Generalized Numerical Solutions of Freezing a Saturated Liquid in Cylinders and Spheres

LUH C. TAO

University of Nebraska, Lincoln, Nebraska

A numerical method and graphs of generalized solutions are presented for a moving interface problem of freezing a saturated liquid inside a cylindrical or a spherical container with a constant heat transfer coefficient, as well as melting a saturated solid. The frozen solid phase has a constant heat capacity.

The moving interface problem of freezing a liquid inside a container is of interest in industrial processes such as consumable electrode melting of reactive metals, casting thermoplastics or metals, freezing foods, and producing ice. A brief review was made by Longwell (*6*). The fundamental transport process can be rigorously formulated by a set of partial differential equations, but the generalized analytical solutions are not readily available for cylinders and spheres.

Using an analog computer, Kreith and Romie (*3*) studied the changes of heat transfer coefficient to maintain a constant interface velocity in a slab, a cylinder, or a sphere. London and Seban (*5, 7*) gave analytic solutions of freezing a liquid in a cylinder or a sphere with negligible heat capacity of solid phase, and Longwell (*6*) proposed a graphical method to include the heat capacity. Baxter (*1*) computed the time required to freeze all the liquid inside a cylinder by using an analog computer. He divided the radius into five increments and the temperature profiles on the time coordinate appeared wavy. Springer and Olson (*8*) proposed a numerical method to solve solidification of materials with heat capacities and in an annular space between two concentric cylinders of finite length. They illustrated the movement of an interface within an annular space but the dimensionless groups were assigned such that finite solutions could not be obtained by letting the inside radius approach zero. The graphic method of reference *6* cannot be used for numerical computation when the interface approaches the vicinity of the center. Also, the usual initial step of assuming a constant temperature gradient in the solid phase could introduce some significant error which may not damp out in a finite radial distance. Therefore, it appears that a complete set of numerical solutions in terms of dimensionless parameters would be useful in that once computed they may serve many practical problems or design work.

This paper presents a numerical method and its solutions of interface position as a function of time during freezing a saturated liquid inside a cylinder or a sphere. The thermal conductivity and heat capacity of solid phase and the convective heat transfer coefficient are assumed to be constants. The temperature profiles at the instant of freezing at the center are also tabulated. The dimensionless groups were chosen so that the numerical solutions can be examined in their convergence toward their respective asymptotic solutions of negligible sensible heat. Also, the computation errors of these solutions given here have been analyzed and were minimized by choosing an optimum increment size. From these generalized solutions the interface position at any given time and the temperature profile at the instant of freezing at the center for a specific problem can be found rapidly.

THEORY

The general problem of freezing a saturated liquid with a constant thermal conductivity and a constant density can be rigorously described by Equation (1) for the heat transport in solid phase and by Equations (2), (3), and (4) for the associated boundary and initial conditions (2). A saturated solution implies that $T = T_L$ for $R \geq \mathrm{r} \geq 0$.

$$\frac{\partial T}{\partial t} = \frac{k}{\rho C} \nabla^2 T \qquad \text{for } R < \mathrm{r} < \mathrm{r}_i \tag{1}$$

$$\frac{dR}{dt} = \frac{k}{\rho L} \nabla T \qquad \text{at } \mathrm{r} = R \tag{2}$$

$$-\nabla T = \frac{U_i}{k} (T_i - T_c) \qquad \text{at } \mathrm{r} = \mathrm{r}_i \tag{3}$$

$$T = T_L \qquad \text{for } t = 0,\ 0 \leq \mathrm{r} \leq \mathrm{r}_i \tag{4}$$

Since we restrict these systems to radial movement only, the radial distance is the only spatial component in the gradient and the Laplacian operator. By a proper combination of variables to form those desired dimensionless parameters, these equations are transformed into the following for both the cylindrical and the spherical coordinate systems:

$$\gamma \frac{\partial T^*}{\partial t^*} = \frac{\partial^2 T^*}{\partial \mathrm{r}^{*2}} + \frac{a}{\mathrm{r}^*} \frac{\partial T^*}{\partial \mathrm{r}^*} \qquad \text{for } R^* < \mathrm{r}^* < 1 \tag{5}$$

$$\frac{dR^*}{dt^*} = \frac{\partial T^*}{\partial \mathrm{r}^*} \qquad \text{at } \mathrm{r}^* = R^* \tag{6}$$

$$-\frac{\partial T^*}{\partial \mathrm{r}^*} = \frac{T^*_i}{\beta} \qquad \text{at } \mathrm{r}^* = 1 \tag{7}$$

$$T^* = 1 \qquad \text{at } t^* = 0, \text{ for } 0 \leq \mathrm{r}^* \leq 1 \tag{8}$$

where

$$\beta = \frac{k}{U_i r_i}$$

$$\gamma = \frac{C}{L}(T_L - T_c) = \text{relative energy content of solid phase}$$

$$T^* = (T - T_c)/(T_L - T_c)$$

$$t^* = tk(T_L - T_c)/r_i^2 \rho L$$

$$r^* = r/r_i,\ R^* = R/r_i$$

$$a = \text{shape factor} = \begin{cases} 1 \text{ for cylinder} \\ 2 \text{ for sphere} \end{cases}$$

If the heat capacity or the energy content of a solid is very small, the time derivative term is negligible and (5) becomes a steady state transport equation. It can be solved with the boundary conditions of (7) and $T^* = 1$ at $r^* = R^*$. These solutions are (9) and (11). Substituting these into (6) and using an initial condition of $R^* = 1$ at $t^* = 0$, one obtains (10) and (12), which are asymptotic solutions for the present numerical solutions. Equations (10) and (12) have been confirmed experimentally (7).

For cylinders

$$T^* = 1 - \frac{\ln(r^*/R^*)}{(\beta - \ln R^*)} \tag{9}$$

$$t^* = (R^{*2}\ln R^*)/2 + (1 - R^{*2})(1 + 2\beta)/4 \tag{10}$$

For spheres

$$T^* = 1 - \frac{1 - R^*/r^*}{1 + (\beta - 1)R^*} \tag{11}$$

$$t^* = (1 - R^{*2})/2 + (1 - R^{*3})(\beta - 1)/3 \tag{12}$$

NUMERICAL METHOD

Numerical methods to solve a set of coupled differential equations [(5) to (8)] consist of converting differentials into differences, choosing a proper relationship between independent parameter increments for the convenience of computation, and then calculating iteratively to obtain a solution.

By using a modified formulation of Binder-Schmidt $\gamma(\Delta r^*)^2 = 2\,\Delta t^*$ (4) and letting N be the number of time increment to move a distance Δr^* (6), the set of partial differential equations is transformed into the following difference equations:

$$T^*_{m,\,n+1} = \left[\left(1 + \frac{a}{2m}\right) T^*_{m-1,\,n} + \left(1 - \frac{a}{2m}\right) T^*_{m+1,\,n} \right]/2 \tag{5a}$$

$$\sum_{n}^{n+N} (T^*_{m-1,\,n} - T^*_{m,\,n}) = 2/\gamma \tag{6a}$$

$$T^*_M = T^*_{M-1}/(1 + \Delta r^*/\beta) \quad \text{at } r^* = 1 \tag{7a}$$

where $M = 1/\Delta r^*$.

To start the computation, the time required for an interface to move r^* from 1 to $1 - \Delta r^*$ was calculated by (13a) or (14a) with (14b) for the surface temperature. These equations are solutions for freezing a semi-infinite liquid pool (2) and may serve as approximate solutions of the present problem with a small Δr^*. They have less errors to be damped out in succeeding computations than does the usual start procedure (6).

For

$$\beta = 0,\ t^* = \gamma\,\Delta R^{*2}/4\,\lambda^2 \tag{13a}$$

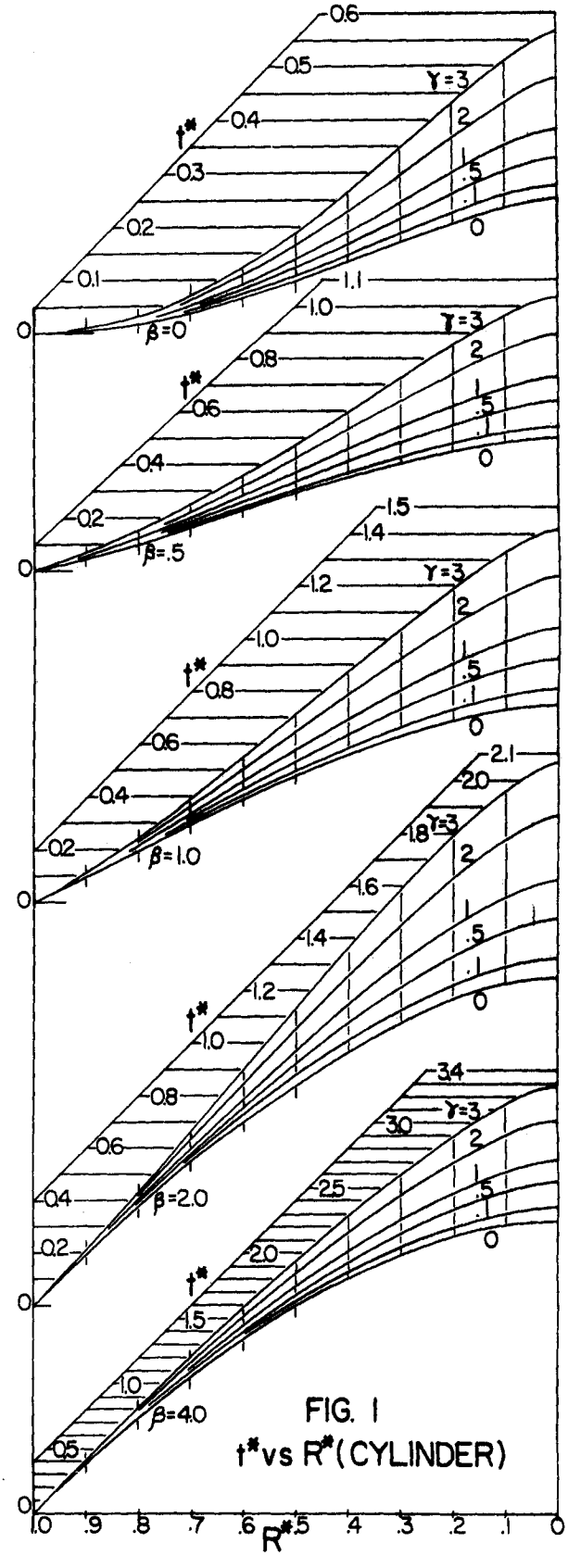

Fig. 1.

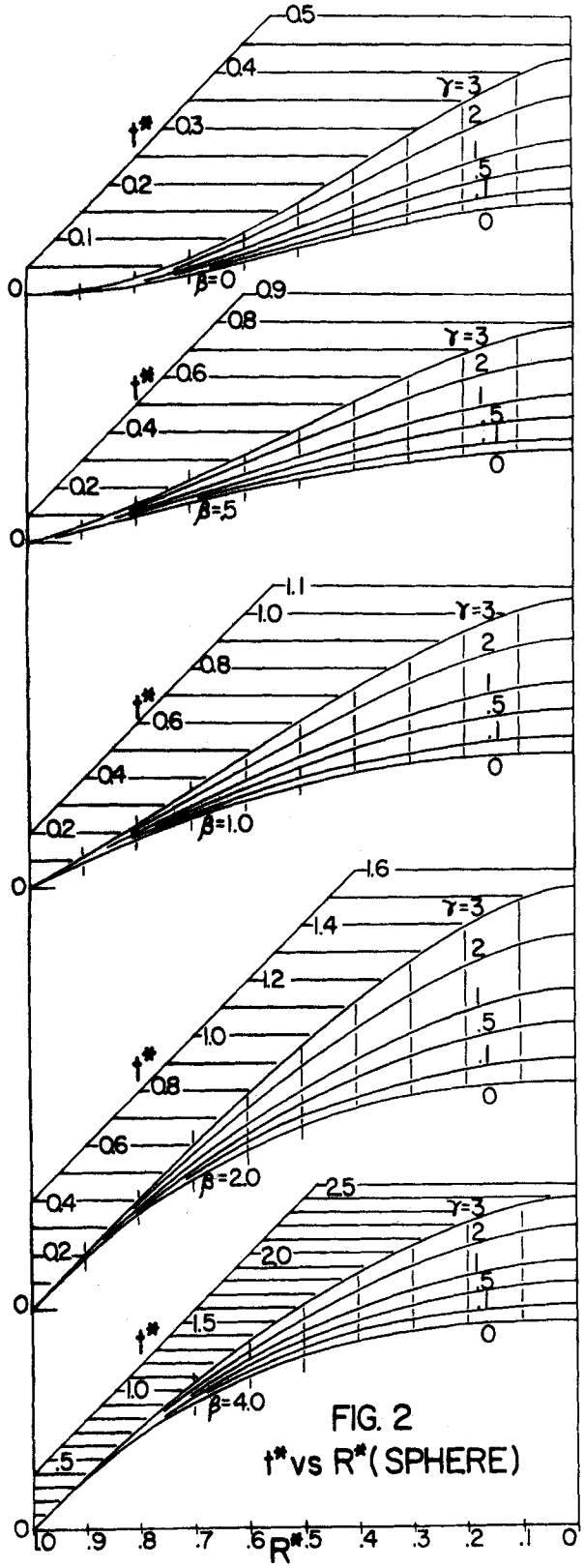

Fig. 2.

where λ is the root of Equation (13b).

$$\lambda \exp \lambda^2 \operatorname{erf} \lambda = \gamma/\sqrt{\pi} \qquad (13b)$$

For

$$\beta \neq 0, t^* = \beta^2 \left(1 - \sqrt{1 - 2\,(1+\gamma)\,\Delta R^*/\beta}\right)/(1+\gamma) \qquad (14a)$$

$$T^* = 1 - t^*/\beta^2 \text{ at } r^* = 1 \qquad (14b)$$

After the time required to reach $1 - \Delta r^*$ was calculated, (5a) was used to calculate temperature T^*_{M-1} for one time increment and (7a) to calculate T^*_M for the succeeding time increment. In this cycle, $T^*_{M-2} = 1.0$. This iteration was continued until (6a) was satisfied and $N\,\Delta t^*$ was obtained as the time to move the interface from $1 - \Delta r^*$ to $1 - 2\Delta r^*$. Then, with $T^*_{M-3} = 1.0$, (5a) and (7a) were iterated to satisfy (6a) in order to move the interface to $1 - 3\,\Delta r^*$. This calculation process was repeated until R^* reached the center. If the last time increment in Equation (6a) for a computation cycle was fractional, a proportional adjustment of all the last temperature increments was also made.

RESULTS AND DISCUSSION

Computation following this proposed method with $\Delta r^* = 0.025$ was performed on an IBM 1620 computer. Output were t^*, the time required for an interface to reach r^* at each succeeding increment and T^*, the temperature profile at the instant of freezing at the center. The calculation results cover ranges of practical systems with γ up to 3 and β up to 5. These results have been tabulated† and are plotted in Figures 1 and 2 to show convergence of these computed values toward their asymptotic solutions, Equations (9) and (11). Figure 3 shows the convergence of temperature profiles at the instant of freezing at the center as γ diminishes. These graphs definitely indicate that these results have correct trends.

With the certainty of these correct trends, a brief analysis of computation errors was made. The round-off and

† The complete tabulation of results has been deposited as document 9159 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and are available for $2.50 for photoprints or $1.75 for 35-mm. microfilm.

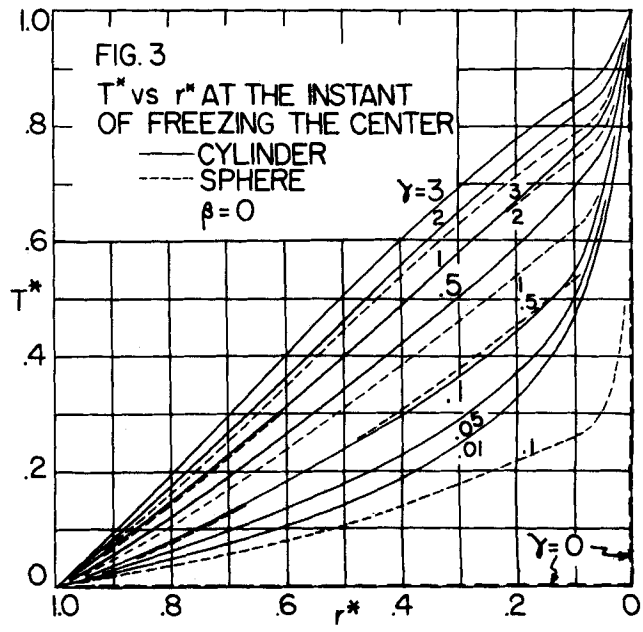

Fig. 3.

Table 1. Effect of Δr^* Size on Computed t^*
(Cylinder: $\gamma = 1.0$, $\beta = 0.0$)

R^*	$r^* = 0.10$	0.05	0.025	0.020
0.9	$t^* = 0.00482$	0.00610	0.00637	0.00640
0.8	0.02377	0.02480	0.02489	0.02486
0.7	0.05379	0.05426	0.05395	0.05411
0.6	0.09312	0.08310	0.09244	0.09264
0.5	0.14074	0.13971	0.13879	0.13886
0.4	0.19437	0.19227	0.19079	0.19080
0.3	0.25120	0.24811	0.24608	0.24618
0.2	0.30909	0.30387	0.30143	0.30168
0.1	0.36347	0.35513	0.34208	0.35228
0.0	0.40586	0.39281	0.38688	0.38647
Estimated truncation error, % of t^* in each column				
Range:	0.03 to 35.3	0.48 to 6.40	0.22 to 1.41	0.01 to 0.78
Average:	5.44	1.37	0.40	0.25

truncation errors, respectively, increase and decrease with a decreasing grid size Δr^*. The round-off error is directly proportional to the total number of time increments in a computation sequence. By assuming $\Delta r^* = 0.025$, the total time increments at $t^*/\Delta t^* = 3{,}200\ t^*/\gamma$ is 48,000 at $t^* = 1.5$ and $\gamma = 0.1$. Since the internal mantissa of IBM 1620 has eight digits, the estimated maximum round-off error of T^* is 0.004 and that of t^* at $R^* = 0.5$ is 0.0004. The truncation error can be estimated by a variation of grid size (4). Since Equation (5*a*) has a second-order truncation error, the true value y can be estimated from $(y - t^*_1)/(y - t^*_2) = (\Delta r^*_1/\Delta r^*_2)^2$. Table 1 shows the effect of grid size and the estimated % truncation errors calculated from 100 $(y - t^*)/t^*$. After considering the required computer time, an apparent optimum of $\Delta r^* = 0.025$ was chosen to obtain the results presented here.

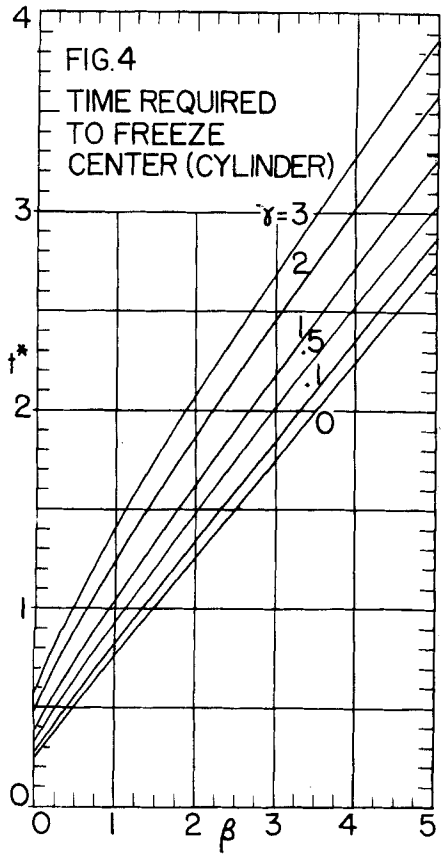

Fig. 4.

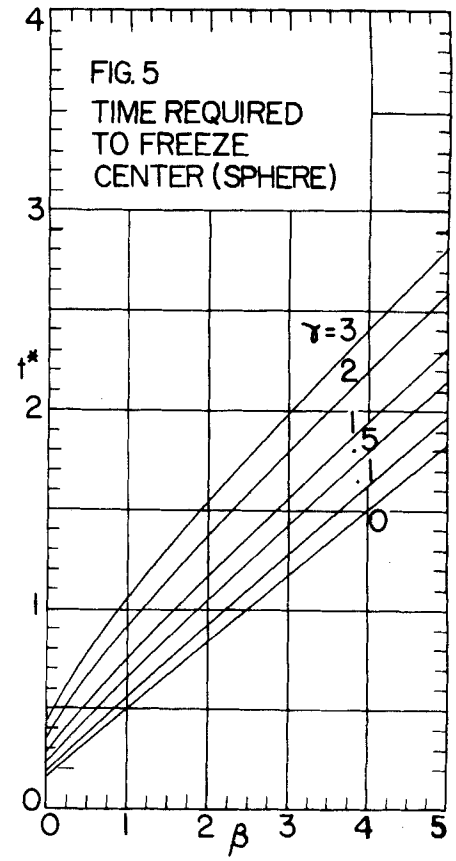

Fig. 5.

The dimensionless groups were chosen to detect the heat capacity effect since the asymptotic solutions of negligible heat capacity are known. An interpretation of these graphs for the effect of γ on t^* should take considerations of the dimensional variables present in both γ and t^*. Since the heat capacity is in γ only, the real time in t^* increases as γ increases according to the graphs shown. However, if the latent heat or the coolant temperature in γ is changed, the real time does not change proportionally with t^* as these two parameters are also present in t^*.

Figures 4 and 5 are time required to freeze the center. They show time increases of 5 to 10% and 7 to 15%, respectively, for cylinders and spheres due to an increase of γ from 0 to 0.1. For $\gamma = 3.0$, the required time may be twice that based on neglecting the heat capacity of solid phase. A comparison of some numerical values from reference *1* with that of this work is shown in Table 2.

Finally, Equations (1) to (4) can also be used to describe the melting of a saturated solid if the solid phase does not move away from its symmetrical position. Therefore, these generalized solutions can also be used for melting a solid inside a cylinder or a sphere by switching the notations of liquid phase and solid phase.

Table 2. A Comparison of $t^*(R^* = 0)$ for a Cylinder

		(*1*)	This work
$\beta = 1.0$	$\gamma = 1.0$	1.00	1.045
	2.0	1.18	1.243
$\beta = 0.5$	$\gamma = 1.0$	0.70	0.736
	2.0	0.82	0.897
$\beta = 0.1$	$\gamma = 1.0$	0.42	0.463
	2.0	0.52	0.580

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NOTATION

a = shape factor, cylinder = 1 and sphere = 2
C = heat capacity of solid
k = thermal conductivity of solid
L = latent heat of fusion
$\mathbf{r}$ = radial distance
R = interface position
t = time
T = temperature
U = overall heat transfer coefficient
ρ = density of solid or liquid, a constant

Superscript

* = dimensionless variable

Subscripts

c = coolant
i = based on radius of inside wall
L = at melting point
m, n = number of radial and time increments
M = total number of radial increments

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A Generalized Differentiation Method for Interpreting Rheological Data of Time-Independent Fluids

J. A. LESCARBOURA, F. J. EICHSTADT, and G. W. SWIFT

University of Kansas, Lawrence, Kansas

A generalized differentiation method for analyzing rheological data of time-independent fluids is presented. The method is demonstrated to be valid and useful in analyzing rheological data and comparing such data obtained on the same time-independent fluid in rheometers of the capillary, annular, coaxial cylinder rotational, and falling cylinder types.

The interpretation of the rheological properties of time-independent fluids is most often approached in terms of the integration method, which requires that a particular ideal model be assumed a priori. Since the ideal models used for this purpose are empirical, one is limited in employing the integration method, since few real fluids are adequately represented by one ideal model over the entire range of shear rate that is of interest.

As pointed out by Savins et al. (*10*) the interpretation can be carried out in a more general manner by employing the differentiation method, which requires no a priori assumption regarding the appropriate rheological model. Instead, the relationship between shear stress and shear rate is expressed as

$$\dot{\gamma} = f(\tau) \qquad (1)$$

In considering a particular rheometer, one obtains an integral equation that contains shear rate as expressed by Equation (1) and differentiates this equation with respect to one of the boundary conditions. The differential equation that results relates the kinematical and dynamical properties measured in the rheometer, for example, Q and ΔP in a capillary instrument, and the derivatives of these properties to the shear rate evaluated at the boundary $f(\tau_b)$. $f(\tau_b)$ can be computed from this expression after determining the derivatives from plots of experimental data and τ_b can be determined from a force balance. From the corresponding values of τ_b and $f(\tau_b)$ over the range of experimental data, one then determines the appropriate functional relationship. Apparently the differentiation method has not achieved widespread acceptance because