EASY WAY TO CALCULATE THE ANZELIUS – SCHUMANN J FUNCTION

by

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The paper deals with the computational aspects of the so called Anzelius function. This special function is the fundamental one for describing the kinetics of a fixed-bed adsorber and is widely used on the theory of breakthrough curves not only in adsorption and ion exchange, but in the other operations with isomorphous mathematical models as well. Instead of the use of graphical and tabular presentations of the numerical values of this function (what is common practice in chemical engineering literature) the paper proposes a simple algorithm as an alternative for its evaluation. The algorithm is very efficient and extremely accurate for entire range of parameters of interest.

Introduction

The central problem in the design of the processes in the fixed-bed adsorption or ion exchange is the one of establishing the dynamic response of packet column to a step change in feed concentration, viz. the problem of predicting the breakthrough curves. It is a well known fact that the socalled Anzelius [1] – Schumann [2] function given by:

$$J(x,y)+1-e^{-y}\int_0^x e^{-\xi} I_0\left(2\sqrt{y\xi}\right)d\xi \tag{1}$$

is the fundamental one for describing the kinetics of a fixed-bed adsorber and is widely used on the theory of breakthrough curves not only in adsorption and ion exchange, but in other operations with isomorphous mathematical models as well. (See [3] for background of the fixed-bed operations.) The arguments x and y (dimensionless distance and time, respectively) usually involve dimensionless groups related to column capacity parameter, throughput parameter and separation factor. Up to date, the chemical engineer is directed to the use of graphical and tabular presentation of this function [3, 4].

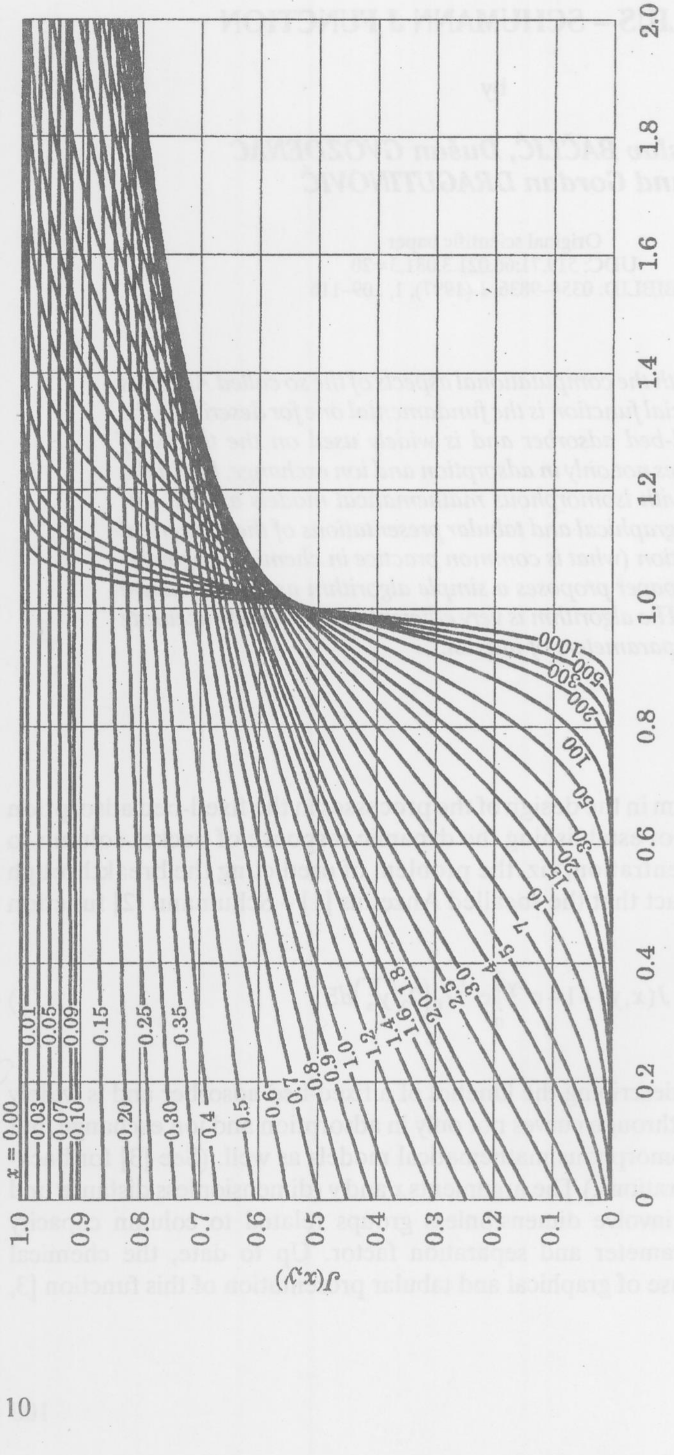

Figure 1. Anzelius-Schumann J function

Figure 1 is a graph of the Anzelius-Schumann function in which we have plotted a dense population of $J(x, y)$ lines at constant x for various y/x so that the whole region of practical interest is covered.

This paper deals with the computational aspects of the function (1) pointing out that there is no need for "new solutions" such as one presented in [5], since the following explicit and very convergent relation holds [6–8],

$$J(x,y) = \mathrm{e}^{-(x+y)} \sum_{n=0}^{\infty} (y/x)^{n/2} I_n\left(2\sqrt{xy}\right) = 1 - \mathrm{e}^{-(x+y)} \sum_{n=1}^{\infty} (x/y)^{n/2} I_n\left(2\sqrt{xy}\right) \qquad (2)$$

This formula is convenient for mini-desk-top computers having a subroutine for the modified Bessel functions of integer order. However, in order to eliminate the use of tabular and nomographic presentations of concentration histories as well as to eliminate the computation of Bessel functions this paper proposes a simple algorithm as an alternative for evaluating $J(x, y)$. The latter is based on Parl's method of calculating the generalized Marcum $Q\left(\sqrt{2x}, \sqrt{2y}\right)$ function [9].

On the search for new solutions for fixed-bed adsorption problem

The problem of predicting breakthrough curves from basic kinetic and equilibrium data has attracted much attention because of its importance not only concerning adsorption columns but also in relation to chromatography and ion exchange. In principle, the breakthrough curve may be calculated, for any system of known kinetics, from the solution of the differential rate equation subject to the boundary conditions imposed by the differential fluid phase mass balance for an element of column.

Recently Liaw et al [5] proposed a "new solution" to a fixed-bed adsorption problem considered previously by Rosen [10]. The problem is that of adsorption of a single adsorbable species from a fluid stream passing through a fixed-bed packed with adsorbents free of adsorbate initially. The isotherm is linear and the rate controlling step is the combination of mass transfer resistances in both fluid and particle phases.

The literature is nowadays fed up with the "new solutions" and various analytical and numerical methods for evaluating the kinetics of these kind of processes. Thus, it seams that the search for new solutions expressible in term of $J(x, y)$ function is absolutely unnecessary. This statement may be supported by the discussions by Camp [11], Rice [12], and Tien [13] that followed the publication of the work [5].

The general expression for the breakthrough curve for a linear isotherm and constant diffusivity involving $J(x, y)$ function was re ported many times in the literature. A review of just ten solutions of this kind is presented in the Table 1.

The description of the nonlinear isothermal breakthrough behaviour of adsorbers reduces to the above linearized results as a special case. Thus, for example, the results obtained for Freundlich isotherm in [2] agree, for $n = 1$, with the solution from [16].

Another well known example is, as given in [4]: the reduction of Thomas' solution for Langumir isotherm to the linearized one by putting the equilibrium constant to be equal to one ($K = 1$). Linearity usually must exist to permit analytical solution for isothermaloperation of a fixed-bed adsorbers. However, the main advantage, from the computational standpoint, of the solutions given by Thomas [20, 22] for Langmuir isotherm, is that they are expressible in the terms of $J(x, y)$ function. See equations (10.31a), (10.31b) and (10.37) in [4] for arguments of J-function in Thomas' solution.

Table 1. Some solutions for linear equilibrium involving $J(x, y)$ function

Reference	Solution	Equation
3	$X = J(N_R, ZN_R)$ $Y = 1 - J(ZN_R, N_R)$	16–123a 16–123b
4	$c/c_0 = J(n, nT)$ $q/q_0 = 1 - J(nT, n)$	10.38 10.39
5	$u = J(Kx/\xi, \theta/\xi)$	28&32
14	$c_A/c_0 = J(s, t)$ $q_A/q_\infty = J(t, s)$	64 65
15	$c_A/c_{A0} = K(s_A, t_A)$	19
16	$y/x_0 = J(ax, \beta\tau)$ $w/w_0 = 1 - J(b\tau, ax)$	21 22
17	$y/y_0 = J(\xi^*, \tau^*)$	25
18	$c/c_{feed} = J(\xi, \tau)$	3
19	$X = J(\xi, \tau)$	22.6–27
20	Saturation: $c/c_0 = 1 - J(Bx, Ay)$ $q/q_0 = J(Ay, Bx)$ Elution: $c/c_0 = J(Bx, Ay)$ $q/q_0 = 1 - J(Ay, Bx)$	 48 49 50 51

* The notation of dependent and independent variables are those from the corresponding reference

The properties of the $J(x, y)$ function have been studied extensively by Goldstein [6] and are obtainable from various texts. At this point it is worthwhile just to notice that beyond the forms given by equations (1) and (2), the following relations hold:

$$J(x,y)=\mathrm{e}^{-(x+y)}I_0(2\sqrt{xy})+\mathrm{e}^{-x}\int_0^y \mathrm{e}^{-\tau}(2\sqrt{xy})d\tau=$$

$$=\mathrm{e}^{-(x+y)}\sum_{n=0}^{\infty}\sum_{k=0}^{n}\frac{y^n x^k}{n!k!}=$$

$$=1-\sum_{n=1}^{\infty}\sum_{k=0}^{n}(-1)^{n+k}\frac{(k+n)!}{(k+1)!k!(n!)^2}x^{k+1}y^n=$$

$$=\mathrm{e}^{-x}\left[1+\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}(-1)^m\frac{(m+n-1)!}{n!m!(n-1)!}x^n\frac{y^{n+m}}{(m+n)!}\right]=$$

$$=1-\mathrm{e}^{-y}\left[\sum_{m=0}^{\infty}(-1)^m\frac{x^{m+1}}{(m+1)!}+\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}(-1)^m\frac{(m+n)!}{m!(n!)^2}y^n\frac{x^{m+n+1}}{(m+n+1)!}\right]=$$

$$=1-\mathrm{e}^{-y}\sum_{n=0}^{\infty}\sum_{i=0}^{n}\frac{(-1)^{n+i}x^{n+1}y^i}{(n+1)(n-i)!(i!)^2} \qquad (3)$$

The $J(x, y)$ function is named as "fundamental" by Carslaw and Jaeger [23], and denoted as $V_1(x, y)$ by Korol'kov [8]. Romie [24, 25] denotes $J(x, y)$ function as $H_0(x, y)$. It is just the J function's different representations that made the solutions of various authors appear different.

The simplest way to prove any of the above equations is by taking the Laplace transform with respect to both variables and using some additional algebra. The choice of one or the other relation is governed by purely computational aspects, *i.e.* the convergence criteria, which we will not discuss here. We just note that the preference of some formula strongly depends on the relative magnitude of the arguments x and y, and for some asymptotic relations the reader should consult the papers by Goldstein [6] and Klinkenberg [7].

Evaluation of *J(x, y)* function on the pocket calculators and home computers

The method proposed here does not employ a power series expansion or a numerical integration for the evaluation of $J(x, y)$ function. Instead, the expansion in modified Bessel functions, as given by equation (2), is used. The latter is evaluated using a forward recursion derived from the backward recursion for the Bessel functions as proposed by Parl [9] for the Marcum function which is related to the noncentral chi-squared distribution with two degrees of freedom.

Calculation of the Anzelius-Schumann function J(x, y) should be performed according to the first expression in (2) when $y < x$ and according to the second expression in (2) when $x \leq y$. This provides a fast convergence. Rearranging the exponential factor

$$\mathrm{e}^{-(x+y)}=\mathrm{e}^{-(\sqrt{x}-\sqrt{y})^2}\mathrm{e}^{-2\sqrt{xy}}$$

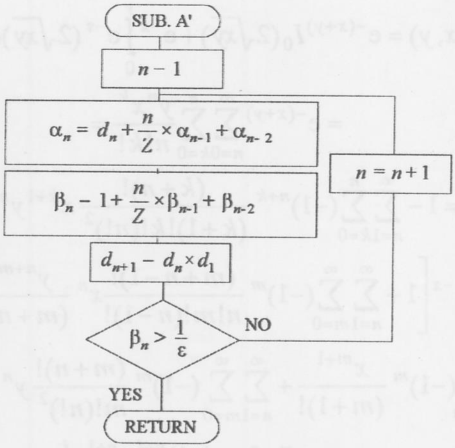

Figure 2. Subroutine A' flow chart

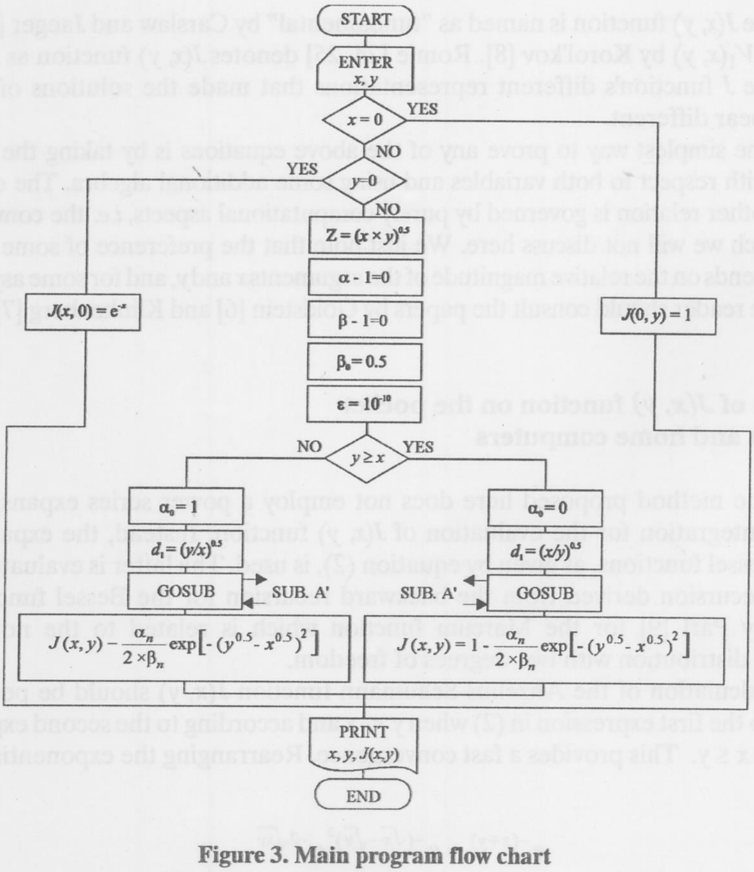

Figure 3. Main program flow chart

one can rewrite equations (2) in the forms

$$J(x,y) = \mathrm{e}^{-\left(\sqrt{x}-\sqrt{y}\right)^2} \sum_{n=0}^{\infty} (y/x)^{n/2} \mathrm{e}^{-2\sqrt{xy}} I_n\left(2\sqrt{xy}\right), \quad \text{for } y < x \tag{4}$$

and

$$J(x,y) = 1 - \mathrm{e}^{-\left(\sqrt{x}-\sqrt{y}\right)^2} \sum_{n=1}^{\infty} (x/y)^{n/2} \mathrm{e}^{-2\sqrt{xy}} I_n\left(2\sqrt{xy}\right), \quad \text{for } y \geq x \tag{5}$$

that lead to a straightforward application of the Parl's algorithm [9]. The reader should consult reference [9] for details of the algorithm development. The flow-chart of the algorithm is given in Fig. 2. It is easily used for either $y < x$ or $x \leq y$ and does not have the dynamic range problem. Further, it is also extremely accurate since the relative error is bounded by $\varepsilon\left(1+\sqrt{\pi\sqrt{xy}}\right)$ where the accuracy is chosen so that $\varepsilon = 10^{-10}$. The algorithm is also very fast and easy to use on the modest calculators.

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