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Gas Phase Dispersion in a Small Rotary Kiln

B. B. Spencer

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Consolidated Fuel Reprocessing Program

GAS PHASE DISPERSION IN A SMALL ROTARY KILN

B. B. Spencer

Fuel Recycle Division

Date Published: July 1981

This report was prepared as a thesis and submitted to the faculty of the Graduate School of The University of Tennessee in partial fulfillment of the degree of Master of Science in the Department of Chemical Engineering.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
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ABSTRACT

A study was made of nonideal flow of gas in a rotary kiln reactor. A rotating tube 0.165 m in diameter by 2.17 m long, with internal lifting flights, was operated at room temperature. Rotational speeds from 2.0 to 7.0 rpm, air flow rates from 0.351 to 4.178 m³/h, and solid contents of 0.0, 5.1, and 15.3% of tube volume were studied.

Residence time distribution of the gas was measured by means of the pulse injection technique using a helium tracer. A model was developed based on dispersive flow that exchanges with a deadwater region. Two parameters, a dispersion number describing bulk gas flow and an interchange factor describing exchange between the flow region and the gas trapped in the solids bed, were sufficient to correlate the data, but these parameters are sensitive to experimental error. The model is applicable to analysis of other flow systems, such as packed beds.

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LIST OF SYMBOLS

A	total cross-sectional area occupied by fluid, m^2
a	chord length or length of interface at a cross section, m
B_0	defined by Eq. (B.16)
B_1	defined by Eq. (B.17)
b	dummy constant
C	concentration in free stream, kg/m^3
C_d	concentration in deadwater region, kg/m^3
C_{in}	inlet concentration, kg/m^3
$C(\theta)$	effluent concentration as a function of dimensionless time, dimensionless
$\cos$	cosine
$\cosh$	hyperbolic cosine
$\cot$	cotangent
$\mathcal{D}$	dispersion number, $D/\bar{u}L$, dimensionless
$\mathcal{D}_e$	equivalent dispersion number computed from tanks in series model
D	dispersion coefficient, m^2/s
d	inside diameter of kiln drum, m , or ordinary differential operator
E	defined by Eq. (44)
E	general exit age distribution or E-curve
E_θ	exit age distribution
$E_{N,a}$	exit age distribution for N active regions
$E_{N,d}$	exit age distribution for N deadwater regions

e	2.71828182845904524
erf	error function, $\text{erf}(y) = 2/\sqrt{\pi} \int_0^y e^{-y^2} dy$
exp	$\exp[y] = e^y$
f	fraction of flow
G(s)	defined by Eq. (5)
G'(s)	general transfer function from Laplace transform of functions of t
i	imaginary number, $\sqrt{-1}$
K	interchange factor, kaL/V , dimensionless
K _e	equivalent interchange factor computed from tanks in series model
k	interchange rate between free stream and deadwater stream, m/s
L	Laplace transform operator
L	length of kiln drum, m
M	defined by Eq. (C.3)
N	number of equal sized tanks
n	integer counter
p	volumetric flow rate of fluid through deadwater region, m^3/s
RPM	revolutions per min. (sometimes written as rpm)
S _n ⁺	defined by Eq. (49)
S _n ⁻	defined by Eq. (50)
s	variable in Laplace transformed domain
sin	sine
sinh	hyperbolic sine
t	time, s

$\bar{t}$	mean time or first moment, s
U	or $U(s)$, defined by Eq. (B.6)
U_d	defined by Eq. (B.7)
$\bar{u}$	mean velocity, m/s
V	volumetric flow rate, m ³ /s
$W(s)$	general transfer function from Laplace transform of functions of θ
x	variable measuring length, m
Y	volume, m ³
y	dummy variable
z	dimensionless length, x/L
∞	infinity

Greek Letters

α	fraction of vessel composed of deadwater region
β	defined by Eq. (21)
γ^3	skewness factor or third moment, s ³
γ_θ^3	normalized skewness factor or third moment, dimensionless
Δ	change
δ	defined implicitly by Eq. (23)
δ_n	n th root of Eq. (23)
$\delta(\theta)$	Dirac delta function
∂	partial differential operator
ϵ	defined implicitly by Eq. (54)
ϵ_n	n th root of Eq. (54)

η	defined by Eq. (6)
θ	dimensionless time, $t/\bar{t}$
$\bar{\theta}$	mean dimensionless time
λ	or $\lambda(s)$, defined by Eq. (C.8)
ν	defined by Eq. (7)
π	3.14159265358979324
$\rho(\theta)$	defined by Eq. (C.9)
σ^2	variance or second moment, s^2
σ_{θ}^2	normalized variance or second moment
ϕ_n	defined by Eq. (53)
χ	defined by Eq. (8)
ψ	or $\psi(s)$, defined by Eq. (C.8)
Ω_n^+	defined by Eq. (51)
Ω_n^-	defined by Eq. (52)
ω	rotational speed, revolutions/s
ω_c	critical rotational speed where centrifuging begins, 0.7052/ $\sqrt{d}$, revolutions/s

CHAPTER 1

INTRODUCTION AND SIGNIFICANCE

Rotary kilns are being evaluated as reactors for the oxidation of spent nuclear fuels as part of a research and development effort in support of a proposed plant to reprocess fuel from nuclear reactors. This work is being conducted in the Consolidated Fuel Reprocessing Program of the Oak Ridge National Laboratory. In such an application, the fuel pellet disintegrates into a powder during oxidation and tritium is irreversibly released from the fuel. Tritiated water is formed, and because containment of the tritium is required, it is desirable to minimize the quantity of gas (i.e., mixtures of oxygen and nitrogen) fed to the reactor and thus reduce the volume of gas to be processed subsequently in a tritium removing step. Because of the slow oxidation reaction, the flow rate of solids is low, and low gas velocities are required for high tritium concentration in the effluent. Under these conditions, axial dispersion could make a major contribution to axial heat and mass transfer.

Axial dispersion, as well as oxygen depletion, would affect the positional concentration of gas phase reactant and would, therefore, affect the length of rotary reactor required to obtain a given mean conversion of solids. Assuming that reaction takes place primarily in the solids bed (the solids have a void fraction) where gaseous reactant is trapped and released (i.e., exchanged), the rate of exchange may be significant in determining solids conversion. The results of

isothermal dispersion experiments quantify this effect even in a case where thermal convection dominates the mixing of the bulk gas phase.

From a control point of view, axial heat fluxes due to dispersion also affect the position of heating and cooling sections along the kiln and the expected thermal load on each portion of the kiln. Such control considerations are important in situations where ionizing radiation fields permit only limited temperature measurement.

This study provides information on the rate of interchange between gas in the bulk (or free stream) and that trapped in the solids region. The interchange rate is expressed in the form of a mass transfer coefficient. The model presented also permits calculation of the degree of mixing (dispersion coefficient) in the bulk. This can permit more detailed kiln modeling than a simple axial dispersion model.

Rotary kilns are among the most widely used equipment for contacting solids with gas in industry. Processing alumina, cement, iron ore, potato starch, and simple heat exchange for subsequent processes are examples of the broad uses of rotary kilns. This work should find application in processes, other than fuel reprocessing, where both the solids and gas flow rates are low. Because the model is not restricted to analysis of rotary kilns, it will also find use in other areas, such as modeling flow through packed beds.

CHAPTER 2

LITERATURE REVIEW

A literature search was conducted and no information on gas phase dispersion or residence time distribution (RTD) in rotary kilns was found. However, several papers on heat transfer and solids RTD in kilns were uncovered, and a few of these contained information of interest here.

Several methods are available for modeling the RTD of nonideal flow. The two most common models are the tanks in series model and the dispersion model. Combinations of these models, either in series, parallel or combinations of both have been used to model flow equipment.

Previous Experimental Work

Tscheng and Watkinson¹ studied heat transfer in a 0.19 m ID $\times$ 2.5 m long, smooth walled rotary kiln. Thermal design and quantification of the effects of gas velocity, temperature, solids flow rate, kiln inclination, rotational speed, solids holdup, and particle size on the convective heat transfer coefficients were stressed. Heat was supplied to the kiln by direct feeding of preheated air ranging from 373 to 650 K at mass velocities of 650 to 3300 kg/m² hr. Solids feed consisted of either ottawa sand or limestone fed at superficial mass velocities of 400 to 1750 kg/m² hr with particle sizes ranging from 0.51 to 1.26 mm. Holdup ranged from 6.5 to 17% of the kiln volume. Kiln inclination

varied between 1.36 and 4.1 degrees. Solids bed motion was described in terms of a critical rotational speed, $\omega_c = 0.7052/\sqrt{J}$, where centrifuging of the solids begins. Rotational speeds greater than ω_c cause the solids to be pressed to the kiln wall throughout a revolution. At values of $\omega < 0.1 \omega_c$ a thin layer of particles is carried up along with the drum wall and then continuously slide back down along the surface of the inclined solids bed. The bulk of the bed (i.e., the core) is thus in a tumbling motion. When values of $\omega < 0.01 \omega_c$ prevail, the solids experience a slumping motion. This motion is characterized by the solids being carried up as a whole with the drum wall and then sliding back down along the wall producing a rocking motion. Particles no longer roll down the surface of the solids continuously.

Wes et al.² studied the dispersion of solids in a rotary kiln and discussed how these results would apply in prediction of mean conversion in a reacting system. Experiments to measure the RTD by impulse-response techniques were carried out in an industrial rotary reactor 0.6 m in diameter $\times$ 9.0 m long. Carbohydrate granulae 15 to 100 μ in size were fed at 285 kg/hr. Air flow rates were 95 and 155 kg/hr. Nine mixing vanes, 6 cm wide, were built into the drum, set at 45° angles to drum wall; the direction of rotation was such that the point of contact was the leading edge of the vane. The degree of filling of the drum varied from 20 to 31%, and the rotational speed varied from 2 to 6 rpm. Model sections of the drum 1.0 m in length and 0.6 and 1.4 m in diameter were used to perform the bulk of the experimentation. In the 0.6 m diameter section nine mixing vanes, mounted at a 45° angle to the wall, 3.5 and

6.0 cm wide were used. In the other section experiments were performed with no mixing strips and with eight strips. Three sizes of strips were used; 5, 8, and 12 cm width strips were mounted in two modes; 45° and 90° to the drum wall. Rotational speed in these sections was varied between 1.6 and 10.0 rpm and the solids holdup varied between 12 and 28%. Dispersion was characterized by the Peclet number, and the effects of mixing vanes, size of vanes, diameter of drum, rotational rate, angle of mounting of the vanes, holdup and particle size on the intensity of mixing were correlated. Slumping and mixing of the solids about a central core were described in qualitative terms. They observed that at very high rotational speeds the solids bed would tend to fluidize due to intake of gaseous phase.

In another paper, Wes et al.³ studied heat transfer in the industrial rotary kiln described above. The purpose of the second study was to measure and correlate heat transfer coefficients for subsequent predictions of temperature profiles. The kiln was heated externally by steam. Granular carbohydrates, 15 to 100 μ in size, were fed at 285 kg/hr, and the solids holdup was varied from 11 to 23%. Countercurrent air flow rates of 95 to 155 kg/hr (considered low enough to give rise to small gas velocities) were employed, in which the air temperature would rise from about 80 to 125°C in passing through the kiln. Rotational speed was varied from 1.6 to 6.0 rpm. The gas to drum wall heat transfer coefficient was determined to be in the magnitude expected for natural convection coefficients, but the gas to solids heat transfer coefficient was found to be approximately an order of magnitude greater.

Friedman and Marshall⁴ studied convective heat transfer in a 0.31 m ID $\times$ 1.83 m long rotary kiln with eight built in mixing flights. The objective was to measure heat transfer coefficients and rates of drying wet solids and correlate these coefficients with operating parameters. Heat was supplied to the kiln by feeding preheated air at 120°C. The first phase of their experimentation concerned itself with the heating of dry solids. Sand, 150 to 2300 μ in size, was fed at 34.5 to 364.5 kg/hr. Holdup varied between 0.8 and 12.4%. Slope of the kiln was varied from 0 to 0.046 m/m, and the rotational speeds ranged between 3.35 and 18.5 rpm. Superficial mass velocities of air were 1.67 to 63.34 kg/m² hr. Second phase experimentation was concerned with the drying of 2300 μ wet sand. Slope of the drum was set to 0.031 m/m and the rotational speed was varied from 3.35 to 15.00 rpm. Solids feed rate varied from 31.8 to 113.2 kg/hr, and superficial mass velocity of air varied from 6.93 to 30.40 kg/m² hr. It was reported that attempts to measure the axial air temperature gradient^c were abandoned because results were not reproducible. They decided that the air probably traveled relatively unmixed between the curtains of falling material giving rise to considerable radial temperature striation.

Bowers and Read⁵ described heat transfer in rotary kilns by developing empirical relationships for overall heat transfer coefficients as a function of kiln dimensions and solids particle size. Data were collected from the literature on kilns used for processing lime, shale, dolomite, and wet and dry cement. Measured heat transfer rates in kilns varying from 1.22 to 3.35 m in diameter and 24.4 to 121.9 m long,

along with a spectrum of particle sizes from 149 μ to 5 cm, comprised the only data given.

Sass⁶ developed a model for heat transfer in kilns which accounted for both convective and radiative heat transfer. The purpose of the model was to allow a designer to predict the length of kiln required for a specified heating of solid material. Two operating gas fired kilns were simulated by the model. The first was a cement kiln 2.0 m in diameter $\times$ 27.3 m long in which the solids flow rate was 10,810 kg/hr and the gas flow rate was 21,311 kg/hr at an inlet temperature of 1343°C. The other unit was an iron ore kiln 2.3 m in diameter $\times$ 45.7 m long. The solids flow rate was 4050 kg/hr and the gas flow rate was 4630 kg/hr at an inlet temperature of 1066°C. Overall heat transfer coefficients were estimated from data in the literature. Kiln length was predicted to within 15%.

Manitus et al.⁷ studied the calcination of basic ammonium aluminum sulfate to aluminum oxide in a direct gas fired rotary kiln. The objective of the study was to generate a steady state model describing convective heat and mass transfer including chemical reaction. Transport of the solids phase was emphasized. Carry-over of solid particles by the moving gas stream was considered, but axial mixing was not. Chemical reaction was described to progress in one of two regimes, diffusive or kinetic controlling, depending upon the temperature. Data were taken on a 1.57 m diameter $\times$ 20.8 m long kiln with no mixing flights operated at rotational speeds of 30 to 70 rpm. Internal chokes were used to increase the solids holdup and bulk solids velocity ranged from 0.20

to 0.27 m/sec. Solids were from 20 to 100 μ in size. Combustion gases were fed to the kiln at 1300 K and 7 m/sec and exited the kiln at 700 K and 4 m/sec. Computed temperature profiles, conversion profiles, and estimated length of kiln were close to experimental values.

Dumont and Bélanger⁸ developed steady state models of the transformation of TiO_2 from anatase to rutile form in direct flame fired rotary kilns. They aimed at improving overall economics of operation by optimizing fuel usage rates and fuel-air ratios. Kilns were considered that ranged from 2 to 4 m in diameter, 36 to 60 m long and operated at 4 to 8 rph. Three sections of the kiln were identified where: (1) drying of anatase slurry occurred, (2) heating of dry material to the reaction temperature took place, and (3) the endothermic transformation occurred. The model was said to be consistent with experimental results. Unfortunately, no flow rates were given because the data were confidential.

Kelly and O'Donnell⁹ performed experiments and developed models to predict the RTD of solids in rotary kilns. Mean cycle time for pumice particles about 2 mm in diameter were determined experimentally in a 0.3 m diameter, 0.3 m long, sealed, dead level rotary drum operated at 19.5 rpm. Eight equal angular distribution mixing flights were built into the drum. These data were coupled to equations they had developed which described particle dynamics (i.e., falling, bouncing, etc.) and subsequently were used to predict residence time. Predictions were then compared to experimental results obtained from a 0.3 m diameter, 1.7 m long drum operated at 8 rpm and a 6° slope. Again, pumice was the solid material fed at about 10 g/sec while the air velocity through the drum

was varied from 0.0 to 1.61 m/sec. Comparison between predicted and actual results were good at low air velocities, but became less favorable at the higher velocities.

In summary, the importance of the above review was to examine the limited information available on gas phase RTD, to determine rotational speeds of general interest in rotary kiln operation, and to obtain further descriptions of solid movement in kilns. The interaction of the gas with solids directly influences the mixing of the gaseous phase in rotary kilns.

It was interesting that operating parameters, such as solid and gas velocities, drum rotational speeds, solids holdup and size of solids covered such wide ranges of values. The difficulties in modeling such complex phenomena have caused some investigators to make simplifying assumptions even when conflicting data were available. For example, Dumont and Bélanger⁸ assumed the solids were in plug flow in a heat transfer study even though Wes et al.² had measured the RTD and reported that dispersion was significant. Gas phase mixing has probably been ignored for similar reasons in some studies. In other cases, assuming plug flow is not bad because of the high gas velocities. The lack of data, of course, frequently resulted in simplifying assumptions. In reacting systems with high velocities of gaseous reactants and an overabundance of such reactant, there would be little concern that the gas is contacting the solids adequately. This is true particularly where solids holdup is small and mixing flights keep essentially all the solid cascading through the gas phase. In those cases, contacting

is not a limiting step. However, in systems where solids residence time is large or where the solids are recirculated and the gas flow rate is low, gaseous reactant concentration gradients and contacting mechanisms become important. There seems to be a lack of data in the literature for predicting these concentration gradients when gas phase mixing is an important factor.

Tanks in Series Models

Some investigators have used tanks in series to model nonideal flow. Levenspiel¹⁰ summarizes much of the mathematics of this model. The exit age distribution is given by:

$$E_{\theta} = \frac{N(N\theta)^{N-1}}{(N-1)!} e^{-N\theta} \quad (1)$$

where N represents the number of equal sized tanks and is the only parameter of the model. The mean and variance are, respectively,

$$\bar{\theta} = 1 \quad (2)$$

and

$$\sigma_{\theta}^2 = \frac{1}{N} \quad (3)$$

Levenspiel¹⁰ goes on to suggest that a model of tanks in series with interacting deadwater zones could be used to describe RTDs with long tails. The method suggested is that the deadwater zones be treated as mixed tanks and that a fraction of the flowing fluid is delayed within these zones. The fraction of fluid delayed once is significant, and

the fraction of fluid delayed more than once is assumed insignificant and ignored. Convolution of N active regions with N deadwater regions would then give the RTD of fluid delayed one time - the remainder of the fluid would have an RTD associated with N active regions. In mathematical form

$$E = (1 - f)E_{N,a} + f[E_{N,a} * E_{N,d}] \quad (4)$$

The mathematics are not pursued beyond this point.

Levich et al.¹¹ developed a model of N tanks in series with interacting deadwater from material balances. The pair of differential equations describing the system were transformed into the Laplace domain, and the transfer function for the outlet concentration from one tank with deadwater was found to be

$$G(s) = \frac{\eta(s + \chi)}{s^2 + (\eta + v + \chi)s + \eta\chi} \quad (5)$$

where

$$\eta = \frac{V}{(1 - \alpha)Y} \quad (6)$$

$$v = \frac{P}{(1 - \alpha)Y} \quad (7)$$

$$\chi = \frac{P}{\alpha Y} \quad (8)$$

First and second moments (i.e., the mean and variance) were calculated from the transform (see Appendix A for the functional relationships) and the mean time was found to be exactly the same as that for a tank

without deadwater. Since the moments are additive, Levich was able to compute the mean and variance for N tanks by multiplying the results by N . Presented in dimensionless form,

$$\bar{\theta} = 1 \quad (9)$$

and

$$\sigma_{\theta}^2 = \frac{1}{N} + \frac{2\alpha^2}{N(p/V)} \quad (10)$$

With numerous simplifying assumptions, the transfer function was back transformed resulting in two equations for the outlet concentration.

When $\theta < (1 - \alpha)$

$$C(\theta) = \left(1 - N \frac{p}{V}\right) \frac{\sqrt{N}}{(1 - \alpha) \sqrt{2\pi}} \exp \left[-\frac{N}{2} \left(\frac{\theta}{(1 - \alpha)} - 1 \right)^2 \right] \\ + \frac{N^2 p^2}{4\alpha V^2} \left[1 - \operatorname{erf} \left(\sqrt{\frac{N}{2}} \left(1 - \frac{\theta}{(1 - \alpha)} \right) \right) \right] \quad (11)$$

and when $\theta > (1 - \alpha)$

$$C(\theta) = \left(1 - N \frac{p}{V}\right) \frac{\sqrt{N}}{(1 - \alpha) \sqrt{2\pi}} \exp \left[-\frac{N}{2} \left(\frac{\theta}{(1 - \alpha)} - 1 \right)^2 \right] \\ + \frac{N^2 p^2}{\alpha V^2} \exp \left(-\frac{Np}{\alpha V} \theta \right) \quad (12)$$

Thus, the solution given is discontinuous at $\theta = (1 - \alpha)$. It was suggested that the three parameters N , α and p/V be estimated from the variance, maximum of the peak, and a fit of the second part of Eq. (12) to the tail of the distribution.

Tanks in series models have the advantage that the C - curves and moments are relatively easy to compute. However, these models are not continuous and are not exact solutions to continuous dispersion processes. They do give good approximations at large values of N.

Dispersion Models

Boundary conditions are important considerations in the use of dispersion models because the choice of boundary conditions depends on the type of experiment one wishes to perform and vice versa. Further, the boundary conditions affect the solution of the differential equation describing dispersive flow to such an extent that the solutions range from simple closed form to complicated infinite series. Obviously, the parameters will not be numerically equivalent if they are derived from solutions developed using different boundary conditions. A discussion of boundary conditions can be found in a paper by Wehner and Wilhelm.¹³ The boundary conditions usually encountered are those of the open-open vessel (or simply open vessel) in which the pipe is pictured to extend to infinity in either direction and the closed-closed vessel (or closed vessel) which is bounded on either end, more closely resembling real systems.¹⁰⁻¹⁹

Levenspiel and Smith¹⁴ solved the diffusion equation

$$\frac{\partial C}{\partial \theta} = D \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} \quad (13)$$

for the open-open vessel boundary conditions as discussed earlier by

Danckwerts.¹⁵ Given an impulse input the outlet concentration as a function of dimensionless time is

$$C(\theta) = \frac{1}{2\sqrt{\pi D\theta}} e^{-\frac{(1-\theta)^2}{4D\theta}} \quad (14)$$

where

$$D = \frac{D}{uL} \quad (15)$$

(L is the length of the experimental section.) The single parameter, D , describes the distribution. The moments were calculated from the solution as the mean

$$\bar{\theta} = 1 + 2D \quad (16)$$

and the variance

$$\sigma_{\theta}^2 = 8D^2 + 2D \quad (17)$$

This provides a means to relate D to the data through the second moment or variance. (See Appendix A for the necessary equations.) Van der Laan¹² later showed that a solution to the differential equations was not required to calculate the moments. The moments could readily be computed from the transfer function; i.e., Laplace transform of the differential equations. Aris,¹⁶ later corrected by Bischoff,¹⁷ showed that the variances computed from the transfer function were independent of the shape of the input forcing function and the parameters could be

inferred from the difference of the variances computed from measured concentrations at the inlet and outlet of the vessel.

Van der Laan¹² computed the moments for several other boundary conditions. For closed-closed vessels, the mean,

$$\bar{\theta} = 1 \quad (18)$$

and the variance

$$\sigma_{\theta}^2 = 2D - 2D^2 \left[1 - e^{-\frac{1}{D}} \right]. \quad (19)$$

The transfer function for this case reduced to the simple form

$$W(s) = \frac{4\beta}{(1 + \beta)^2 e^{-\frac{1}{2D}(1-\beta)} - (1 - \beta)^2 e^{-\frac{1}{2D}(1+\beta)}} \quad (20)$$

where

$$\beta = \sqrt{1 + 4Ds} \quad (21)$$

as also listed in Wen and Fan.¹⁰ Wen and Fan¹⁰ gave the analytic solution of the differential equation [i.e., back transformation of Eq. (20)] as

$$C(\theta) = \sum_{n=1}^{\infty} \frac{2\delta_n \left(\frac{1}{2D} \sin \delta_n + \delta_n \cos \delta_n \right) e^{\left[\frac{1}{2D} - \left(\frac{4D^2 \delta_n^2 + 1}{4D} \right) \theta \right]}}{\left(\frac{1}{4D^2} + \frac{1}{D} + \delta_n^2 \right)} \quad (22)$$

where δ_n 's are given implicitly as the roots of

$$\cot \delta = \frac{i}{2} \left(2D\delta - \frac{1}{2D\delta} \right) . \quad (23)$$

They also report an expression for the third moment, or skewness factor,

$$\gamma_{\theta}^3 = 24D^3 \left[\left(\frac{1}{2D} - 1 \right) + \left(\frac{1}{2D} + 1 \right) e^{-\frac{1}{D}} \right] . \quad (24)$$

Bischoff and Levenspiel¹⁹ summarize the variances and means computed for a variety of boundary conditions and derive what are perhaps the most general functions of such available for simple dispersion models. The general functions reduce to the expressions given above for closed and open vessels upon introduction of the corresponding boundary conditions. The models were compared and discussed further.

There appears to be no solution published for the dispersion models with an interacting deadwater. The closest model is the tanks in series with interactive deadwater discussed earlier. Although Levich¹¹ attempts to compare such a model with the corresponding dispersion model, the comparison is approximate at best because the moments were not computed for the continuous model. For instance, the closed-closed vessel model can be compared to the tanks in series model via Eqs. (3) and (19) to determine how N and D compare.

CHAPTER 3

DEVELOPMENT OF MODEL — DISPERSIVE FLOW WITH INTERACTING DEADWATER

A continuous flow model is developed which describes flow through a vessel in which some of the fluid undergoes dispersed flow and some of the fluid is held back in a stagnant or deadwater zone. Matter is allowed to exchange between these zones. If the exchange rate is small enough, then the concentration-time curve will have a long, slowly decaying tail.

The model contains three parameters; fraction of vessel that is a deadwater zone, a dispersion coefficient and an interchange factor. This may be reduced to a two parameter model if one parameter, say the deadwater fraction, can be measured independently.

Derivation of Differential Equations and Boundary Conditions

Consider a differential element of a tube where fluid enters and leaves by both bulk flow and dispersion as shown in Fig. 1. Further, assume that within the element there exists a deadwater region occupying some fraction, α , of the tube and a region of unobstructed flow occupying the remainder of the tube. These two regions interchange matter across some interface at a net rate proportional to the difference of the concentrations in the two regions. The unsteady state material balance

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- C = the concentration in the free stream region
- C_d = the concentration in the deadwater region
- r = the radius of the tube
- a = the cord length subtended by the interface

Fig. 1. Differential element considered for material balance.

for the free stream where forced convective flow and dispersion takes place is

$$(1 - \alpha)A\Delta x \frac{\Delta C}{\Delta t} = VC|_x - VC|_{x+\Delta x} - (1 - \alpha)AD \left. \frac{\partial C}{\partial x} \right|_x + (1 - \alpha)AD \left. \frac{\partial C}{\partial x} \right|_{x+\Delta x} - ka\Delta x(C - C_d) . \quad (25)$$

Divide by $(1 - \alpha)A\Delta x$ and take the limit as Δx approaches zero to obtain

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \frac{V}{(1 - \alpha)A} \frac{\partial C}{\partial x} - \frac{ka}{(1 - \alpha)A} (C - C_d) . \quad (26)$$

A material balance on the deadwater region yields

$$\alpha A\Delta x \frac{\Delta C_d}{\Delta t} = ka\Delta x(C - C_d) . \quad (27)$$

Division by $\alpha A\Delta x$ followed by taking the limit as Δx approaches zero gives

$$\frac{\partial C_d}{\partial t} = \frac{ka}{\alpha A} (C - C_d) . \quad (28)$$

Equations (26) and (28) are the basic partial differential equations that describe the system. Two initial conditions and two boundary conditions are required. The initial conditions are

$$\text{at } t = 0, C = 0, \text{ and } C_d = 0 \quad (29)$$

or may be put in this form by substitution of the proper deviation variables for C and C_d in case the concentrations at the prevailing steady state are not zero. Closed vessel boundary conditions may be

derived from Eq. (25) as follows. At the vessel inlet, matter does not enter or leave by dispersion so

$$D \left. \frac{\partial C}{\partial x} \right|_{x=0^-} = 0 \quad (30)$$

and

$$VC|_{x=0^-} = VC_{in} \quad (31)$$

Substitutions of Eqs. (30) and (31) into Eq. (25) and letting Δx shrink to zero from the positive side yields

$$\text{at } x = 0^+, (1 - \alpha)D \frac{\partial C}{\partial x} = \frac{V}{A} C - \frac{V}{A} C_{in} \quad (32)$$

At the outlet, matter does not disperse back into the vessel, although it may leave that way, thus

$$D \left. \frac{\partial C}{\partial x} \right|_{x=L+\Delta x} = 0 \quad (33)$$

and

$$VC|_{x=L+\Delta x} = VC_{out} = VC|_{x=L} \quad (34)$$

Again, substitute Eqs. (33) and (34) into Eq. (25) and let Δx shrink to zero to obtain

$$\text{at } x = L, \frac{\partial C}{\partial x} = 0 \quad (35)$$

For convenience, the differential equations, boundary and initial conditions will be put in dimensionless form. Let $z = x/L$ and

$\theta = t/\bar{t} = t\bar{u}/L$. Recognize that $V/A = \bar{u}$. Equations (26), (28), (29), (32), and (35) may be written

$$\frac{\partial C}{\partial \theta} = D \frac{\partial^2 C}{\partial z^2} - \frac{1}{(1 - \alpha)} \frac{\partial C}{\partial z} - \frac{K}{(1 - \alpha)} (C - C_d) \quad (36)$$

$$\frac{\partial C_d}{\partial \theta} = \frac{K}{\alpha} (C - C_d) \quad (37)$$

$$\theta = 0, C = 0, \text{ and } C_d = 0 \quad (38)$$

$$z = 0^+, (1 - \alpha) \frac{\partial C}{\partial z} = C - C_{in} \quad (39)$$

$$z = 1, \frac{\partial C}{\partial z} = 0 \quad (40)$$

where

$$D = \frac{D}{\bar{u}L} \quad (41)$$

and

$$K = \frac{kaL}{\bar{u}A} = \frac{kaL}{V} \quad (42)$$

Relation of the Moments of the Concentration-Time Curve to Model Parameters

As Van der Laan¹² first showed, the moments of the concentration-time curve for the dispersion model are simply related to the transfer function (i.e., Laplace transforms) of the defining differential

equations. The transfer function relating the outlet concentration with time for the present model is obtained from Eqs. (36) through (40) and may be written

$$U = \frac{4E}{(1+E)^2 e^{\frac{-(1-E)}{2D(1-\alpha)}} - (1-E)^2 e^{\frac{-(1+E)}{2D(1-\alpha)}}} \quad (43)$$

where

$$E = \sqrt{1 + \frac{4D(1-\alpha)(\alpha s^2 - \alpha^2 s^2 + Ks)}{(\alpha s + K)}} \quad (44)$$

See Appendix B for details. Evaluating the first three derivatives of Eq. (43) and performing the operations indicated by Eqs. (A.8) through (A.10) in the Appendix is straightforward and yields the first three moments

$$\bar{\theta} = 1, \quad (45)$$

$$\sigma_{\theta}^2 = 2D(1-\alpha) - 2D^2(1-\alpha)^2 \left[1 - e^{-\frac{1}{D(1-\alpha)}} \right] + \frac{2\alpha^2}{K}, \quad (46)$$

and

$$\begin{aligned} \gamma_{\theta}^3 = & 24D^3(1-\alpha)^3 \left[\left(\frac{1}{2D(1-\alpha)} - 1 \right) + \left(\frac{1}{2D(1-\alpha)} + 1 \right) e^{-\frac{1}{D(1-\alpha)}} \right] \\ & + \frac{24\alpha^2 D^2 (1-\alpha)^2}{K} \left[\frac{1}{2D(1-\alpha)} + 1/2 \left(\frac{1}{D(1-\alpha)} - 1 \right) \right] + \frac{6\alpha^3}{K^2}. \end{aligned} \quad (47)$$

[Because the derivatives of Eq. (43) are large and cumbersome, they are not presented in this paper.] When $\alpha = 0$, Eqs. (46) and (47) reduce to

Eqs. (19) and (24), respectively, the moments of the ordinary dispersion model. If $K = 0$ it is necessary to return to the transfer function and modify the transfer function for $K = 0$. The reason is that the transfer function is a function of two variables (i.e., s and K) and, therefore, the order with which the limits are taken is important. Upon doing the analysis for this case, $\bar{\theta} = (1 - \alpha)$ and σ_{θ}^2 and γ_{θ}^3 are the same as given by Eqs. (46) and (47) except the terms involving K are not present. Or, put another way, the results in this limiting case are the same as for the ordinary dispersion model in which the vessel size has been modified by a factor of $(1 - \alpha)$. In the general case, the new model shows that the mean time is independent of the deadwater fraction and the interchange factor, however small.

With actual data one can calculate values of σ_{θ}^2 and γ_{θ}^3 . Equations (46) and (47) are not sufficient to then solve for D , K and α simultaneously. However, if one of the three parameters can be set, the other two can then be calculated. The equation for the fourth moment could be derived which would give a third equation with which to compute all three parameters. However, because small errors in data would be magnified, particularly at large values of time, this approach does not appear to be practical for determining values of the parameters.

Solution to the Differential Equations

Back transformation of Eq. (43) into the time domain will give the outlet concentration as a function of dimensionless time, θ , for an impulse input. The complex inversion integral and theory of residues

are often used to back transform from the Laplace domain.^{20,21} With no simplifying assumptions, the solution is

$$C(\theta) = \sum_{n=1}^{\infty} \frac{2\epsilon_n \left[\frac{1}{2\mathcal{D}(1-\alpha)} \sin \epsilon_n + \epsilon_n \cos \epsilon_n \right] e^{\frac{1}{2\mathcal{D}(1-\alpha)} + S_n^+ \theta}}{\Omega_n^+ \left[\frac{1}{4\mathcal{D}^2(1-\alpha)^2} + \frac{1}{\mathcal{D}(1-\alpha)} + \epsilon_n^2 \right]} + \sum_{n=1}^{\infty} \frac{2\epsilon_n \left[\frac{1}{2\mathcal{D}(1-\alpha)} \sin \epsilon_n + \epsilon_n \cos \epsilon_n \right] e^{\frac{1}{2\mathcal{D}(1-\alpha)} + S_n^- \theta}}{\Omega_n^- \left[\frac{1}{4\mathcal{D}^2(1-\alpha)^2} + \frac{1}{\mathcal{D}(1-\alpha)} + \epsilon_n^2 \right]} \quad (48)$$

where

$$S_n^+ = \frac{1}{2(1-\alpha)} \left[\left(\phi_n - \frac{K}{\alpha} \right) + \left(\phi_n + \frac{K}{\alpha} \right) \sqrt{1 - \frac{4\alpha^2 \phi_n K}{(\alpha \phi_n + K)^2}} \right] \quad (49)$$

$$S_n^- = \frac{1}{2(1-\alpha)} \left[\left(\phi_n - \frac{K}{\alpha} \right) - \left(\phi_n + \frac{K}{\alpha} \right) \sqrt{1 - \frac{4\alpha^2 \phi_n K}{(\alpha \phi_n + K)^2}} \right] \quad (50)$$

$$\Omega_n^+ = 1 - \frac{\alpha^2 S_n^+ (\alpha S_n^+ + 2K)}{(\alpha S_n^+ + K)^2} \quad (51)$$

$$\Omega_n^- = 1 - \frac{\alpha^2 S_n^- (\alpha S_n^- + 2K)}{(\alpha S_n^- + K)^2} \quad (52)$$

$$\phi_n = \frac{-4\mathcal{D}^2(1-\alpha)^2 \epsilon_n^2 - 1}{4\mathcal{D}(1-\alpha)} \quad (53)$$

and ϵ_n given implicitly by

$$\cot \epsilon = \frac{1}{2} \left[2D(1 - \alpha)\epsilon - \frac{1}{2D(1 - \alpha)\epsilon} \right] \quad (54)$$

(See Appendix C for details.) The notation ϵ_n is used since there are infinitely many values of ϵ for which Eq. (54) is valid. Although the solution appears complicated, values of $C(\theta)$ can be calculated rapidly on modern digital computers. The first series in the solution converges rapidly, particularly at large values of θ , and the second series converges less rapidly. Both series will always converge for $\theta > 0$.

The first series generates a curve that is responsible for the bell shaped portion of the concentration-time curve, whereas, the second series generates the slowly decaying tail. However, the results from each series cannot be decoupled and examined separately because one series may generate a negative number and the other, a positive number in such a way that the sum is a real, positive value of concentration. Figures 2 through 4 show the individual effects of varying α , D , and K while the two parameters not being varied are held constant. An increasing dispersion number, D , has the expected effect of causing the curve to be skewed to the left, of making the peak lower and the width greater with a long tail. As interchange factor, K , increases, the curve is skewed some to the right, the peak gets lower and the tail decays rapidly. At small values of K , the tail decays rather slowly. The effect of an increasing deadwater fraction, α , is to skew the curve to the left, make the peak higher and narrower and cause the tail to

Fig. 2. Effect of varying dispersion number.

Fig. 3. Effect of varying interchange factor.

Fig. 4. Effect of varying deadwater fraction.

decay very slowly at a set value of K . These plots show that considerable adjustment in the shape of the curve can be obtained, depending on the values of the parameters.

The solution can aid in the determination of the model parameters. Suppose all three parameters, α , $\mathcal{D}$, and K must be determined from experimental concentration-time data. (That is, there is no independent way to determine one of the parameters.) Values of α can be picked (a good choice since α must be bounded between zero and unity) by successive approximations, $\mathcal{D}$ and K computed from Eqs. (46) and (47), concentrations then computed from the solution and the sum of squares of errors between experimental data and computed results used as an index to update values of α until a satisfactory fit can be obtained.

Comparison with Previous Models

The model that compares most favorably with the model developed in the preceding section is the tanks in series model with interactive deadwater due to Levich et al.¹¹ In that model, net flow through the deadwater zone corresponds to a net interchange in the present model, or

$$p(C - C_d) = ka\Delta x(C - C_d) . \quad (55)$$

Assuming that Δx is approximated by L/N ,

$$p(C - C_d) = \frac{kaL}{N} (C - C_d) . \quad (56)$$

Divide through by $(C - C_d)$, use Eq. (42) to introduce K and rearrange to obtain

$$N \frac{p}{V} = K . \quad (57)$$

The correspondence between $\mathcal{D}$ and N can be visualized by comparing Eqs. (10) and (46). With Eq. (57) to aid in removing parts involving K from the comparison,

$$\frac{1}{N} = 2\mathcal{D}(1 - \alpha) - 2\mathcal{D}^2(1 - \alpha)^2 \left[1 - e^{-\frac{1}{\mathcal{D}(1-\alpha)}} \right] . \quad (58)$$

If $\mathcal{D}$ is small then

$$\frac{1}{N} \cong 2\mathcal{D}(1 - \alpha) . \quad (59)$$

Thus, Eqs. (57) and (59) can be used as a basis for comparing the parameters of the two models. Of course, α is the same in each model. [Henceforth, denote K and $\mathcal{D}$ calculated by Eqs. (57) and (59), respectively, as K_e and $\mathcal{D}_e$; equivalency parameters.]

In order to calculate the parameters of Levich's model independently, an equation for the third moment is needed since Levich computed only the first two moments [see Eqs. (9) and (10)]. By the method outlined in Appendix A, the dimensionless skewness factor for that model is calculated from the derivatives of Eq. (5) to be,

$$\gamma_0^3 = \frac{2}{N^2} + \frac{6\alpha^3}{N^2(p/V)^2} + \frac{6\alpha^2}{N^2(p/V)} . \quad (60)$$

Again, if α can be set by another means, then N and p/V can be computed from the second and third moments of the data using Eqs. (10) and (60).

CHAPTER 4

EXPERIMENTAL APPARATUS AND PROCEDURES

Measured RTDs of the gas phase in a rotary kiln are required data for this study. A flowsheet of the experimental equipment is shown in Fig. 5. The rotary kiln is an experimental Bartlett-Snow unit which has a 0.165 m inside diameter and a 2.17 m long retort tube. Six equally spaced mixing flights, each 2.54 cm in height and 0.64 cm wide, are attached internally over the length of the kiln. The unit has an electric clamshell furnace and a water cooled zone, but these were not needed for these experiments, because each run was performed at room temperature. The kiln drum can be rotated at speeds of 2 to 8 rpm with the variable speed drive motor.

Air is metered to the kiln with two rotameters in parallel. One rotameter carries the main air flow to the kiln through a diverging diffuser which insures that injected helium tracer fills the entire cross section upon entering the kiln. The other rotameter feeds a small quantity of air to the breaching section associated with the gas entrance end of the drum. This air flows through any small gaps that exist between the stationary diverger and the rotating entrance to the drum. The back pressure, thus imposed, keeps any tracer from backmixing into the breaching section and subsequently bleeding back into the drum causing the concentration-time curves to have long tails. It is desired that long tails indicate the entrapment-release mechanism discussed previously and not be a product of entrance deadspace. Ordinarily,

Fig. 5. Flowsheet of RTD measurement apparatus.

the function of the breaching section is to seal the drum against the atmosphere via a grease seal and still allow solids to exit the drum. Total flow rate through the kiln is the sum of the flows through the two rotameters.

The gas stream exits the kiln through a small tube (approximately 2.54 cm I.D.) and is exhausted to the atmosphere. A small quantity of sample is continuously withdrawn from the exhaust tube and analyzed. A Varian Model 936-70 helium leak detector used in the "sniffer" mode served as the gas analyzer. This instrument's principle of operation is mass spectrometry enabling fast response and high sensitivity. Only 5 to 10 ml of helium tracer was required for full scale readings, depending on air flow rates. The total lag time due to the interval required for the sample to travel through the sample line plus instrument response time was measured experimentally to be 1.71 s. Lag time for the main air flow to travel from the tracer injection point through the small inlet line into the kiln and later out of the kiln through the exhaust tube to the sampling point was calculated from the flow rates and the volume of these two lines (429 ml). Analog output from the leak detector was recorded on strip charts providing concentration-time data after tracer injection.

Quartz sand was used as an inert solid material to simulate solid feed. The drum was set dead level so that the inventory of solid was constant along the axial length. A measured charge of sand was placed in the drum and then the gas lines were reconnected causing the solids to be captive. This prevents axial dispersion of gas due to trapped

gas being carried along with solid flow. The sand used in the experiments had an average particle size of 780 microns and a void fraction of 48.9%.

Each end of the drum was constrained, as described above, so that plug flow prevails before the gas enters and after it leaves the drum. By definition, the dispersion coefficient is zero for plug flow. Therefore, dispersive mixing of the gas occurs only inside the kiln, and the experiment qualifies for analysis by closed vessel models.

CHAPTER 5

RESULTS AND DISCUSSION OF RESULTS

With the experimental apparatus as described in the previous chapter, 71 runs were performed in which the following three parameters were varied: (1) rotational speed, (2) fraction of kiln loaded with solid or simply holdup, and (3) air flow rate. The data were analyzed by four models: (1) open vessel dispersion model, (2) closed vessel dispersion model, (3) tanks in series with interacting deadwater model, and (4) the new closed vessel dispersion with interacting deadwater model developed in Chapter 3. The first two models are one parameter models, whereas, the last two are three parameter models. These three parameter models were reduced to two parameter models by calculating the deadwater fraction based on the internal volume of the vessel and the void volume of the solid region. Thus, only the experiments performed with solids contained in the kiln were analyzed by these multiparameter models. In each case, model parameters were obtained from the moments of the experimental concentration-time curve.

Experimental Data and Description of Results

A summary of experimental conditions with calculated results is shown in Tables 1, 2, and 3. (See Appendix D for a graphical compilation of the concentration-time data for each run.) Model parameters D and K were calculated from the second and third moments of the concentration-time curve with the aid of a computer program (see Appendix E for a

Table 1. Experimental conditions and some calculated results for runs performed with no solids holdup

Title	RPM	Flowrate (m ³ /h)	Bulk mean time (min)	From moments			Closed vessel $\bar{D}$	Open vessel $\bar{D}$
				$\bar{t}$ (min)	σ (min ²)	γ (min ³)		
GPRTD-29	7.0	0.411	6.78	6.21	1.61486	1.21967	0.0214	0.0209
GPRTD-30	7.0	0.884	3.15	3.03	0.44725	0.24731	0.0246	0.0240
GPRTD-31A	7.0	1.765	1.58	1.53	0.13604	0.03803	0.0301	0.0292
GPRTD-31B	7.0	1.765	1.58	1.52	0.12631	0.03820	0.0282	0.0274
GPRTD-32	7.0	2.887	0.97	0.91	0.06824	0.01575	0.0427	0.0409
GPRTD-33	7.0	4.276	0.65	0.65	0.05339	0.02045	0.0674	0.0629
GPRTD-34	5.0	4.276	0.65	0.59	0.05422	0.01981	0.0841	0.0770
GPRTD-35	5.0	2.889	0.97	0.91	0.08402	0.02942	0.0532	0.0504
GPRTD-36	5.0	1.766	1.58	1.48	0.15117	0.05596	0.0356	0.0344
GPRTD-37	5.0	0.885	3.15	3.09	0.47340	0.25116	0.0255	0.0248
GPRTD-38	5.0	0.412	6.78	6.30	1.68655	1.55740	0.0217	0.0213
GPRTD-39	3.0	0.413	6.76	6.03	1.75952	1.19797	0.0248	0.0242
GPRTD-40	3.0	0.887	3.14	3.07	0.56467	0.30343	0.0310	0.0300
GPRTD-41	3.0	1.771	1.58	1.53	0.20192	0.09317	0.0452	0.0431
GPRTD-42	3.0	2.897	0.96	0.88	0.09592	0.03385	0.0657	0.0614
GPRTD-43	3.0	4.290	0.65	0.64	0.05596	0.01708	0.0738	0.0684
GPRTD-44	2.0	4.305	0.65	0.59	0.05788	0.02139	0.0928	0.0842
GPRTD-45	2.0	2.906	0.96	0.94	0.11166	0.06034	0.0677	0.0631
GPRTD-46	2.0	1.777	1.57	1.51	0.19949	0.11145	0.0459	0.0438
GPRTD-47	2.0	0.890	3.13	2.98	0.54487	0.32587	0.0316	0.0306
GPRTD-48	2.0	0.414	6.74	6.09	2.58818	3.62569	0.0362	0.0348

Table 2. Experimental conditions and some calculated results for runs performed with a 5.1% solids holdup

Title	RPM	Flostrate (m ³ /h)	Bulk mean time (min)	From moments				Closed vessel D	Open vessel D	New model		Tanks model		Equivalency variables	
				$\bar{t}$ (min)	$\bar{t}^2$ (min ²)	$\bar{t}^3$ (min ³)	$\bar{t}^4$ (min ⁴)			D	K	N	p/v	D _e	K _e
GPRTD-49 ^a	2.0	0.402	6.76	6.67	4.01864	5.94236	0.0475	0.0452	0.0475	0.5948	12.26	0.01209	0.0419	0.1482	
GPRTD-50	2.0	0.858	3.17	3.21	0.56884	0.32723	0.0285	0.0277	0.0264	0.2489	21.42	0.00709	0.0240	0.1519	
GPRTD-51	2.0	1.714	1.59	1.55	0.14320	0.05469	0.0307	0.0298	0.0261	0.1315	21.03	0.00519	0.0244	0.1092	
GPRTD-52	2.0	2.956	0.92	0.87	0.08595	0.03921	0.0601	0.0565	0.0491	0.0596	11.58	0.00458	0.0451	0.0521	
GPRTD-53	2.0	4.161	0.65	0.64	0.06170	0.02703	0.0832	0.0763	0.0680	0.0454	8.37	0.00370	0.0613	0.0394	
GPRTD-54	3.0	4.161	0.65	0.66	0.05296	0.02050	0.0651	0.0609	0.0450	0.0527	10.66	0.00358	0.0481	0.0367	
GPRTD-55	3.0	2.966	0.92	0.92	0.07253	0.03147	0.0450	0.0430	0.0350	0.0652	15.61	0.00382	0.0329	0.0397	
GPRTD-56	3.0	1.720	1.58	1.54	0.14483	0.06648	0.0316	0.0306	0.0255	0.1037	21.29	0.00433	0.0241	0.0921	
GPRTD-57 ^a	3.0	0.861	3.16	3.17	0.61125	0.41556	0.0314	0.0304	0.0281	0.1738	19.83	0.00632	0.0259	0.1253	
GPRTD-58 ^a	3.0	0.403	6.73	6.75	4.67341	9.00993	0.0342	0.0313	0.0542	0.5285	11.15	0.00910	0.0460	0.1015	
GPRTD-59	5.0	0.404	6.73	6.65	5.14317	12.68682	0.0620	0.0582	0.0576	0.1263	10.14	0.00727	0.0506	0.0737	
GPRTD-60	5.0	0.861	3.15	3.22	0.62781	0.39549	0.0312	0.0302	0.0289	0.2305	19.58	0.00712	0.0262	0.1195	
GPRTD-61	5.0	1.721	1.58	1.58	0.11844	0.03677	0.0243	0.0237	0.0207	0.1687	26.36	0.00827	0.0195	0.1390	
GPRTD-62	5.0	2.968	0.92	0.91	0.05920	0.01787	0.0368	0.0355	0.0301	0.0942	18.16	0.00454	0.0283	0.0825	
GPRTD-63	5.0	4.178	0.65	0.64	0.04008	0.01090	0.0312	0.0485	0.0426	0.0748	13.06	0.00489	0.0393	0.0639	
GPRTD-64	7.0	4.135	0.66	0.64	0.03869	0.01078	0.0497	0.0473	0.0408	0.0716	13.59	0.00460	0.0378	0.0625	
GPRTD-65	7.0	4.135	0.66	0.64	0.03605	0.00876	0.0454	0.0433	0.0379	0.0842	14.61	0.00491	0.0351	0.0717	
GPRTD-66	7.0	2.938	0.92	0.94	0.06255	0.01956	0.0364	0.0351	0.0297	0.0938	18.41	0.00448	0.0279	0.0825	
GPRTD-67	7.0	1.703	1.60	1.58	0.12228	0.03896	0.0252	0.0245	0.0214	0.1609	25.50	0.00522	0.0268	0.1332	
GPRTD-68	7.0	0.853	3.19	3.19	0.63114	0.41037	0.0320	0.0310	0.0294	0.2104	19.17	0.00685	0.0268	0.1333	
GPRTD-69 ^a	2.0	0.400	6.80	6.83	6.19667	18.76022	0.0716	0.0665	0.0651	0.0924	8.97	0.00681	0.0572	0.0611	
GPRTD-70 ^a	2.0	0.400	6.79	6.60	4.22778	7.36018	0.0511	0.0485	0.0511	0.5869	11.73	0.00833	0.0437	0.1118	
GPRTD-71 ^a	2.0	0.854	3.18	3.17	0.34535	0.27607	0.0279	0.0271	0.0279	0.9701	21.35	0.00825	0.0240	0.1762	
GPRTD-72	2.0	1.705	1.59	1.58	0.14721	0.05342	0.0302	0.0293	0.0262	0.1463	21.07	0.00555	0.0244	0.1170	
GPRTD-73	2.0	2.942	0.92	0.91	0.08080	0.02938	0.0514	0.0497	0.0436	0.0814	12.82	0.00525	0.0400	0.0673	

^aValues for D and K estimated.

Table 3. Experimental conditions and some calculated results for runs performed with a 15.3% solids holdup

Title	RPM	Flowrate (m ³ /h)	Bulk mean time (min)	From moments			Closed vessel D	Open vessel D	New model		Tanks model		Equivalency variables	
				$\bar{t}$ (min)	σ (min ²)	γ (min ³)			D	K	N	p/v	D _e	K _e
GPRTD-74	2.0	0.362	7.11	6.82	2.97395	3.56492	0.0330	0.0319	0.0330	2.6201	20.53	0.04221	0.0265	0.8663
GPRTD-75	2.0	0.742	3.46	3.54	0.57990	0.38694	0.0236	0.0231	0.0170	0.8481	34.61	0.02198	0.0157	0.7607
GPRTD-76	2.0	1.523	1.69	1.71	0.20650	0.18886	0.0366	0.0353	0.0162	0.3186	34.92	0.00899	0.0156	0.5159
GPRTD-77	2.0	2.644	0.97	0.99	0.09514	0.05311	0.0512	0.0485	0.0283	0.2827	20.43	0.01337	0.0266	0.2731
GPRTD-78	2.0	3.642	0.71	0.67	0.05327	0.01780	0.0624	0.0585	0.0430	0.3194	13.94	0.02084	0.0390	0.2905
GPRTD-79	2.0	3.642	0.71	0.70	0.05032	0.01537	0.0549	0.0519	0.0380	0.3605	15.69	0.02088	0.0347	0.3277
GPRTD-80	3.0	3.650	0.70	0.69	0.04613	0.01381	0.0515	0.0488	0.0344	0.3605	17.20	0.01936	0.0316	0.3329
GPRTD-81	3.0	2.651	0.97	0.97	0.07075	0.02345	0.0393	0.0378	0.0261	0.4578	23.44	0.01991	0.0242	0.4244
GPRTD-82	3.0	1.527	1.68	1.65	0.14471	0.05667	0.0275	0.0267	0.0185	0.6600	31.41	0.01939	0.0173	0.6090
GPRTD-83	3.0	0.744	3.46	3.50	0.71216	0.75140	0.0299	0.0290	0.0181	0.5215	31.73	0.01565	0.0171	0.4965
GPRTD-84	3.0	0.363	7.09	7.08	4.01410	6.75262	0.0418	0.0401	0.0384	1.0884	16.97	0.03644	0.0321	0.6184
GPRTD-85	5.0	0.363	7.09	6.94	5.08368	11.67518	0.0559	0.0528	0.0480	0.6228	13.25	0.03299	0.0411	0.4372
GPRTD-86	5.0	0.744	3.45	3.54	1.00736	1.73729	0.0418	0.0401	0.0224	0.3303	25.53	0.01256	0.0213	0.3205
GPRTD-87	5.0	1.527	1.68	1.66	0.12392	0.03909	0.0230	0.0225	0.0161	0.8338	36.29	0.02087	0.0180	0.7573
GPRTD-88	5.0	2.652	0.97	0.99	0.06207	0.01844	0.0324	0.0314	0.0209	0.5237	27.81	0.01766	0.0196	0.4910
GPRTD-89	5.0	2.652	0.97	0.96	0.07149	0.02427	0.0405	0.0388	0.0268	0.4430	21.90	0.01878	0.0248	0.4112
GPRTD-90	5.0	1.527	1.68	1.69	0.11435	0.02687	0.0205	0.0201	0.0164	1.2612	36.57	0.02801	0.0149	1.0243
GPRTD-91	5.0	3.652	0.70	0.69	0.04430	0.01205	0.0484	0.0461	0.0334	0.4031	17.76	0.02067	0.0306	0.3671
GPRTD-92	5.0	3.530	0.73	0.70	0.04351	0.01185	0.0460	0.0439	0.0310	0.4067	19.02	0.01968	0.0286	0.3743
GPRTD-93	7.0	3.530	0.73	0.69	0.04455	0.01349	0.0485	0.0461	0.0311	0.5591	18.83	0.01785	0.0289	0.3361
GPRTD-94	7.0	3.530	0.73	0.70	0.04366	0.01279	0.0469	0.0447	0.0303	0.3732	19.33	0.01804	0.0282	0.3487
GPRTD-95	7.0	2.563	1.00	0.96	0.06234	0.02113	0.0352	0.0340	0.0213	0.4438	27.12	0.01859	0.0201	0.4227
GPRTD-96	7.0	1.476	1.74	1.67	0.12802	0.02945	0.0235	0.0229	0.0213	1.7606	29.83	0.03868	0.0182	1.0634
GPRTD-97 ^a	7.0	0.720	3.57	3.49	0.85579	0.58994	0.0364	0.0351	0.0364	2.3952	18.91	0.04028	0.0288	0.7618
GPRTD-98 ^a	7.0	0.351	7.33	7.03	6.25321	15.83642	0.0678	0.0632	0.0678	1.3740	10.55	0.03934	0.0516	0.4150

^aValues of D and K estimated.

listing of the program). A trial and error approach for calculating D and K from Eqs. (46) and (47), for example, was employed because these equations could not be written explicit in these parameters. Those cases where the code failed to find the zeros of Eqs. (46) and (47) are indicated in the tables and the best estimate is listed. However, these points are not considered in the correlation of the data.

The dispersion numbers computed by the open and closed vessel models compare favorably for all cases. This is not surprising since the dispersion numbers are small. The dispersion number is somewhat larger for the closed vessel model than for the open vessel model. Figures 6, 7, and 8 depict the effect of operating parameters on the closed vessel dispersion number. When no solids are present the dispersion number is a monotonically increasing function of flow rate and increases with decreased kiln rotational speed. Presumably, at higher rotational speed, the flow is stabilized. However, when solids are in the drum, the dispersion number decreases with increased flow rate up to approximately $1.5 \text{ m}^3/\text{h}$ and then increases with flow rate. Furthermore, at low flow rate the dispersion number appears to increase with rotational speeds and at high flow rates decrease with increased rotational speed. It appears that a change in controlling mixing mechanism is occurring. It can be speculated that at high gas flow rates convective forces dominate, whereas, at low flow rates the solids cascading through the gas phase is the major mixing force. In comparing Figs. 7 and 8, the effect of increased holdup seems to be to decrease the dispersion number.

Fig. 6. Dispersion number from closed vessel model at zero solids holdup.

Fig. 7. Dispersion number from closed vessel model at 5.1% solids holdup.

Fig. 8. Dispersion number from closed vessel model at 15.3% solids holdup.

The parameters from the new model, dispersive flow with interactive deadwater, may be compared with the parameters of the tanks in series with interactive deadwater model. In Tables 2 and 3, pages 38 and 39, it is shown that D and D_e compare to within 20%; D_e is smaller. Values of K and K_e compare even less favorably. The effects of operating parameters on the dispersion number and interchange rate of the new model are shown in Figs. 9 and 10, and Figs. 11 and 12, respectively. The dispersion number behaves as described above for the closed vessel model and is slightly smaller in magnitude. An interchange rate is obtained from the interchange factor as follows:

$$ka = \frac{kaL}{V} \left(\frac{V}{L} \right) = K \left(\frac{V}{L} \right) . \quad (61)$$

The term, k , is not isolated by itself in case a is a function of rotational speed as well (i.e., the simple chord length, a , may not exist between active and deadwater regions). As shown in Fig. 11, the interchange rate initially rises with increased flow rate but quickly levels until there is practically no further effect. The interchange rate increases with rotational speed; this is particularly noticeable at the higher flow rates. Figure 12 does not show this trend as well as Fig. 11 due to greater scatter in the data. However, the interchange rates do appear to be greater with an increase in holdup, as seen by comparing Figs. 11 and 12. The same observations can be drawn from similar plots of the equivalent variables obtained from the tanks in series with deadwater model (see Figs. 13 through 16).

Fig. 9. Dispersion number from new model at 5.1% solids holdup.

Fig. 10. Dispersion number from new model at 15.3% solids holdup.

Fig. 11. Interchange rate from new model at 5.1% holdup.

Fig. 12. Interchange rate from new model at 15.3% holdup.

Fig. 13. Equivalent dispersion number from tanks model at 5.1% holdup.

Fig. 14. Equivalent dispersion number from tanks model at 15.3% holdup.

Fig. 15. Equivalent interchange rate from tanks model at 5.1% holdup.

Fig. 16. Equivalent interchange rate from tanks model at 15.3% holdup.

Comparison of Experimental Data with Models

Three closed vessel type models are compared with the data and each other in Figs. 17, 18, and 19. With a small deadwater fraction, the new model and the ordinary closed vessel dispersion model fit the data essentially equally well, provided that the tail of the distribution is short as shown in Fig. 17. When this condition is not met and the deadwater fraction becomes more significant, then the new model describes the data considerably better (see Fig. 18). The tanks in series with interactive deadwater model should describe the data as well as the current model. However, since the equations for the C curve for that model were derived with several simplifying assumptions, this is not the case as shown by Fig. 19.

Plotted comparisons between the data and the new model for each run may be found in Appendix D.

Sensitivity of Model to Errors in Data

Data from two runs were altered synthetically to simulate an error in zero line in the concentration data. An error equivalent to 2.0% of full instrument scale was either added to or subtracted from the concentration data and the resulting data were reanalyzed. The results appear in Table 4. As shown in the table, a 2% shift in the data can make a threefold change in the calculated interchange factor and about a twofold change in the dispersion number. The dispersion number was affected in like manner in the ordinary dispersion models as well. This

GPRTD-50

ORNL-DWG.80-18764

Fig. 17. Comparison of data (crosses) with new model (solid line) and ordinary dispersion model, $D = 0.028$ (dashed line), for run no. GPRTD-50.

GPRTD-77

ORNL-DWG.80-18765

Fig. 18. Comparison of data (crosses) with new model (solid line) and ordinary dispersion model, $D = 0.051$ (dashed line), for run no. GPRTD-77.

Fig. 19. Comparison of data (crosses) with new model (solid line) and tanks in series with deadwater model, $N = 21.42$ and $p/V = 0.0709$ (dashed line), for run no. GPRTD-50.

Table 4. Sensitivity of model to errors in the data

Title	RPM	Holdup (% full)	Flowrate (m ³ /h)	Bulk mean time (min)	From moments			Closed vessel $\bar{D}$	Open vessel $\bar{D}$	New model		Tanks model		Equivalency variables	
					$\bar{t}$ (min)	σ (min ²)	γ (min ³)			$\bar{D}$	K	N	μ/V	D_0	K_0
GPRD-53	2.0	5.1	4.161	0.65	0.64	0.06170	0.02703	0.0832	0.0763	0.0680	0.0454	8.37	0.00470	0.0613	0.0394 ^a
GPRD-53	2.0	5.1	4.161	0.65	0.61	0.03918	0.00811	0.0560	0.0529	0.0519	0.1341	11.18	0.00718	0.0459	0.0803 ^b
GPRD-53	2.0	5.1	4.161	0.65	0.72	0.14450	0.09922	0.1666	0.1399	0.1462	0.0391	4.32	0.00656	0.1188	0.0283 ^c
GPRD-80	3.0	15.3	3.650	0.70	0.69	0.04613	0.01381	0.0515	0.0418	0.0344	0.3605	17.20	0.01936	0.0316	0.3329 ^d
GPRD-80	3.0	15.3	3.650	0.70	0.66	0.03177	0.00468	0.0376	0.0361	0.0331	0.9911	19.15	0.03422	0.0284	0.6553 ^e
GPRD-80	3.0	15.3	3.650	0.70	0.73	0.07913	0.03876	0.0814	0.0748	0.0533	0.2327	11.29	0.01910	0.0482	0.2155 ^e

^aOriginal data.^bTwo percent of full scale subtracted from concentration reading, points deleted if then less than zero.^cTwo percent of full scale added to concentration reading.

is a high degree of sensitivity and shows a possible cause for the scatter in the data presented in the previous section.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

Gas phase RTD experiments have been performed using a rotary kiln with a 0.165 m inside diameter and a 2.17 m long retort tube operated isothermally at room temperature. Kiln rotational speeds were varied from 2.0 to 7.0 rpm, air flow rate through the kiln varied from 0.351 to 4.178 m³/h, and settled solid contents of 0.0, 5.1, and 15.3% of kiln volume were featured. A continuous flow model was developed to aid in the data analysis. The model describes a system with a region of dispersive flow that exchanges matter with a deadwater region. This model has three parameters, but was reduced to a two parameter model by assuming that the deadwater fraction, α , was calculable from the settled solids volume and porosity. The dispersion number, D , and the interchange factor, K , were then computed from the moments of the experimental data. Values of D ranged from 0.0161 to 0.0680, and values of K ranged from 0.0454 to 2.6201.

Conclusions

The following conclusions can be drawn from the results of this study:

1. The developed model represents the experimental data well over the range of variables tested.

2. Although there is some scatter in the dispersion numbers and interchange factors presented, these data represent the best available information on such a system.
3. The interchange factor can be in error by as much as a factor of three if the zero line in the data is shifted by 2.0% of full instrument scale. This is a high degree of sensitivity. Additionally, the assumption that the deadwater fraction can be calculated from the porosity of the settled solids may introduce some error since the solids may be partially fluidized by kiln rotation. In the range of deadwater fractions imposed (a maximum of 8.1%), K does not affect the concentration-time curves very much and, therefore, is not known precisely.

Recommendations

The following recommendations are made:

1. The new model should be used to analyze data from other continuous flow systems in which an interactive deadwater region is suspected to be present (e.g., packed beds).
2. Experimentation should be continued to obtain data on larger kilns, both in diameter and length, which should be analyzed with the model.
3. The model should be used to estimate the parameters D and K as input to subsequent design of rotary reactors.
4. Mechanistic theories should be developed that explain and/or predict how D and K behave.

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APPENDIXES

APPENDIX A

RELATIONSHIP OF THE MOMENTS TO THE CONCENTRATION-TIME CURVE AND TO THE TRANSFER FUNCTION

The first three moments, the mean, the variance, and the skewness factor can be computed from concentration-time data with formulae given in the literature. See, for example, Wen and Fan.¹⁸ These equations are

$$\bar{t} = \frac{\int_0^{\infty} t C dt}{\int_0^{\infty} C dt}, \quad (A.1)$$

$$\sigma^2 = \frac{\int_0^{\infty} (t - \bar{t})^2 C dt}{\int_0^{\infty} C dt} = \frac{\int_0^{\infty} t^2 C dt}{\int_0^{\infty} C dt} - \bar{t}^2, \quad (A.2)$$

and

$$\gamma^3 = \frac{\int_0^{\infty} (t - \bar{t})^3 C dt}{\int_0^{\infty} C dt} = \frac{\int_0^{\infty} t^3 C dt}{\int_0^{\infty} C dt} - 3\bar{t}\sigma^2 - \bar{t}^3 \quad (A.3)$$

Each of these quantities can be related to the dimensionless time variable, θ , thus:

$$\bar{\theta} = \frac{\bar{t}}{\bar{t}} = 1 \quad (\text{A.4})$$

$$\sigma_{\theta}^2 = \frac{\sigma^2}{\bar{t}^2} \quad (\text{A.5})$$

$$\gamma_{\theta}^3 = \frac{\gamma^3}{\bar{t}^3} \quad (\text{A.6})$$

For purposes of data analysis, it is convenient to put the integrals of Eqs. (A.1) through (A.3) into finite form. As an example, Eq. (A.1) becomes

$$\bar{t} = \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} \quad (\text{A.7})$$

The moments can be related to the transfer function (i.e., Laplace transform of the RTD function) in the following way. Suppose $W(s)$ is the normalized transfer function where s is the transform variable related to the dimensionless time, θ . The normalized moments are then given by

$$\bar{\theta} = - \lim_{s \rightarrow 0} \frac{dW(s)}{ds} \quad (\text{A.8})$$

$$\sigma_{\theta}^2 = \lim_{s \rightarrow 0} \left[\frac{d^2 W(s)}{ds^2} - \left(\frac{dW(s)}{ds} \right)^2 \right] \quad (\text{A.9})$$

$$\gamma_{\theta}^3 = \lim_{s \rightarrow 0} \left\{ -\frac{d^3 W(s)}{ds^3} - 3 \left[-\frac{dW(s)}{ds} \right] \left[\frac{d^2 W(s)}{ds^2} - \left(\frac{dW(s)}{ds} \right)^2 \right] - \left[-\frac{dW(s)}{ds} \right]^3 \right\}. \quad (\text{A.10})$$

Nonnormalized moments, $\bar{t}$, σ^2 , and γ^3 would be given by the same equations when $W(s)$ is replaced by $G(s)$, the nonnormalized transfer function associated with the variable t . Then, if desired, Eqs. (A.4) through (A.6) could be used to normalize the moments calculated in this way. This last method is outlined because some authors prefer to work in dimensional variables.

APPENDIX B

DERIVATION OF TRANSFER FUNCTION

The dimensionless pair of partial differential equations for which a solution is sought are:

$$\frac{\partial C}{\partial \theta} = \mathcal{D} \frac{\partial^2 C}{\partial z^2} - \frac{1}{(1 - \alpha)} \frac{\partial C}{\partial z} - \frac{K}{(1 - \alpha)} (C - C_d) \quad (B.1)$$

$$\frac{\partial C_d}{\partial \theta} = \frac{K}{\alpha} (C - C_d) \quad (B.2)$$

with initial and boundary conditions

$$\theta = 0, C = 0, \text{ and } C_d = 0 \quad (B.3)$$

$$z = 0^+, (1 - \alpha) \mathcal{D} \frac{\partial C}{\partial z} = C - C_{in} \quad (B.4)$$

$$z = 1, \frac{\partial C}{\partial z} = 0. \quad (B.5)$$

Both C and C_d are functions of θ and z . Adapting the convention that the Laplace transform with respect to θ is $L\{C(\theta, z)\} = U(s, z) = U$, then the transform of Eqs. (B.1) and (B.2) are

$$sU - C(0, z) = \mathcal{D} \frac{d^2 U}{dz^2} - \frac{1}{(1 - \alpha)} \frac{dU}{dz} - \frac{K}{(1 - \alpha)} (U - U_d) \quad (B.6)$$

$$sU_d - C_d(0, z) = \frac{K}{\alpha} (U - U_d) \quad (B.7)$$

Applying the initial conditions given in Eq. (B.3), then solving Eq. (B.7) for U_d and substituting the result into Eq. (B.6) gives, upon rearrangement,

$$\mathcal{D} \frac{d^2 U}{dz^2} - \frac{1}{(1-\alpha)} \frac{dU}{dz} - \left(\frac{\alpha s^2 - \alpha^2 s^2 + Ks}{(1-\alpha)(\alpha s + K)} \right) U = 0 \quad (B.8)$$

The solution to this ordinary differential equation is not difficult and may be written as

$$U = B_0 e^{\frac{(1+E)z}{2\mathcal{D}(1-\alpha)}} + B_1 e^{\frac{(1-E)z}{2\mathcal{D}(1-\alpha)}} \quad (B.9)$$

where

$$E = \sqrt{1 + \frac{4\mathcal{D}(1-\alpha)(\alpha s^2 - \alpha^2 s^2 + Ks)}{(\alpha s + K)}} \quad (B.10)$$

B_0 and B_1 must now be determined from the two boundary conditions. Let $C_{in} = \delta(\theta)$, an impulse, for which $L\{\delta(\theta)\} = 1$. Taking the Laplace transform with respect to θ of the boundary conditions, Eqs. (B.4) and (B.5), yields

$$z = 0^+, (1-\alpha)\mathcal{D} \frac{dU}{dz} = U - 1 \quad (B.11)$$

$$z = 1, \frac{dU}{dz} = 0 \quad (B.12)$$

From Eq. (B.9)

$$\frac{dU}{dz} = B_0 \frac{(1+E)}{2\mathcal{D}(1-\alpha)} e^{\frac{(1+E)z}{2\mathcal{D}(1-\alpha)}} + B_1 \frac{(1-E)}{2\mathcal{D}(1-\alpha)} e^{\frac{(1-E)z}{2\mathcal{D}(1-\alpha)}} \quad (B.13)$$

Substitute Eqs. (B.13) and (B.9) into Eq. (B.11), set $z = 0$ and combine like terms to obtain

$$B_0(1 - E) + B_1(1 + E) = 2 . \quad (B.14)$$

Upon substituting Eq. (B.13) into Eq. (B.12), putting $z = 1$ and multiplying each side of the equation by $2D(1 - \alpha)(1 + E)$, the result is

$$B_0(1 + E)^2 e^{\frac{1+E}{2D(1-\alpha)}} + B_1(1 - E)(1 + E)e^{\frac{1-E}{2D(1-\alpha)}} = 0 . \quad (B.15)$$

Solving Eqs. (B.14) and (B.15) simultaneously for B_0 and B_1 yields

$$B_0 = \frac{2(1 - E)}{(1 - E)^2 - (1 + E)^2 e^{\frac{E}{D(1-\alpha)}}} \quad (B.16)$$

and

$$B_1 = \frac{-2(1 + E)e^{\frac{E}{D(1-\alpha)}}}{(1 - E)^2 - (1 + E)^2 e^{\frac{E}{D(1-\alpha)}}} \quad (B.17)$$

Substitute these results into Eq. (B.9) to obtain

$$U = \frac{2(1 - E)e^{\frac{(1+E)z}{2D(1-\alpha)}} - 2(1 + E)e^{\frac{E}{D(1-\alpha)}} e^{\frac{(1-E)z}{2D(1-\alpha)}}}{(1 - E)^2 - (1 + E)^2 e^{\frac{E}{D(1-\alpha)}}} . \quad (B.18)$$

The concentration at the outlet of the vessel is required. Therefore, set $z = 1$ and simplify. Now

$$U = \frac{4E}{(1 + E)^2 e^{\frac{-(1-E)}{2D(1-\alpha)}} - (1 - E)^2 e^{\frac{-(1+E)}{2D(1-\alpha)}}} \quad (\text{B.19})$$

which is the desired result.

APPENDIX C

INVERSE TRANSFORMATION OF TRANSFER FUNCTION TO OBTAIN EFFLUENT CONCENTRATION AS A FUNCTION OF TIME FOR AN IMPULSE INPUT

Rewrite the transfer function derived in Appendix B as

$$U = \frac{4Ee^M}{(1 + E)^2 e^{ME} - (1 - E)^2 e^{-ME}} \quad (C.1)$$

where

$$E = \sqrt{1 + \frac{4D(1 - \alpha)(\alpha s^2 - \alpha^2 s^2 + Ks)}{\alpha s + K}} \quad (C.2)$$

and

$$M = \frac{1}{2D(1 - \alpha)} \quad (C.3)$$

The terms M and e^M in Eq. (C.1) are constants since the variable s appears only in E . Recall the identities

$$e^{by} = \cosh by + \sinh by \quad (C.4)$$

and

$$e^{-by} = \cosh by - \sinh by \quad (C.5)$$

Replace the exponentials in the denominator of Eq. (C.1) by the hyperbolic functions. Upon expansion and collection of like terms

$$U = \frac{2Ee^M}{E^2 \sinh ME + 2E \cosh ME + \sinh ME} \quad (C.6)$$

The back transformation of Eq. (C.6) can be determined using the complex inversion integral and theory of residues. Since U is analytic, except for singularities which are poles only,

$$C(\theta) = L^{-1}\{U(s)\} = (\text{applicable constant}) \sum \rho_n(\theta) \quad (C.7)$$

where $\rho_n(\theta)$ are the residues of $U(s)$ at each of its poles. Equation (C.6) may be written

$$U = 2e^M \frac{\lambda(s)}{\psi(s)}, \quad (C.8)$$

where $\lambda(s)$ and $\psi(s)$ are defined by comparison with Eq. (C.6). When written as a power series in s the degree of $\psi(s)$ minus the degree of $\lambda(s)$ is greater than unity. In this case, the residues are calculated by

$$\rho_n(\theta) = \left. \frac{\lambda(s)}{\frac{d}{ds} \psi(s)} e^{s\theta} \right|_{s=s_n} \quad (C.9)$$

where s_n are the simple poles of U . These simple poles are the zeros of $\psi(s)$. Proceed as follows:

$$\psi(s) = (E^2 + 1) \sinh ME + 2E \cosh ME \quad (C.10)$$

where E is given by Eq. (C.2). Use the identities

$$\cosh y = \cos iy \quad (C.11)$$

$$\sinh y = -i \sin iy \quad (C.12)$$

and write

$$\psi(s) = -i(E^2 + 1) \sin iME + 2E \cos iME = 0. \quad (C.13)$$

Divide through by $\sin iME$, recall the identity

$$\cot y = \frac{\cos y}{\sin y}, \quad (C.14)$$

and back substitute for M from Eq. (C.3).

$$\cot \frac{iE}{2D(1 - \alpha)} = \frac{i(E^2 + 1)}{2E} \quad (C.15)$$

Let

$$\epsilon = \frac{iE}{2D(1 - \alpha)}. \quad (C.16)$$

Combine Eqs. (C.15) and (C.16) and rearrange to obtain

$$\cot \epsilon = \frac{1}{2} \left[2D(1 - \alpha)\epsilon - \frac{1}{2D(1 - \alpha)\epsilon} \right]. \quad (C.17)$$

There are an infinite number of values of ϵ for which this equation is true, call them ϵ_n . Thus, from Eq. (C.16)

$$E = \frac{2D(1 - \alpha)\epsilon_n}{i}. \quad (C.18)$$

Substitute Eq. (C.2) for E , square both sides of the equation, rearrange, solve the resulting quadratic for s and denote the result as s_n . Thus,

$$s_n = \frac{1}{2\alpha(1-\alpha)} \left[(\alpha\phi_n - K) \pm (\alpha\phi_n + K) \sqrt{1 - \frac{4\alpha^2\phi_n K}{(\alpha\phi_n + K)^2}} \right] \quad (C.19)$$

where

$$\phi_n = \frac{-4\mathcal{V}^2(1-\alpha)^2\epsilon_n^2 - 1}{4\mathcal{V}(1-\alpha)}. \quad (C.20)$$

As indicated, there is a positive and negative square root with which to deal, leading to two different sets of s_n . Designate these by

$$s_n^+ = \frac{1}{2\alpha(1-\alpha)} \left[(\alpha\phi_n - K) + (\alpha\phi_n + K) \sqrt{1 - \frac{4\alpha^2\phi_n K}{(\alpha\phi_n + K)^2}} \right] \quad (C.21)$$

and

$$s_n^- = \frac{1}{2\alpha(1-\alpha)} \left[(\alpha\phi_n - K) - (\alpha\phi_n + K) \sqrt{1 - \frac{4\alpha^2\phi_n K}{(\alpha\phi_n + K)^2}} \right]. \quad (C.22)$$

Take the derivative of $\psi(s)$ [i.e., Eq. (C.10)] with respect to s to obtain

$$\frac{d}{ds} [\psi(s)] = \Omega \left[\left(E + \frac{2}{ME} + \frac{1}{E} \right) \cosh ME + \left(\frac{2}{M} + 2 \right) \sinh ME \right] \quad (C.23)$$

where

$$\Omega = 1 - \frac{\alpha^3 s^2 + 2\alpha^2 K s}{(\alpha s + K)^2}. \quad (C.24)$$

As shown by Eq. (C.9), these last two expressions are to be evaluated at s_n . To make the algebra easier, realize that $\psi(s)|_{s_n} = 0$ and write

$$\frac{d}{ds} \psi(s)|_{s_n} = \frac{d}{ds} \psi(s)|_{s_n} - \Omega \psi(s)|_{s_n} \quad (C.25)$$

Now consider functions involving S_n^+ first. Substitute Eq. (C.25) into Eq. (C.9) and further substitute Eqs. (C.10), (C.18), (C.23), (C.24), and (C.21) to obtain

$$\rho_n^+(\theta) = \frac{\frac{\epsilon_n}{iM} e^{S_n^+ \theta}}{\Omega_n^+ \left[\left(-\frac{\epsilon_n}{iM} + \frac{2i}{\epsilon_n} + \frac{iM}{\epsilon_n} \right) \cosh \frac{\epsilon_n}{i} + \left(\frac{\epsilon_n^2}{M^2} + \frac{2}{M} + 1 \right) \sinh \frac{\epsilon_n}{i} \right]} \quad (C.26)$$

where

$$\Omega_n^+ = 1 - \frac{\alpha^2 S_n^+ (\alpha S_n^+ + 2K)}{(\alpha S_n^+ + K)^2} \quad (C.27)$$

Multiply both numerator and denominator of Eq. (C.26) by iM and use the identities given in Eqs. (C.11) and (C.12) to simplify to

$$\rho_n^+(\theta) = \frac{\epsilon_n e^{S_n^+ \theta}}{\Omega_n^+ \left[M \left(\frac{\epsilon_n^2}{M^2} + \frac{2}{M} + 1 \right) \sin \epsilon_n - \frac{M^2}{\epsilon_n} \left(\frac{\epsilon_n^2}{M^2} + \frac{2}{M} + 1 \right) \cos \epsilon_n \right]} \quad (C.28)$$

Multiply numerator and denominator by $M \sin \epsilon_n + \epsilon_n \cos \epsilon_n$ and rewrite

$$\rho_n^+(\theta) = - \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^+ \theta}}{\Omega_n^+ \left[M^2 \left(\frac{\epsilon_n^2}{M^2} + \frac{2}{M} + 1 \right) (\sin^2 \epsilon_n - \cos^2 \epsilon_n) + \left(\epsilon_n M - \frac{M^3}{\epsilon_n} \right) \left(\frac{\epsilon_n^2}{M^2} + \frac{2}{M} + 1 \right) \sin \epsilon_n \cos \epsilon_n \right]} \quad (C.29)$$

Add zero to the part within brackets in the form of $M^2(\epsilon_n^2/M^2 + 2/M + 1)(\cos^2 \epsilon_n - \cos^2 \epsilon_n)$ and invokes the identity

$$\sin^2 y + \cos^2 y = 1 \quad (C.30)$$

to obtain

$$\rho_n^+(\theta) = \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^+ \theta}}{\Omega_n^+ \left[(M^2 + 2M + \epsilon_n^2) - 2(M^2 + 2M + \epsilon_n^2) \cos^2 \epsilon_n + \left(2\epsilon_n + \frac{\epsilon_n^3}{M} - \frac{2M^2}{\epsilon_n} - \frac{M^3}{\epsilon_n} \right) \sin \epsilon_n \cos \epsilon_n \right]} \quad (C.31)$$

Rewrite Eq. (C.17) as

$$\sin \epsilon_n = 2 \cos \epsilon_n \left(\frac{M \epsilon_n}{\epsilon_n^2 - M^2} \right) \quad (C.32)$$

Substitute Eq. (C.32) for $\sin \epsilon_n$ in the denominator of Eq. (C.31) and simplify to

$$\rho_n^+(\theta) = \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^+ \theta}}{\Omega_n^+ (M^2 + 2M + \epsilon_n^2)} \quad (C.33)$$

Now, considering functions involving S_n^- , begin at Eq. (C.25) and in similar manner obtain

$$\rho_n^-(\theta) = \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^- \theta}}{\Omega_n^- (M^2 + 2M + \epsilon_n^2)} \quad (C.34)$$

where

$$\Omega_n^- = 1 - \frac{\alpha^2 S_n^- (\alpha S_n^- + 2K)}{(\alpha S_n^- + K)^2} \quad (C.35)$$

Comparing Eqs. (C.7) and (C.8) and observing that all the residues, ρ_n , are described by ρ_n^+ and ρ_n^- , the final solution is given by

$$C(\theta) = 2e^M \left\{ \sum_{n=1}^{\infty} \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^+ \theta}}{\Omega_n^+ (M^2 + 2M + \epsilon_n^2)} + \sum_{n=1}^{\infty} \frac{\epsilon_n (M \sin \epsilon_n + \epsilon_n \cos \epsilon_n) e^{S_n^- \theta}}{\Omega_n^- (M^2 + 2M + \epsilon_n^2)} \right\} \quad (C.36)$$

APPENDIX D

EXPERIMENTAL DATA AND COMPARISON WITH MODEL

The data are shown on the following plots by crosses and the solid line represents the model fit to the data. Runs GPRTD-29 through GPRTD-48 were performed with no solids holdup and are compared to the ordinary closed vessel dispersion model, hence, only one parameter, D , appears on the plot. The remaining runs are compared to the new dispersive flow with interacting deadwater model: GPRTD-49 through GPRTD-98. When a plot appears with no line representing the model, this means that the series solution did not converge satisfactorily or that five digit accuracy was not sufficient. This latter problem occurs when the two series generate numbers of about 10^3 or more in magnitude, but of opposite sign, such that their sum gives a poor value for concentration. Such a problem usually develops when D is less than about 0.025. However, the model parameters are accurate since they were calculated from the moments of the data.

GPRTD-29

ORNL-DWG. 80-18767

Fig. D-1. Experimental and calculated effluent concentration for run no. GPRTD-29.

GPRTD-30

ORNL-DWG. 80-18768

Fig. D-2. Experimental and calculated effluent concentration for run no. GPRTD-30.

GPRTD-31A

ORNL-DWG. 80-18769

Fig. D-3. Experimental and calculated effluent concentration for run no. GPRTD-31A.

GPRTD-31B

ORNL-DWG.80-18770

Fig. D-4. Experimental and calculated effluent concentration for run no. GPRTD-31B.

GPRTD-32

ORNL-DWG. 80-18771

Fig. D-5. Experimental and calculated effluent concentration for run no. GPRTD-32.

GPRTD-33

ORNL-DWG.80-18772

Fig. D-6. Experimental and calculated effluent concentration for run no. GPRTD-33.

GPRTD-34

ORNL-DWG.80-18773

Fig. D-7. Experimental and calculated effluent concentration for run no. GPRTD-34.

Fig. D-8. Experimental and calculated effluent concentration for run no. GPRTD-35.

GPRTD-36

ORIG-DWG. 80-18775

Fig. D-9. Experimental and calculated effluent concentration for run no. GPRTD-36.

GPRTD-37

ORNL-DWG.80-18776

Fig. D-10. Experimental and calculated effluent concentration for run no. GPRTD-37.

GPRTD-38

ORNL-DWG.80-18777

Fig. D-11. Experimental and calculated effluent concentration for run no. GPRTD-38.

Fig. D-12. Experimental and calculated effluent concentration for run no. GPRTD-39.

Fig. D-13. Experimental and calculated effluent concentration for run no. GPRTD-40.

GPRTD-41

ORNL-DWG 80-18780

Fig. D-14. Experimental and calculated effluent concentration for run no. GPRTD-41.

GPRTD-42

ORNL-DWG.60-18781

Fig. D-15. Experimental and calculated effluent concentration for run no. GPRTD-42.

GPRTD-43

ORNL-DWG. 80-18782

Fig. D-16. Experimental and calculated effluent concentration for run no. GPRTD-43.

GPRTD-44

ORNL-DWG 80-18783

Fig. D-17. Experimental and calculated effluent concentration for run no. GPRTD-44.

GPRTD-45

ORNL-DWG. 80-18784

Fig. D-18. Experimental and calculated effluent concentration for run no. GPRTD-45.

GPRTD-46

ORNL-DWG. 80-18785

Fig. D-19. Experimental and calculated effluent concentration for run no. GPRTD-46.

GPRTD-47

ORNL-DWG. 80-18786

Fig. D-20. Experimental and calculated effluent concentration for run no. GPRTD-47.

GPRTD-48

ORNL-DWG 80-18787

Fig. D-21. Experimental and calculated effluent concentration for run no. GPRTD-48.

GPRTD-49

ORNL-DWG 80-18788

Fig. D-22. Experimental and calculated effluent concentration for run no. GPRTD-49.

GPRTD-50

ORNL-DWG. 80-18789

Fig. D-23. Experimental and calculated effluent concentration for run no. GPRTD-50.

GPRTD-51

ORNL-DWG.60-18790

Fig. D-24. Experimental and calculated effluent concentration for run no. GPRTD-51.

GPRTD-52

ORNL-DWG. 80-18791

Fig. D-25. Experimental and calculated effluent concentration for run no. GPRTD-52.

GPRTD-53

ORNL-DWG.80-18792

Fig. D-26. Experimental and calculated effluent concentration for run no. GPRTD-53.

GPRTD-54

ORNL-DWG.80-18793

Fig. D-27. Experimental and calculated effluent concentration for run no. GPRTD-54.

GPRTD-55

ORNL-DWG.60-16794

Fig. D-28. Experimental and calculated effluent concentration for run no. GPRTD-55.

GPRTD-56

ORNL-DWG.80-18795

Fig. D-29. Experimental and calculated effluent concentration for run no. GPRTD-56.

GPRTD-57

ORNL-DWG 80-18796

Fig. D-30. Experimental and calculated effluent concentration for run no. GPRTD-57.

GPRTD-58

ORNL-DWG.80-18797

Fig. D-31. Experimental and calculated effluent concentration for run no. GPRTD-58.

GPRTD-59

ORNL-DWG.80-18798

Fig. D-32. Experimental and calculated effluent concentration for run no. GPRTD-59.

GPRTD-60

ORNL-DWG.80-18799

Fig. D-33. Experimental and calculated effluent concentration for run no. GPRTD-60.

Fig. D-34. Experimental and calculated effluent concentration for run no. GPRTD-61.

GPRTD-62

ORNL-DWG 80-18801

Fig. D-35. Experimental and calculated effluent concentration for run no. GPRTD-62.

GPRTD-63

ORNL-DW3.60-18802

Fig. D-36. Experimental and calculated effluent concentration for run no. GPRTD-63.

GPRTD-64

ORNL-DWG.80-18803

Fig. D-37. Experimental and calculated effluent concentration for run no. GPRTD-64.

GPRTD-65

ORNL-DWG 80-18804

Fig. D-38. Experimental and calculated effluent concentration for run no. GPRTD-65.

GPRTD-66

ORNL-DWG 80-18805

Fig. D-39. Experimental and calculated effluent concentration for run no. GPRTD-66.

GPRTD-67

ORNL-DWG.80-18806

Fig. D-40. Experimental and calculated effluent concentration for run no. GPRTD-67.

GPRTD-68

ORNL-DWG. 80-18907

Fig. D-41. Experimental and calculated effluent concentration for run no. GPRTD-68.

GPRTD -69

ORNL-DWG 80-18808

Fig. D-42. Experimental and calculated effluent concentration for run no. GPRTD-69.

GPRTD-70

ORNL-DWG.80-18809

Fig. D-43. Experimental and calculated effluent concentration for run no. GPRTD-70.

GPRTD-71

ORNL-DWG 80-18810

Fig. D-44. Experimental and calculated effluent concentration for run no. GPRTD-71.

GPRTD-72

ORNL-DWG 80-18811

Fig. D-45. Experimental and calculated effluent concentration for run no. GPRTD-72.

GPRTD-73

ORNL-DWG.80-18812

Fig. D-46. Experimental and calculated effluent concentration for run no. GPRTD-73.

GPRTD-74

ORNL-DWG 80-18913

Fig. D-47. Experimental and calculated effluent concentration for run no. GPRTD-74.

GPRTD-75

ORNL-DWG 80-18814

Fig. D-48. Experimental effluent concentration for run no. GPRTD-75.

GPRTD-76

ORNL-DWG 80-18815

Fig. D-49. Experimental effluent concentration for run no. GPRTD-76.

GPRTD-77

ORNL-DWG 80-10816

Fig. D-50. Experimental and calculated effluent concentration for run no. GPRTD-77.

GPRTD-78

ORNL-DWG 80-18817

Fig. D-51. Experimental and calculated effluent concentration for run no. GPRTD-78.

GPRTD-79

ORNL-DWG 80-18818

Fig. D-52. Experimental and calculated effluent concentration for run no. GPRTD-79.

GPRTD-80

ORNL DWG 80-18819

Fig. D-53. Experimental and calculated effluent concentration for run no. GPRTD-80.

Fig. D-54. Experimental and calculated effluent concentration for run no. GPRTD-81.

GPRTD-82

ORNL-DWG. 80-18821

Fig. D-55. Experimental effluent concentration for run no. GPRTD-82.

GPRTD-83

ORNL-DWG 80-18822

Fig. D-56. Experimental effluent concentration for run no. GPRTD-83.

GPRTD-84

ORNL-DWG 80-18823

Fig. D-57. Experimental and calculated effluent concentration for run no. GPRTD-84.

GPRTD-85

ORNL-DWG 80-18824

Fig. D-58. Experimental and calculated effluent concentration for run no. GPRTD-85.

GPRTD-86

ORNL-DWG 80-18825

Fig. D-59. Experimental effluent concentration for run no. GPRTD-86.

GPRTD-87

ORNL-DWG 80-13626

Fig. D-60. Experimental effluent concentration for run no. GPRTD-87.

GPRTD-88

ORNL-DWG. 80-18827

Fig. D-61. Experimental and calculated effluent concentration for run no. GPRTD-88.

GPRTD-89

ORNL-DWG 80-18828

Fig. D-62. Experimental and calculated effluent concentration for run no. GPRTD-89.

GPRTD-90

ORNL-DWG 80-18829

Fig. D-63. Experimental effluent concentration for run no. GPRTD-90.

GPRTD-91

ORNL-DWG 80-18830

Fig. D-64. Experimental and calculated effluent concentration for run no. GPRTD-91.

GPRTD-92

ORNL-DWG 80-18831

Fig. D-65. Experimental and calculated effluent concentration for run no. GPRTD-92.

GPRTD-93

ORNL-DWG 80-18832

Fig. D-66. Experimental and calculated effluent concentration for run no. GPRTD-93.

GPRTD-94

ORNL-DWG 80-18833

Fig. D-67. Experimental and calculated effluent concentration for run no. GPRTD-94.

GPRTD-95

ORNL-DWG 80-18834

Fig. D-68. Experimental and calculated effluent concentration for run no. GPRTD-95.

GPRTD-96

ORNL-DWG 80-18835

Fig. D-69. Experimental effluent concentration for run no. GPRTD-96.

GPRTD-97

ORNL-DWG 80-18836

Fig. D-70. Experimental and calculated effluent concentration for run no. GPRTD-97.

GPRTD-98

ORNL-DWG 80-18837

Fig. D-71. Experimental and calculated effluent concentration for run no. GPRTD-98.

APPENDIX E

COMPUTER PROGRAM

The computer code, written in FORTRAN language, that does the computations is listed on the following pages. It has several options (see comment statements) including the ability to plot the results using the DISSPLA software package.

```

C-----GASRTG
C-----CLOSED VESSEL MODELS
C-----**DISPERSIVE FLOW WITH INTERACTIVE DEADWATER**
C-----DATE: 10-14-80
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/XXXX/T(300),C(300),TH(300),E(300),TITL(5),S
      COMMON/I100/THETA(300),CE(300),ALPHA,DISWUM,CAPK,DISPM,WHOD
      COMMON/COMP/CTHE(300),THKUM,PO2,EDISH,ECAPE,PI
      DIMENSION RUNUM(100),RESULT(15,100)
C-----V FT/HR
      V(S,TT,PP,A)=6.575*200*(TT+273.D0)*S/PP/A
      PI=4.D0*DATAH(1.D0)
C-----MOLECULAR WT. OF AIR & HELIUM
      WHAIR=28.9690
      WHCH4=4.D0
C-----KILN LENGTH FT
      ZLEN=7.12500
C-----KILN I.D. INCHES
      DI=6.500
C-----AREA SQFT
      AREA=DI/2.D0/12.D0
      AREA=PI*AREA*AREA
C-----ENTRANCE AND EXIT TUBE VOLUME(ML) CHS TO (CUFT)
      EEVOL=429.400
      EEVOL=EEVOL*3.5310-05
C-----INSTRUMENT LAG (SEC) CHS TC (MIN)
      HLAG=1.7100
      HLAG=HLAG/60.D0
C-----DENSITY OF SAND, LB/CUFT
      RHO=84.3300
C-----VOID FRACTION SAND
      VOID=.48900
      CALL CALCHP
      WRITE(6,103)
103  FORMAT(' ',34X,'BULK',8X,'FROM MOMENTS',8X,'DISPERSION ',/,
14X,'TITL',4X,'RPM',3X,'HLDP',3X,'FLOWRATE',X,'THLAP',2X,'THEAN',
22X,'SIGNA',4X,'GAMMA',3X,'CLOSED',3X,'CPEV',4X,'DISWUM',3X,'CAPK',
33X,'HTANK',5X,'P/V',3X,'EDISH',3X,'ECAPE',/,
418X,'(VFULL)',1X,'(H**3/H)',1X,'(MIN)',2X,'(MIN)',X,'(MIN**2)',
5X,'(MIN**3)')
      DO 9 LOOP=1,100
      READ(18,100,END=1)TITL
100  FORMAT(5A10)
      READ(18,102)RPM
      READ(18,102)SCPM
      READ(18,102)BP
      READ(18,102)AT
      READ(18,102)TML
      READ(18,102)HLDP
102  FORMAT(D10.4)
      ALAG=SCPM*(AT+273.D0)*29.9200/273.D0/BP
      ALAG=EEVOL/ALAG
      TOTLAG=ALAG+HLAG
      DO 3 IJK=1,300
      READ(18,101)D1,D2
101  FORMAT(2D10.4)

```

```

      IF((D1+D2).EQ.0.D0) GO TO 4
      N=IJK
      T(N)=D1/60.D0-TOTLAG
      C(N)=D2
3     CONTINUE
4     Q=0.D0
      DO 5 K=2,N
5     Q=Q+((C(K-1)+C(K))/2.D0)*(T(K)-T(K-1))
      TBAR=0.D0
      SIG=0.D0
      GAN=0.D0
      DO 7 I=2,N
      INH=I-1
      DELT=T(I)-T(INH)
      TBAR=TBAR+DELT*(T(INH)+C(INH)+T(I)+C(I))/2.D0
      TSQ1=T(INH)*T(INH)
      TSQ2=T(I)*T(I)
      SIG=SIG+DELT*(TSQ1+C(INH)+TSQ2+C(I))/2.D0
      TCU1=TSQ1*T(INH)
      TCU2=TSQ2*T(I)
7     GAN=GAN+DELT*(TCU1+C(INH)+TCU2+C(I))/2.D0
      TBAR=TBAR/Q
      TTT=TBAR*TBAR
      SIG=SIG/Q-TTT
      GAN=GAN/Q-3.D0*TBAR*SIG-TTT*TBAR
      RAT=SIG/TTT
      DO 12 ISEE=1,N
      TH(ISEE)=T(ISEE)/TBAR
12    E(ISEE)=TBAR*C(ISEE)/Q
C-----DEBUG
C      WRITE(6,108)TTT(1)
C 108  FORMAT(' ',A10)
C      WRITE(6,105)
C 105  FORMAT('/', ' ITRY',8X,'DISPN',6X,'ERROR')
C
      DISP=GAN/2.D0
      SAVE=DISP
      A=1.500*DISP
      B=.500*DISP
      SPAN=A
      KOFF=1
      ZZZ=DISP/SPAN
      DO 10 ITRY=1,15
      DISP=SPAN*ZEXP(KOFF,ZZZ)
      ZZZ=1.D0-DEXP(-1.D0/DISP)
      ZZZ=2.D0*DISP-2.D0*DISP*DISP*ZZZ-RAT
C-----DEBUG
C      WRITE(6,106)ITRY,DISP,ZZZ
C 106  FORMAT(2X,I2,3X,F9.4,3X,F9.4)
C
      IF(KOFF.LT.0)GO TO 11
10    CONTINUE
11    CK=DABS(SAVE-DISP)*100.D0/SAVE
      VEL=V(SCP,AT,BP,A*EA)
      VEL=VEL/60.D0
      TMEAN=ZLZN/VEL

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```

HLDP=HLDP/453.59DO/RHO/ZLEN
HLDP=100.DO*HLDP/AREA
ALPHA=VOID*HLDP/100.DO
OHWELL=(1.DO-HLDP/100.DO*ALPHA)
THEAN=THEAN*OHWELL
ALPHA=ALPHA/OHWELL
SIGNA=RAT
GAMMA=GAM/TTT/TBAR
DISNUM=0.DO
CAPK=0.DO
TKNUM=0.DO
POQ=0.DO
EDISN=0.DO
ECAPK=0.DO
IF (ALPHA.EQ.0.DO) GO TO 15
CALL FINDEH (SIGNA,GAMMA,DISPN)
CALL TANKEH (SIGNA,GAMMA)
15 SCFMET=VEL*AREA*2.831685D-02*67.DO
LOOPER=LOOP
RUNNUM (LOOP) =TITL (1)
RESULT (1,LOOP) =RPH
RESULT (2,LOOP) =HLDP
RESULT (3,LOOP) =SCFMET
RESULT (4,LOOP) =THEAN
RESULT (5,LOOP) =TBAR
RESULT (6,LOOP) =SIG
RESULT (7,LOOP) =GAM
RESULT (8,LOOP) =DISPN
RESULT (9,LOOP) =SAVE
RESULT (10,LOOP) =DISNUM
RESULT (11,LOOP) =CAPK
RESULT (12,LOOP) =TKNUM
RESULT (13,LOOP) =POQ
RESULT (14,LOOP) =EDISN
RESULT (15,LOOP) =ECAPK
WRITE (6,104) TITL (1),RPH,HLDP,SCFMET,THEAN,TBAR,SIG,GAM,DISPN,SAVE,
1DISNUM,CAPK,TKNUM,POQ,EDISN,ECAPK
104 FORMAT (' ',A10,F5.1,F7.1,5X,F5.3,2F7.2,2F9.5,F7.4,F8.4,2X,
1F6.4,2X,F7.4,2X,F5.2,2X,F7.5,1X,F6.4,2X,F6.4)
IF (CAPK.LT.0.DO) GO TO 9
TIMLIN=TH (1)
CALL GOODUN (TIMLIN)
CALL FIGURE
9 CONTINUE
1 CALL DONEPL
WRITE (6,200)
200 FORMAT (1H1)
WRITE (6,103)
WRITE (12,103)
DO 14 I=1,LOOPER
WRITE (12,104) RUNNUM (I), (RESULT (J,I),J=1,15)
14 WRITE (6,104) RUNNUM (I), (RESULT (J,I),J=1,15)
STOP
END

```

```

      FUNCTION ZEROUP(KID,TRY)
C     KEEPS VALUE OF ZEROUP BETWEEN ZERO AND ONE
C     ***ZEROUP BY H. E. WHATLEY***
C     *** MODIFIED DEC 1973 ***
C     *** MAJOR MODIFICATION FEB 2, 1977 ***
C     *** CHANGED TO ZEROUP FROM NULONE AUG 1, 1977
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION XCF(4), YCF(5)
      IF(KID) 3, 1, 2
      1 YCF(4) = TRY
      IF(DABS(YCF(4) - YCF(3)) - 1. D - 30) 30, 30, 40
      40 IF(TRY * YPOS * YNEG) 6, 41, 5
      41 IF(TRY * YPOS) 5, 42, 44
      42 IF(TRY) 43, 30, 6
      43 IF(YNEG) 45, 5, 33
      44 IF(YPOS - TRY) 46, 33, 6
      45 IF(TRY - YNEG) 46, 33, 5
      46 XCF(2) = XCF(4)
      YCF(2) = TRY
      BS = 1.0D0
      GOTO 9
      5 XNEG = XCF(4)
      YNEG = TRY
      BS = BS * .85D0 - 1. D0
      GOTO 7
      6 XPOS = XCF(4)
      YPOS = TRY
      BS = BS * .85D0 + 1. D0
      7 DO8J = 1, 3
      YCF(J) = YCF(J+1)
      8 XCF(J) = XCF(J+1)
      9 DBS = DABS(BS)
      IF(XPOS * XNEG .GT. 0. D0) GOTO 11
      IF(YCF(2) .EQ. 0. D0) GOTO 31
C     *** BEPOPE BOTH XPOS AND XNEG ARE ESTABLISHED ***
      IF(XCF(3) * (1. D0 - XCF(3)) .LE. 0. D0) GOTO 33
      XCF(4) = XCF(3) - DBS * (XCF(2) - XCF(3)) * YCF(3) / (YCF(2) - YCF(3))
      DO12 J = 1, 10
      IF(XCF(4) * (1. D0 - XCF(4))) 12, 12, 36
      12 XCF(4) = (XCF(4) + XCF(3)) / 2. D0
      GOTO 33
      11 CUT = CUT + 1. D0
C     *** THIS IS THE WAY WE FUN ***
      IF(CUT .LT. 1.9D0 .OR. DBS .GT. 4.0D0) BS = 0. D0
      IF(DBS .GT. 3.5D0) GOTO 22
      IF(DBS .GT. 2.3D0) GOTO 27
C     *** SIMPLE LINEAR INTERPOLATION ***
      14 NBS = (BS - .8D0) * (.95 + .8D0)
      AAA = NBS * DEXP(-CUT)
      IF(NBS * BS) 24, 26, 25
      24 YPOS = YPOS * 2. D0 ** (1. D0 - DBS)
      GOTO 26
      25 YNEG = YNEG * 2. D0 ** (1. D0 - DBS)
      26 XCF(4) = XPOS - (XNEG - XPOS) * (YPOS - AAA * YNEG) / (YNEG - YPOS) / (1. D0 + AAA)
      GOTO 29
C     *** TRIES A PARABOLIC FIT ***

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```

27 AAA=0.D0
   CCC=0.D0
   BBB=0.D0
   XCF(4)=XCF(1)
   YCF(4)=YCF(1)
   YCF(5)=YCF(2)
   DO28J=1,3
   AAA=AAA+XCF(J)*YCF(J+1)-YCF(J)*XCF(J+1)
   BBB=BBB+YCF(J)*XCF(J+1)+XCF(J+1)-YCF(J+1)*XCF(J)*XCF(J)
28 CCC=CCC+YCF(J+2)*(XCF(J)+XCF(J+1)+XCF(J+1)-XCF(J+1)*XCF(J)+XCF(J))
   RAD= BBB*BBB-4.D0*AAA*CCC
   IF(RAD.LE.0.D0 .OR. DABS(AAA).LT.1.D-25) GOTO 22
   RAD= 0.5D0*DSQRT(RAD)/AAA
   BBB= -0.5D0*BBB/AAA
   XCF(4)= BBB+RAD
   IF((XCF(4)-XNEG)*(XCF(4)-XPOS).LT.0.D0) GOTO 36
   XCF(4)= BBB-RAD
29 IF((XCF(4)-XNEG)*(XCF(4)-XPOS).LT.0.D0) GOTO 36
C *** BISECTS INTERVAL ***
22 XCF(4)=(XPOS+XNEG)/2.D0
C THIS WAY OUT
36 IF(DABS((XPOS-XNEG)/(XPOS+XNEG)) -DEL)30,30,3
30 KID = -1
   3 ZERUF= XCF(4)
   RETURN
C *** INITIALIZES WHEN KID .GT. ZERO ***
2 XCF(4)= TRY
   CUT = 0.D0
   XPCS= 0.D0
   XNEG= 0.D0
   YPOS= 0.D0
   YNEG= 0.D0
   YCF(3)= 0.D0
   DEL = KID* .0000001D0
   DEL = DABS(DEL)
   KID = 0
   IF((1.D0-TRY)*TRY)33,33,3
C FIRST STEP
31 XCF(4)= 0.9D0*XCF(3)
   BS= 0.D0
   IF(XCF(3)*(1.D0-XCF(3)).GT.0.D0) GOTO 36
33 WRITE(6,133)
   GOTO 30
133 FORMAT( ' VIOLATION OF ZERUF')
   END

```

```
      FUNCTION BIG(ARRAY,N)
C-----FINDS LARGEST VALUE IN AN ARRAY OF N POINTS
      DIMENSION ARRAY(N)
      BIG=ARRAY(1)
      DO 400 K=2,N
      IF (BIG.GT.ARRAY(K)) GO TO 400
      BIG=ARRAY(K)
400    CONTINUE
      RETURN
      END
```



```

SUBROUTINE FINDEN(SIGNA,GAMMA,BOUNDH)
C-----FINDS VALUOS OF CAPK AND DISNUH FROM SECOND
C-----AND THIRD MOMENTS
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/I100/THETA(300),CE(300),ALPHA,DISNUH,CAPK,DISPK,WHOD
      FONE=1.00-ALPHA
      A2=ALPHA*ALPHA
      A3=ALPHA*A2
      BOUNDL=.00100
      SPAN=BOUNDH-BOUNDL
      DELTA=SPAN/100.00
      A=BOUNDL
      FH=CRSOVR(A,FONE,A2,A3,SIGNA,GAMMA,CAPK)
      ESTD=A
      ESTK=CAPK
      ERR=FH
      NTRY=100
6     DO 4 I=1,NTRY
      B=A+DELTA
      AH=CRSOVR(B,FONE,A2,A3,SIGNA,GAMMA,CAPK)
      IF(DABS(AH).GT.DABS(FH))GO TO 7
      ESTD=B
      ESTK=CAPK
      ERR=FH
7     FLIP=FH-AH
      IF(FLIP.LE.0.00)GO TO 3
      A=B
      FH=AH
4     CONTINUE
      WRITE(6,200)
200    FORMAT(' FINDEN:ROOTS NOT IN GIVEN INTERVAL')
      IF(NTRY.EQ.10)GO TO 5
      NTRY=10
      ESTDK=ESTD
      ESTKK=ESTK
      ERRK=ERR
      WRITE(6,201)
201    FORMAT('      WILL INCRZASE UPPER BOUND BY 10%')
      GO TO 6
      5     DISNUH=ESTDK
      CAPK=ESTKK
      WRITE(6,202)ERRK
202    FORMAT(' PARAMETERS ESTIMATED:ERROR=',E10.4)
      RETURN
      3     KOFF=1
      SPAN=B-A
      ZZZ=.500
      DO 1 ITRY=1,35
      DISNUH=SPAN*ZZZ*(KOFF,ZZZ)+A
      ZZZ=CRSOVR(DISNUH,FONE,A2,A3,SIGNA,GAMMA,CAPK)
      IF(KOFF.LT.0)GO TO 2
      1     CONTINUE
      WRITE(6,100)
100    FORMAT(' FINDEN:POOR CONVERGENCE')
      2     RETURN
      END

```

```

FUNCTION CRSOVR(DISHUE,POKE,A2,A3,SIGMA,GAMMA,CAPK)
IMPLICIT REAL*8(A-H,O-Z)
C-----USED BY FINDER
DF1=DISHUE*POKE
DF2=DF1*DF1
DF3=DF1*DF2
TUF=DEXP(-1.DO/DF1)
TUPH=1.DO-TUF
CAPK=2.DO*A2/(SIGMA-2.DO*DF1+2.DO*DF2*TUPH)
ZZZ=12.DO*DF2*(1.DO+TUF)-24.DO*DF3*TUPH-12.DO*DF2*A2*TUFH/CAPK
1+6.DO*A3/CAPK/CAPK+12.DO*DF1*A2/CAPK-GAMMA
CRSOVR=ZZZ
RETURN
END

```

```

SUBROUTINE GOODMUN (TIMLIN)
C-----CALCULATES CONC. VS. TIME CURVE; DISPERSION MODEL
C-----WITH DEADWATER
      IMPLICIT REAL*8 (A-H,O-Z)
      LOGICAL*1 PTEST
      COMMON/I100/THETA (300),CE (300),ALPHA,DISNUM,CAPK,DISPN,WMOD
      DIMENSION EPSN (200),SN (200),PREN (200),SMN (200),PRENN (200),
      1CEH (300),KOP (300)
      DCOTAN (ARG) =DCOS (ARG) /DSIN (ARG)
      PTEST=ALPHA.EQ.0.DO
C-----SET UP VALUES FOR THETA
      DELT=.01D0
      INLIN=TIMLIN*100.DO-10.DO
      TINLOW=INLIN/100.DO
      IF (TINLOW.GE.0.DO) GO TO 20
      TINLOW=0.DO
      WMOD=300
      GO TO 21
20  WMOD=300-INLIN
21  DO 22 I=1,WMOD
      THETA (I) =TINLOW+I*DELT
      CE (I) =0.DO
      CEH (I) =0.DO
22  KOP (I) =I
      NPASS=0
      IKOP=WMOD
C-----FIND VALUES OF EPSILON FROM IMPLICIT FORMULA
      A=.001D0
      H=.15D0
      TTT=2.DO*DISNUM*(1.DO-ALPHA)
      IF (PTEST) TTT=2.DO*DISPN
      ART=TTT*A
      PH=DSIN (A) * (ART-1.DO/ART) /2.DO-DCOS (A)
16  DO 1 I=1,200
3    B=A+H
      ART=TTT*B
      AH=DSIN (B) * (ART-1.DO/ART) /2.DO-DCOS (B)
      FLIP=PH-AH
      IF (FLIP.LE.0.DO) GO TO 2
      A=B
      PH=AH
      GO TO 3
2    KOFF=1
      SPAN=B-A
      ZZZ=.5D0
      DO 4 ITRY=1,25
      EPS=SPAN*ZERUP (KOFF,ZZZ) +A
      ART=TTT*EPS
      ZZZ=DSIN (EPS) * (ART-1.DO/ART) /2.DO-DCOS (EPS)
      IF (KOFF.LT.0) GO TO 5
4    CONTINUE
      WRITE (6,500) I
500  FORMAT (' TROUBLE WITH ZERUP ON',I3,'TH FOOT')
5    A=B
      PH=AH
      EPSN (I) =EPS

```

```

1  CONTINUE
C-----DEBUG
C      DO 10 J=1,200
C      ART=TTT*EPSN(J)
C      EPROR=(ART-1.00/ART)/2.00-DCOTAN(EPSN(J))
C      WRITE(6,200) J,EPSN(J),ERROR
C 200  FORMAT(3X,I3,2(2X,1PE12.5))
C 10  CONTINUE
      IF (FTEST) GO TO 30
      IF (NPASS.GT.0) GO TO 17
C-----FIRST SERIES
C-----COMPUTE PREMULTIPLIERS, ETC. FOR SUBSEQUENT CALCULATIONS
      AL2=ALPHA*ALPHA
      AL3=ALPHA*AL2
      T1=TTT
      T=1.00/TTT
      PONE=1.00-ALPHA
      PD1=T*T+2.00*T
      AK=CAPK/ALPHA
      DO 6 I=1,200
      EPS2=EPSN(I)*EPSN(I)
      PHI=(-T1*T1*EPS2-1.00)/T1/2.00
      PROOT=ALPHA*PHI+CAPK
      ROOT=DSQRT(1.00-4.00*AL2*PHI*CAPK/PROOT/PROOT)
      SN(I)=(PHI*(ROOT+1.00)+AK*(ROOT-1.00))/2.00/PONE
      OMEGA=ALPHA*SN(I)+CAPK
      OMEGA=1.00-(AL3*SN(I)*SN(I)+2.00*AL2*CAPK*SN(I))/OMEGA/OMEGA
      PRE=2.00*EPSN(I)*(T*DSIN(EPSN(I))+EPSN(I)*DCOS(EPSN(I)))
      PREN(I)=PRE/OMEGA/(PD1+EPS2)
      ROOT=-ROOT
      SNH(I)=(PHI*(ROOT+1.00)+AK*(ROOT-1.00))/2.00/PONE
      OMEGA=ALPHA*SNH(I)+CAPK
      OMEGA=OMEGA*OMEGA
      OMEGA=OMEGA/(OMEGA-(AL3*SNH(I)*SNH(I)+2.00*AL2*CAPK*SNH(I)))
      PRENH(I)=PRE*OMEGA/(PD1+EPS2)
C      WRITE(6,300) I,SN(I),PREN(I),EPSN(I),SNH(I),PRENH(I)
C 300  FORMAT(3X,I4,5(2X,1PE12.5))
6  CONTINUE
C-----CALCULATE CONCENTRATION AS FUNCTION OF TIME
      DO 7 I=1,NMOD
      DO 8 J=1,200
      TERM=PREN(J)*DEXP(I+SN(J)*THETA(I))
      CE(I)=CE(I)+TERM
      CONVER=DABS(TERM/CE(I))
      IF (CONVER.LE.1.D-5 .AND. J.GT.10) GO TO 9
8  CONTINUE
      WRITE(6,100) THETA(I)
100  FORMAT(' FIRST SERIES DID NOT CONVERGE FOR THETA=',1PE10.3)
9  WRITE(6,400) I,THETA(I),CE(I),J
400  FORMAT(3X,I4,2(2X,1PE12.5),I6)
7  CONTINUE
      GO TO 18
C-----SECOND SERIES
C-----PREMULTIPLIERS
17  DO 15 I=1,200
      EPS2=EPSN(I)*EPSN(I)

```

```

PHI = (-T1*T1*EPS2-1.D0)/T1/2.D0
PROOT = ALPHA*PHI*CAPK
ROOT = DSQRT(1.D0-4.D0*AL2*PEI*CAPK/PROOT/PROOT)
PRE = 2.D0*EPSN(I)*(T*DSIN(EPSN(I))+EPSN(I)*DCOS(EPSN(I)))
ROOT = -ROOT
SNH(I) = (PHI*(ROOT+1.D0)+AK*(ROOT-1.D0))/2.D0/FOH2
OMEGA = ALPHA*SNH(I)*CAPK
OMEGA = OMEGA*OMEGA
OMEGA = OMEGA/(OMEGA-(AL3*SNH(I)*SNH(I)+2.D0*AL2*CAPK*SNH(I)))
PRENH(I) = PRE*OMEGA/(PD1+EPS2)
C      WRITE(6,700) I,SNH(I),PRENH(I)
C 700  FORMAT(3X,I4,2(2X,1PE20.13))
      15 CONTINUE
C-----CALCULATE CONCENTRATION
      18 IFAIL=0
      DO 12 I=1,IKOP
      DO 11 J=1,200
      TERM=PRENH(J)*DEXP(T*SNH(J)*THETA(KOP(I)))
      CEN(KOP(I))=CEN(KOP(I))+TERM
      CONVER=DABS(TERM/CEN(KOP(I)))
      IF(CONVER.LE.1.D-5 .AND. J.GT.10) GO TO 14
      11 CONTINUE
      IF(DABS(CEN(KOP(I))) .LT. 1.D-10) GO TO 12
      IFAIL=IFAIL+1
      KOP(IFAIL)=KOP(I)
      14 WRITE(6,400) KOP(I),THETA(KOP(I)),CEN(KOP(I)),J
      12 CONTINUE
      IKOP=IFAIL
      NPASS=NPASS+1
      IF(IKOP.EQ.0) GO TO 999
      IF(NPASS.LE.10) GO TO 16
      WRITE(6,600) IFAIL
      600 FORMAT(' 2ND SERIES DID NOT CONVERGE FOR ',I3,' VALUES OF THETA')
C-----ADD RESULTS FROM EACH SERIES
      999 DO 900 IFIN=1,NMOD
      900 CE(IFIN)=CE(IFIN)+CEN(IFIN)
      RETURN
C-----ORDINARY DISPERSION MODEL
C-----COMPUTE MULTIPLIERS, ETC. FOR SUBSEQUENT CALCULATIONS
      30 T=1.D0/TTT
      PD2=T*T
      PD3=2.D0*T
      PD1=PD2+PD3
      DO 31 I=1,200
      EPS2=EPSN(I)*EPSN(I)
      SN(I) = -(PD2+EPS2)/PD3
      PRE=2.D0*EPSN(I)*(T*DSIN(EPSN(I))+EPSN(I)*DCOS(EPSN(I)))
      PREN(I)=PRE/(PD1+EPS2)
C      WRITE(6,3001) I,SN(I),PREN(I)
C 3001 FORMAT(3X,I4,2(2X,1PE12.5))
      31 CONTINUE
C-----CALCULATE CONCENTRATION AS FUNCTION OF TIME
      DO 32 I=1,NMOD
      DO 33 J=1,200
      TERM=PREN(J)*DEXP(T*SN(J)*THETA(I))
      CE(I)=CE(I)+TERM

```

```
CONVER=DAPS(TEMP/CE(I))  
IF(CONVER.LE.1.D-5 .AND. J.GT.10) GO TO 34  
33 CONTINUE  
WRITE(6,100) THETA(I)  
34 WRITE(6,400) I, THETA(I), CE(I), J  
32 CONTINUE  
END
```

```

SUBROUTINE FIGURE
C-----USES DISPLA TO PLOT RESULTS AND DATA
COMMON/TIOO/THETA (2,300),CE (2,300),ALPHA (2,1),DISNUM (2,1),
ICAPK (2,1),DISPN (2,1),NMOD
COMMON/XXXX/T (2,300),C (2,300),TH (2,300),E (2,300),TITL (10),N
DIMENSION X (300),Y (300),HEAD (4)
DATA NUMBER/0/
DATA HEAD/'+' ',' ',' ' '
DO 2 I=1,2
2 HEAD(I+1)=TITL(I)
DO 1 I=1,N
1 X(I)=TH(1,I)
Y(I)=E(1,I)
CALL SIMPLX
CALL HX1ALF('L/CSTD','+')
CALL HX2ALF('STANDA','+')
CALL HX3ALF('L/CGRE','+')
CALL HX4ALF('SCRIPT','E')
CALL TITLE(HEAD,-100,'!Q+S',100,'+C(!Q+S',100,9.,6.2)
CALL XTICKS(5)
CALL YTICKS(5)
YHI=BIG(Y,N)
IYHI=10.*YHI+1.
YHI=IYHI/10.
CALL YAXANG(0.0)
CALL BLNK1(-.1,0.,-.1,6.3,0)
CALL BLNK2(-.1,9.1,-.1,0.,0)
CALL GRAP(0.,1.,3.,0.,'SCALE',YHI)
CALL RESET('BLNKS')
CALL BLNK1(-.1,.7,-.1,6.3,0)
CALL YGRAXS(0.,'SCALE',YHI,6.2,' S',-100,0.,0.)
CALL BLNK1(-.1,9.2,5.9,6.1,0)
CALL XGRAXS(0.,1.,3.,9.,' S',100,0.,6.2)
CALL BLNK1(-.1,9.2,-.1,.3,0)
CALL XGRAXS(0.,1.,3.,9.,' S',-100,0.,0.)
CALL BLNK1(8.3,8.9,-.1,6.3,0)
CALL YGRAXS(0.,'SCALE',YHI,6.2,' S',100,9.,0.)
CALL RESET('BLNK1')
A=ALPHA(1,1)
D=DISNUM(1,1)
IF(A.EQ.0.)D=DISPN(1,1)
CC=CAPK(1,1)
CALL MESSAG('E D+S',100,6.7,5.2)
CALL REALNO(D,3,7.,5.2)
IF(A.EQ.0.)GO TO 4
CALL MESSAG('! A+S',100,6.7,5.5)
CALL REALNO(A,3,7.,5.5)
CALL MESSAG('! K+S',100,6.7,4.9)
CALL REALNO(CC,3,7.,4.9)
4 CALL MARKER(4)
CALL CURVE(X,Y,N,-1)
DO 3 I=1,NMOD
3 X(I)=THETA(1,I)
Y(I)=CE(1,I)
CALL CURVE(X,Y,NMOD,0)
C-----TO COMPARE WITH OTHER MODELS,REMOVE LEADING C FROM NEXT LINES

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C      IF(A.GT.0.) CALL WRTANK(X,Y)
C      IF(A.GT.0.) CALL WORD(X,Y)
      NUMBER=NUMBER+1
      CALL ENQPL(NUMBER)
      RETURN
      END
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SUBROUTINE TANKER (SIGMA,GAMMA)
C-----CALCULATES NUMBER OF TANKS AND CROSSFLOW RATIO FROM
C-----SECOND AND THIRD MOMENTS FOR TANKS IN SERIES
C-----MODEL
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/IIOO/THETA (300),CE (300),ALPHA,DISNUM,CAPK,DISP,NMOD
      COMMON/COMP/CTNK (300),TNKNUM,POQ,EDISN,PCAPK,PI
      DIMENSION PQ (2)
      AL2=ALPHA*ALPHA
      AL3=ALPHA*AL2
      AL4=ALPHA*AL3
      SIGSQ=SIGMA*SIGMA
      DENOM=GAMMA-2.DO*SIGSQ
      B1=AL2*(4.DO*GAMMA-6.DO*SIGSQ)/DENOM
      B2=(4.DO*AL4*GAMMA-6.DO*AL3*SIGSQ)/DENOM
      ARG=B1*B1-4.DO*B2
      IF (ARG.GE.0.DO) GO TO 2
      TNKNUM=0.DO
      POQ=0.DO
      EDISN=0.DO
      ECAPK=0.DO
      RETURN
2    ROOT=DSQRT (ARG)
      PQ (1) = (-B1+ROOT)/2.DO
      PQ (2) = (-B1-ROOT)/2.DO
      DO 1 I=1,2
      IF (PQ (I) .LT. 0.DO) GO TO 1
      POQ=PQ (I)
      TNKNUM=(1.DO+2.DO*AL2/PQ (I))/SIGMA
      EDISN=.5DO/TNKNUM/(1.DO-ALPHA)
      ECAPK=PQ (I) *TNKNUM
1    CONTINUE
      RETURN
      END

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      SUBROUTINE NETANK (X,Y)
C-----CALCULATES E-CURVE FROM TANKS IN SERIES
C      WITH DEADWATER MODEL
C-----USED WITH FIGURE FOR PLOTTING
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 X(300),Y(300)
      COMMON/XXXX/T(300),C(300),TH(300),E(300),TITL(5),N
      COMMON/IIOO/THETA(300),CE(300),ALPHA,DISNUH,CAPK,DISPN,NHOD
      COMMON/COMP/CTNK(300),TNKNUH,POQ,EDISN,ECAPE,PI
      FONE=1.DO-ALPHA
      POQN=TNKNUH*POQ
      RTNK=DSQRT(TNKNUH)
      PRE1=(1.DO-POQN)*RTNK/FONE/DSQRT(2.DO*PI)
      PRE2=POQN*POQN/ALPHA
      PRE3=PRE2/4.DO
      PRE4=-TNKNUH/2.DO
      PRE5=DSQRT(TNKNUH/2.DO)
      PRE6=-POQN/ALPHA
      DO 1 I=1,NHOD
      A=THETA(I)/FONE-1.DO
      CTNK(I)=PRE1*DEXP(PRE4+A*A)
      IF(A) 2,3,3
2     CTNK(I)=CTNK(I)+PRE3*(1.DO-DEXP(PRE5*(-A)))
      GO TO 1
3     CTNK(I)=CTNK(I)+PRE2*DEXP(PRE6+THETA(I))
1     CONTINUE
      DO 4 J=1,NHOD
4     Y(J)=CTNK(J)
      CALL DASH
      CALL CURVE(X,Y,NHOD,0)
      CALL RESET('DASH')
      RETURN
      END

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      SUBROUTINE WORD(X,Y)
C-----USED WITH FIGURE TO PLOT ORDINARY DISPERSION
C      MODEL FOR COMPARISON WITH NEW MODEL
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 X(300),Y(300)
      COMMON/XXXX/T(300),C(300),TH(300),Z(300),TITL(5),N
      COMMON/IIOO/THETA(300),CE(300),ALPHA,DISNUN,CAPF,DISPN,NMOD
      SAVAL=ALPHA
      ALPHA=0.00
      TIMLIN=TH(1)
      CALL GOODUN(TIMLIN)
      ALPHA=SAVAL
      DO 1 I=1,NMOD
1      Y(I)=CE(I)
      CALL DASH
      CALL CURVE(X,Y,NMOD,0)
      CALL RESET('DASH')
      RETURN
      END

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