int_0^R q(r,z,t)r^2dr \quad (3)$$

The introduction of an average concentration eliminates the radial dependence of the solid-phase concentration from Eq. 1.

The initial and boundary conditions are written as

$$C(0,t) = C_0 \quad (4)$$

$$C(\infty,t) = 0 \quad (5)$$

$$C(z,0) = 0 \quad (6)$$

$$q_i(0,z,t) \neq \infty \quad (7)$$

$$q_i(R,z,t) = q_s(z,t) \text{ given by } \frac{\partial \overset{\Delta}{q}}{\partial t} = \frac{3k_f}{R}\left(C - \frac{q_s}{K}\right) - \lambda\overset{\Delta}{q} \quad (8)$$

$$q_i(r,z,0) = 0 \quad (9)$$

Equations 2 through 9 can be solved formally using Duhamel's theorem for arbitrary concentrations $q_s(z,t)$ on the surface of the pellets:

$$q(r,z,t) = \int_0^t q_s(z,\tau)\frac{\partial}{\partial t}F(r,t-\tau)d\tau \quad (10)$$

where $F(r,t)$ is the solution of Eq. 2 for a step increase of the concentration at the surface of the pellets (i.e., $r = R$). Then substituting Eq. 10 into Eq. 3 and performing the integration over r, we obtain

$$\overset{\Delta}{q} = \frac{3}{R^3}\int_0^R\int_0^t q_s(z,\tau)\frac{\partial}{\partial t}F(r,t-\tau)r^2d\tau dr \quad (11)$$

Taking the Laplace transform of Eqs. 8 and 11, we have

$$s\tilde{\overset{\Delta}{q}} = \frac{3k_f}{R}\left(\tilde{C} - \frac{\tilde{q}_s}{K}\right) - \lambda\tilde{\overset{\Delta}{q}} \quad (12)$$

and

$$\tilde{\overset{\Delta}{q}} = \frac{3}{R^3}\int_0^R q_s(z,\tau)\frac{R}{r}\frac{\sinh r\sqrt{\dfrac{\lambda+s}{D_s}}}{\sinh R\sqrt{\dfrac{\lambda+s}{D_s}}}r^2dr \quad (13)$$

$$= \frac{3D_s\tilde{q}_s(z,\tau)}{R^2(\lambda+s)}\left(R\sqrt{\frac{\lambda+s}{D_s}}\coth R\sqrt{\frac{\lambda+s}{D_s}} - 1\right) \quad (14)$$

Again, taking the Laplace transform of Eq. 1 and using Eqs. 13 and 14 to eliminate $\tilde{q}_s$ and $\tilde{\overset{\Delta}{q}}$, we have

$$\frac{\partial^2\tilde{C}}{\partial z^2} - \frac{u}{D_L}\frac{\partial\tilde{C}}{\partial z} - \left(\frac{s}{D_L} + \frac{Y_T(s)}{mD_L}\right)\tilde{C} = 0 \quad (15)$$

where

$$Y_T(s) = \frac{Y_D(s)}{1 + R_F Y_D(s)} \quad (16)$$

$$Y_D(s) = \frac{3K(s+\lambda)}{\sigma^2}(\sigma\coth\sigma - 1) \quad (17)$$

Present address of J. C. Huang: General Electric Co., Corporate Research & Development, P.O. Box 8, Schenectady, NY 12301.