Zeros of the Dutkai and Ruckenstein Equation

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INTRODUCTION

The spread of liquid in a packed column by a dispersion model leads to the following partial differential equation:

$$\frac{\delta L}{\delta z} = D_r\left(\frac{1}{r}\frac{\delta L}{\delta r} + \frac{\delta^2 L}{\delta r^2}\right) \tag{1}$$

Solutions of this PDE are dependent on both the initial conditions and the boundary conditions. The initial conditions at $z = 0$ can be a continuous point source on the axis of the column, $r = 0$ or a uniformly distributed source. The first initial condition is important for spreading measurements to determine the coefficient D_r. The second condition is the normal operating condition. The boundary conditions at $r = R$ have been considered by a number of authors. Cihla and Schmidt (1957) have used,

$$\frac{\delta L}{\delta r} = 0 \tag{2}$$

Porter and Jones (1963) have used,

$$L = KW \tag{3}$$

where W is the wall flow rate at $r = R$. Dutkai and Ruckenstein (1968) have used,

$$-2\Pi R\, D_r \frac{\delta L}{\delta r} = k_p L - k_w W \tag{4}$$

Onda et al. (1973) have used,

$$-2\Pi R\, D_r \frac{\delta L}{\delta r} = C(W^* - W) \tag{5}$$

where W^* is the equilibrium wall flow rate in an infinitely deep column. Other boundary conditions at the base of the column where $z = Z$ have been considered by Gunn (1978). When there is no spreading below the base of the column, the boundary condition becomes,

$$\frac{\delta L}{\delta z} = 0 \tag{6}$$

The analogous case with heat conduction leads to a PDE similar to that given by Eq. 1. The initial and boundary conditions are discussed by Carslaw and Jaeger (1962). In this case the initial conditions are the radial distribution of temperature in the solid at $t = 0$, while the boundary conditions can take a number of forms. If the outer surface, $r = R$, is at a constant temperature then,

$$T(R) = T_c \tag{7}$$

If a radiation condition applies,

$$\frac{\delta T}{\delta r} + hT = 0 \tag{8}$$

If the surface is impervious to heat,

$$\frac{\delta T}{\delta r} = 0 \tag{9}$$

If there is a constant heat flux,

$$-K\frac{\delta T}{\delta r} = F_o \tag{10}$$

If there is contact with a well-stirred fluid with heat loss,

$$-2\Pi\, R\, K\frac{\delta T}{\delta r} = MC_p\frac{dT_f}{dt} + HT_f \tag{11}$$

The analogous case with diffusion leads also to a similar PDE, and the initial and boundary conditions are discussed by Crank (1975). The initial conditions correspond to the radial distribution of the concentration at $t = 0$. The boundary conditions at $r = R$ can be:

A constant concentration,

$$C = C_c \tag{12}$$

A surface transfer

$$-D\frac{\delta c}{\delta r} = \alpha_M(C - C_o) \tag{13}$$

An impermeable surface,

$$\frac{\delta C}{\delta r} = 0 \tag{14}$$

A constant flux,

$$-D\frac{\delta c}{\delta r} = F_o \tag{15}$$

While there are many similarities between the heat conduction and diffusion boundary conditions, there is only one example of zero surface gradient at $r = R$ in common with the spread of liquid in packed columns. Some of the other boundary conditions are only in partial agreement. This complication of

the boundary condition for the spread of a liquid is due to the complexity of the wall-packing interaction.

Solutions of the heat conduction and diffusion cases in cylinders are available in a Dini series and the coefficients obtained to satisfy the boundary conditions. When the surface condition is constant, as given by Eqs. 7 and 12, then the boundary conditions leads to

$$J_o(R\alpha_n) = 0 \tag{16}$$

The zeros of this equation α_1, α_2, . . . etc are available from the British Association Mathematical Tables (1937), Carslaw and Jaeger (1962), and Abramovich and Stegun (1965).

In the radiation or surface transfer condition as given by Eq. 8 or Eq. 13 with $C_o = 0$ we have,

$$\alpha_n J_o'(R\alpha_n) + h J_o(R\alpha_n) = 0 \tag{17}$$

or

$$-\alpha_n J_1(R\alpha_n) + h J_o(R\alpha_n) = 0 \tag{18}$$

The zeros of this equation are given by Carslaw and Jaeger (1962) and Crank (1975).

In the constant surface flux conditions given by Eq. 10 we have

$$J_1(\alpha_n) = 0 \tag{19}$$

The zeros of this equation are available from the above sources. With a zero gradient condition at the surface we have,

$$J_1(R\alpha_n) = 0 \tag{20}$$

For contact with a well-stirred fluid the zeros are obtained from an equation of the form given by Eq. 18.

SPREADING LIQUID MODEL

The Porter and Jones boundary condition at the wall given by Eq. 3 leads to the following equation.

$$2J_1(\alpha_n) + k\alpha_n J_o(\alpha_n) = 0 \tag{21}$$

where

$$k = \frac{1}{\Pi R^2 K} \tag{22}$$

The zeros of this equation have been given by Crank (1975) resulting from an analysis of diffusion to a cylinder in a stirred solution of limited volume.

The Dutkai and Ruckenstein model for the spread of liquid in a packed column gives the radial distribution at a depth (z) by,

$$\frac{L}{L(0)} = \frac{1}{1+a}\left\{1 + 2(1+a)\sum \frac{\alpha_n}{\left(2b\alpha_n^2 - \frac{2}{a}\right)^2 + \alpha_n^2 + \frac{4}{a}} \frac{J_o\left[\frac{\alpha_n r}{R}\right]}{J_1[\alpha_n]} \exp\left[-\alpha_n^2 \frac{D_r z}{R^2}\right]\right\} \tag{23}$$

The Dutkai and Ruckenstein boundary condition given by Eq. 4 leads to,

$$2\left[b\alpha_n - \frac{1}{a\alpha_n}\right] J_1(\alpha_n) - J_o(\alpha_n) = 0 \tag{24}$$

where

$$a = \frac{1}{\Pi R^2}\frac{k_p}{k_w} \tag{25}$$

$$b = \frac{\Pi D_r}{k_p} \tag{26}$$

when $b \to 0$

$$J_1(\alpha_n) + \frac{a}{2}\alpha_n J_o(\alpha_n) = 0 \tag{27}$$

The zeros of this equation are obtained in a similar manner to the zeros of Eq. 18.

When $a \to 0$

$$J_1(\alpha_n) = 0 \tag{28}$$

The zeros are obtained as for Eq. 19. These two limiting cases provide valuable information of the location of the zeros. When both (a) and (b) are not zero the Dutkai and Ruckenstein equation (Eq. 24) may be rearranged to give,

$$2[ab\alpha_n^2 - 1] J_1(\alpha_n) - a\alpha_n J_o(\alpha_n) = 0 \tag{29}$$

This equation has a zero at the origin.

$$\alpha_1 = 0 \tag{30}$$

EVALUATION OF THE ZEROS

The location of a zero of Eq. 29 in an interval described by a lower and upper limit (LL and UL) can be evaluated by a combination of methods based on linear interpolation, extrapolation, and bisection as described by Bus and Dekker (1975). The Numerical Algorithm Group (NAG) (1984) uses this procedure in program C05ADF. This program searches successfully for the second zero, α_2, when the low limit is incrementally greater than zero and the upper limit is π, for $a = 0.1$ and $b = 1.0$. However, the method fails when $a = 0.1$ and $b = 0.1$ because the upper limit was less than α_2. If this limit is increased to 4 the method works for most examples but fails when $a = 0.5$ and $b = 1$. The program C05AGF improves the method by using an estimate of α_2 and a step h to locate an interval by a binary search technique, then searches for the zero. This method is successful with $a = 0.1$ and $b = 1.0$, but fails with $a = 0.1$ and $b = 0.1$ by returning to the zero $\alpha_1 = 0$ with the starting value of $\alpha_2 = 1$ and $h = \pi/2$. The program C05AJF uses a robust second interaction to locate the root as described by Swift and Lindfield (1978) given an initial estimate. With an estimate $\alpha_2 = 1$ for starting, the method gave the zero $\alpha_1 = 0$ for a wide range of a,b values. For higher numbered zeros the method would give two equal zeros in the middle of a series of zeros.

These difficulties can be overcome by noting that the zeros of Eq. 27 are approximately separated by π, and program C05AJF is successful in locating the series of zeros when a has values from 0.1 to 1.0 and $b = 0$. If these zeros are used as estimates for the zeros for nonzero values of b, then program C05AJF is successful for increments in b, which can be reused for larger values of b.

For a larger number of evaluations of these zeros the improved convergence of a Newton-Raphson procedure can be used, as the gradient can be determined explicitly.

TABLE 1. ZEROS OF DUTKAI-RUCKENSTEIN EQUATION; $a = 0.10$, $\alpha_1 = 0.0$

b	α_2	α_3	α_4	α_5	α_6
0.00	3.65515985	6.69955262	9.73009826	12.76646520	15.81332953
0.05	3.64377101	6.62512361	9.48336342	12.18535649	14.80203423
0.10	3.63102134	6.51752333	9.03292534	11.32097951	13.96996530
0.15	3.61669926	6.36311250	8.47257126	10.81235293	13.68971753
0.20	3.60056188	6.15606989	8.01473609	10.58424795	13.57354128
0.25	3.58233524	5.91135363	7.71242821	10.46972274	13.51230788
0.30	3.56171864	5.65777258	7.52536655	10.40346037	13.47488976
0.35	3.53839556	5.41811669	7.40796461	10.36086811	13.44975516
0.40	3.51205380	5.20290360	7.33079831	10.33136642	13.43174105
0.45	3.48241719	5.01465671	7.27742425	10.30978995	13.41820983
0.50	3.44928796	4.85232490	7.23878240	10.29335082	13.40767900
0.55	3.41259441	4.71358299	7.20971533	10.28042222	13.39925298
0.60	3.37243235	4.59578007	7.18715077	10.26999460	13.39235954
0.65	3.32908524	4.49628059	7.16917340	10.26140979	13.38661623
0.70	3.28301187	4.41257806	7.15453866	10.25422095	13.38175787
0.75	3.23480099	4.34234175	7.14240779	10.24811441	13.37759484
0.80	3.18510528	4.28344989	7.13219723	10.24286361	13.37398805
0.85	3.13457371	4.23401680	7.12348961	10.23830095	13.37083311
0.90	3.08379796	4.19240766	7.11597912	10.23429980	13.36805021
0.95	3.03328040	4.15723708	7.10943692	10.23076273	13.36557726
1.00	2.98342240	4.12735270	7.10368855	10.22761359	13.36336526

Let

$$f = 2[ab\alpha^2 - 1]\,J_1(\alpha) - a\alpha\,J_o(\alpha) \tag{31}$$

Then

$$f' = [a(1 - 2b)\alpha + \frac{2}{\alpha} + 4ab]\,J_1(\alpha) + [2(ab\alpha^2 - 1) - a]\,J_o(\alpha) \tag{32}$$

$$\alpha_{new} = \alpha_{old} - \frac{f}{f'} \tag{33}$$

The magnitude of the error between successive iterations on α is given by,

$$e = \frac{f}{f'} \tag{34}$$

It has been found that the Newton-Raphson method can be unstable and miss a zero if the initial estimate of the zero is too inaccurate. A suitable procedure in selecting these initial estimates is to evaluate the series of zeros when $b = 0$ using program CO5AJF for values of b close to zero, and to reuse existing stored zeros when b deviates substantially from zero. The Newton-Raphson method using this initial value procedure was also successful, with excellent convergence characteristics, to provide an error condition,

$$|e| < 10^{-8} \tag{35}$$

The results for $a = 0.1$ and (b) ranging from 0 to 1.0 are given in Table 1. A similar result for $a = 0.5$ is given in Table 2. The numerical values in the table were checked by reducing the error condition. The difference between the higher zeros approaches (π). The difference

$$\Delta\alpha_{32} = \alpha_3 - \alpha_2 \tag{36}$$

depends on the value of (b), while the difference $\Delta\alpha_{43}$ has a minimum value which can be obtained from the tables.

TABLE 2. ZEROS OF DUTKAI-RUCKENSTEIN EQUATION; $a = 0.50$, $\alpha_1 = 0.0$

b	α_2	α_3	α_4	α_5	α_6
0.00	3.20751837	6.07780873	9.06057947	12.10660800	15.18633802
0.05	3.10350934	5.65849585	8.31063722	11.12932852	14.06794400
0.10	2.98636561	5.23663074	7.81003165	10.70051587	13.71632729
0.15	2.86170061	4.90723918	7.55551839	10.52470522	13.58470679
0.20	2.73607216	4.67281137	7.41668214	10.43460459	13.51827538
0.25	2.61482326	4.50795632	7.33232244	10.38069470	13.47856476
0.30	2.50116531	4.39005152	7.27644381	10.34502658	13.45223425
0.35	2.39644237	4.30351402	7.23697111	10.31974720	13.43352207
0.40	2.30079552	4.23824544	7.20770633	10.30091985	13.41954949
0.45	2.21373480	4.18774217	7.18518776	10.28636488	13.40872243
0.50	2.13450397	4.14775653	7.16734526	10.27478148	13.40008824
0.55	2.06227959	4.11545295	7.15287050	10.26534665	13.39304305
0.60	1.99626780	4.08889234	7.14089841	10.25751486	13.38718577
0.65	1.93574499	4.06671649	7.13083518	10.25091045	13.38223966
0.70	1.88007013	4.04795228	7.12226020	10.24526639	13.37800767
0.75	1.82868355	4.03188769	7.11486744	10.24038777	13.37434570
0.80	1.78110000	4.01799174	7.10842910	10.23612898	13.37114593
0.85	1.73689986	4.00586146	7.10277216	10.23237911	13.36832612
0.90	1.69572026	3.99518622	7.09776293	10.22905220	13.36582241
0.95	1.65724687	3.98572308	7.09329649	10.22608056	13.36358452
1.00	1.62120680	3.97727961	7.08928936	10.22341024	13.36157226

CONCLUSION

The Dutkai and Ruckenstein boundary conditions lead to a radial liquid distribution function which requires the zeros of the Dutkai-Ruckenstein equation. These values of α_n are given as the zeros of Eq. 31 and are tabulated in Tables 1 and 2 for selected values of (*a*) and (*b*). Several procedures using existing NAG programs and a Newton-Raphson procedure have been successful in obtaining the zeros. This allows the radial liquid distribution in a packed column to be obtained for values of the transfer parameters k_p and k_w.

NOTATION

a = Dutkai and Ruckenstein coefficient
b = Dutkai and Ruckenstein coefficient
C = Onda et al. coefficient, m^{-2}
C_c = constant concentration, kg/m^3
D_r = spreading coefficient, m
e = error estimate
f = function
f' = derivative of function F with respect to α
F_o = heat or mass transfer flux, W/m^2, $kg/m^2 \cdot s$
h = radiation coefficient, m^{-1}
H = heat loss coefficient W/K
k = coefficient related to K
k_p = transfer coefficient from the packing, m
k_w = transfer coefficient from the wall, m^{-1}
K = Porter and Jones constant, m^{-2}
L = liquid loading, $kg/m^2 \cdot s$
M = mass stirred fluid, kg
r = radius, m
R = outer radius, m
T = temperature, K
T_c = constant temperature, K
T_f = fluid temperature, K
W = wall flow, kg/s
W^* = equilibrium wall flow, kg/s
z = packing depth, m
Z = total packing depth, m
α_m = mass transfer coefficient, m/s
α_n = zeros of the appropriate equation, m^{-1}

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