DIFFUSION AND CHEMICAL REACTION IN A

TUBULAR REACTOR WITH NON-NEWTONIAN

LAMINAR FLOW

BY

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NOMENCLATURE

A   – dimensionless diffusion parameter = $D/KR^2 c_o^{n-1}$

a_n – coefficients of series expansion

C   – dimensionless concentration of reactant = c/c_o

$\bar{C}$ – dimensionless integral average concentration of reactant

c   – concentration of reactant at (z,r), mole/ft^3

c_o – inlet concentration of reactant, mole/ft^3

D   – molecular diffusivity, ft^2/sec

F   – difference equations vector

f   – scalar function values of difference equations

H   – progress vector

I   – integer

i   – one of the chemical components undergoing reaction

J   – Jacobian

j   – subscript for grid station in radial direction

K   – homogeneous reaction constant, $(mole/ft^3)^{1-n}$ sec^{-1}

κ – consistency index, lbm sec^{s-2} ft^{-1}

K'   – dimensionless homogeneous first order rate parameter as defined by KR^2/D

K"   – heterogeneous first order rate constant, sec^{-1}

k	— subscript for grid station in axial direction
L	— length of tubular reactor, ft
M	— dimensionless heterogeneous first order rate parameter as defined by K"R/D
m	— iteration index
N	— radial grid number
n	— chemical reaction order
p	— pressure, lbf/ft^2
R	— reactor radius, ft
Rn	— rate of chemical reaction, sec^{-1} $(mole/ft^3)$
r	— radial position in reactor measured from reactor axis
s	— rheology index (flow behavior index)
τ	— shear stress, lbf/ft^2
t	— time, sec
t_o	— time of contact of central stream line, sec
μ	— viscosity, lbm/ft sec
U	— dimensionless radial coordinate measured from reactor axis = r/R
v_z	— axial velocity of fluid within reactor, ft/sec
v_o	— velocity of central streamline, ft/sec
$\langle v \rangle$	— average velocity of fluid within reactor, ft/sec
w_n	— eigenvalues
x	— axis of rectangular coordinates
y	— axis of rectangular coordinates, perpendicular to x axis
z	— dimensionless time of contact $= Kzc_o^{n-1}/v_o$

Z'   – dimensionless time of contact $= Kzc_o^{n-1}/\langle v \rangle$

z   – distance coordinate measured from reactor inlet, ft

ψ_n – eigenfunctions

CHAPTER I

INTRODUCTION

In a tubular reactor in which a given chemical
reaction takes place in a continuous manner, the reactants
flow in steadily at one end and the products out at the
other. Thus, the composition varies with both axial and,
to a lesser extent, radial direction, due to the radial
velocity gradient, assuming the fluid flows in the laminar
flow region. Under constant conditions of flow the
composition at any point in the tube will usually approach
a stationary, time-independent value. This type of system
is thus characterized by changes of composition in the
space coordinates.

To solve the chemical conversion of a reacting fluid
flowing inside a circular tube, three factors determine
the difficulty and complexity of obtaining an analytical
solution. These include diffusion effects, reaction
kinetics and fluid characteristics (rheology index). All
of the previous works dealing with these concerns were
limited to specified conditions when either analytical or
numerical solution were sought.

The purpose of this research is to develop a
convenient computer program, which is capable of handling

all kinds of problems by keying in those characteristic parameters at the beginning of computer execution. A major drawback of the traditional numerical techniques is that they have been developed for large computer systems. Therefore, they are expensive to run and can be difficult to access. The program in this work is designed to run on IBM compatible Personal Computers, which are inexpensive and widely available. This user-friendly and interactive package can be easily used by a chemical engineer to obtain all the data required for the design of an isothermal tubular reactor where entrance effects can be ignored. The Crank-Nicolson finite difference method is the main tool applied in this paper in solving the partial differential equations. The results have been compared with some cases for which analytical solutions or experimental data exist.

Appendix E shows a brief survey about what has been and what has not been done in this field. It is clear that almost nothing has been studied for non-Newtonian fluids with chemical reaction other than first order. The program developed in this study has almost no restrictions on the fluid characteristics or the reaction order. This generality makes it possible to obtain data for non-Newtonian fluids undergoing a non-first order chemical reaction as easy as for other systems.

CHAPTER II

LITERATURE REVIEW

For isothermal laminar flow inside a circular tube, it is well known that different annular elements of the stream travel at different speeds. The different sections of the fluid will therefore have different reactor residence times, i.e. different chemical conversion if a chemical reaction is involved. The problem of the distribution of reactor residence times includes both the velocity distribution and the problem of diffusion effects that results from radial and axial concentration gradients.

Modeling work by previous investigators have taken a number of different approaches which have produced limited solutions to the problem. Some investigators have presented advanced analytical solutions for first order chemical reactions. However, only a few papers have considered the non-Newtonian fluids as their flowing media and even fewer have attempted to resolve the problem for non-first-order chemical reactions.

Reactors built on different scales will not give comparable results unless they show the same distribution curve for reaction residence times. Generally it is not

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sufficient to use the mean reaction time for all cases.

The distribution of residence times for Poiseuille flow in unpacked cylindrical reactors was first dealt with systematically by Bosworth in 1946 (1). Both axial and radial diffusion were taken into account separately in his work. For laminar flow and in the absence of molecular diffusion, the distribution curve of residence time varies as an inverse cube with a sharp cut-off at the minimum residence time. Criteria to decide if radial or axial diffusional effects could be neglected (within 1.0 percent range of distribution time variation) were developed:

Neglect radial diffusion if $R > 18(Dt_o)^{1/2}$

Neglect axial diffusion if $L > 360(Dt_o)^{1/2}$

Thus, the modifying effect of diffusion on the reaction time distribution curve is most pronounced in the smallest vessels. Use of these inequalities applies principally in the area of liquid flow systems. Even in modest size gaseous reaction systems, turbulent flow exists and it is not necessary to use this criteria since the radial velocity and concentration profiles are uniform.

In chemical engineering practice, it is almost always true that if the first condition is satisfied then the second is satisfied automatically, since reactor length is

typically at least twenty times the radius.

A complete investigation involving both calculated and experimental results was presented by Cleland and Wilhelm in 1956 (2). This study considered Newtonian fluid flow with irreversible first order chemical reaction in an isothermal tubular reactor with radial diffusion. A finite difference method was used to solve the continuity equation. This equation was of the form of a partial differential equation involving axial and radial coordinates. Accuracy of the numerical method was checked with the analytical solution neglecting radial diffusion.√ The criterion for neglecting radial diffusion derived in the paper agreed quite well with that of Bosworth (1). They also concluded that radial diffusion was negligible when the unconverted fraction was less than one percent lower than it would be in the absence of diffusion. A diffusion parameter, A, for fixed contact time, Z, which decreases average concentration, $\bar{C}$, by one percent from its value at A = 0 was introduced. The product of Z and A were calculated and found to be nearly constant at 0.00195 (Table I). Converted to Bosworth's notation, radial diffusion may be neglected when

$$A \times Z = Dt_o/R^2 < 0.00195$$

A criterion that the plug flow assumption is valid was also derived when A x Z > 1.0 ; appreciable errors are intreduced only at high conversions. Their experimental

TABLE I

VALUES OF Dt_o/R^2 REQUIRED TO LOWER $\bar{C}$ BY 1%

Z	$\bar{C}$ at A=0	A when $\bar{C}=.99*(C$ at A=0)	$AZ=Dt_o/R^2$ x10³
0.2	0.7037	0.00977	1.95
0.5	0.4432	0.00382	1.91
0.8	0.2887	0.00244	1.95
1.0	0.2194	0.00195	1.95
1.5	0.1135	0.00128	1.92
2.0	0.0603	0.000955	1.91

work bring out three factors that separate the real world from an ideal one: first, the entrance effect, where the parabolic velocity profile is not well developed ; the second, the existence of a non-isothermal situation (which violates their previous assumption used to derive the overall partial differential equation); third, natural convection caused by density gradients within the reactor. Density gradients may be due to a temperature gradient, a concentration gradient, or a combination of the two. The convective processes always increase mass and heat transfer rates, so that, in effect, conductivities and diffusivities are increased. According to Cleland and Wilhelm, two factors that may cause a radial density gradient within the reactors are:

1. Concentration gradients due to greater depletion of reactant near the wall compared with that at the center of the reactor,

2. Radial temperature gradients caused by heat released during reaction.

Instead of using numerical methods, Lauwerier (3) treated the same problem and partial differential equation, by using separation of variables. He was the first to recognize that a separation of variables was possible and that the resulting characteristic value problem was of the confluent hypergeometric type. The

solution is expressed as

$$C(U,Z) = \sum_{n=1}^{\infty} a_n \exp(-w_n Z)\psi_n(U)$$

where ψ_n form an orthogonal set of eigenfunctions with eigenvalues w_n.

A drawback of this solution is that when Z is small, a tremendous number of eigenfunctions must be taken into account. A simplified model was therefore considered where the cylindrical wall is replaced by a flat wall. In this case, an explicit power series solution for the concentration at the wall was obtained by means of Laplace transformation.

The analysis of Lauwerier was extended by Wissler and Schechter(4) in 1960 to cover the case of consecutive irreversible, first order reactions. Wissler and Schechter also completed Lauwerier's formal solution by performing the numerical labor of computing the eigenvalues which Lauwerier had approximated only for limited cases.

The work of Cleland and Wilhelm (2) was extended to include homogeneous second order chemical reactions by Vignes and Trambouze (5) using a similar approach in 1961.

Krongelb and Strandberg (6) used numerical methods similar to those of Cleland and Wilhelm (2) to investigate specific examples of second-order homogeneous reaction with first-order wall reaction but neglecting axial diffusion. Axial and radial diffusion with first-order

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homogeneous and heterogeneous reaction in Poiseuille flow
were investigated by Walker (7). A velocity profile
feature coupled with wall reaction creates radial
concentration gradients; the magnitude of these gradients
will depend on the flow rate and the diffusion
coefficient. Investigators who have included
heterogeneous wall reaction always include the additional
wall chemical reaction in the boundary conditions and
leave the original equation unchanged.

The identical case was studied by Soloman and Hudson
(8) in 1967, but they did not consider axial diffusion in
their equation. The eigenvalues and eigenfunctions were
determined using Galerkin's method to solve an ordinary
differential equation of the Sturm-Liouville form after
separation of variables. Cosine functions were used as
the trial function in Galerkin's method. Results of
limited cases agree well with those of Brown (9) and Hsu
(10) for no homogeneous reaction and no heterogeneous
reaction, respectively. Having calculated accurate
eigenvalues and eigenfunctions they give a criteria to
determine whether homogeneous reaction can be neglected
compared to the heterogeneous reaction or the converse.
Their conclusions are:

1. Homogeneous reaction is the controlling factor
   when $K' > 10$ and $M < 0.1$;

2. **Heterogeneous reaction is the controlling factor**

when K'< 0.1 and M > 10 ;

3.   When both K'and M lie between 0.1 and 10
      individual concentration profiles must be
      computed to prevent extreme error.

The dimensionless heterogeneous rate parameter, M, is
defined as RK''/D and K'is the dimensionless homogeneous
rate parameter KR^2/D.

Neglecting diffusional effects Johnson (11) related
chemical conversion to some known factors such as the rate
constant, initial concentrations, etc. for general n-th
order chemical reactions and first-order consecutive
reactions.

Though some profound work has been done in this field
as stated above, none of them has considered a non-
Newtonian fluid as their reacting media. Wein and
Ulbrecht (12) first discussed the residence time
distribution for non-Newtonian laminar flow in tubes
without mass transport by diffusion. The extent of
applicability of the results obtained for the 'power law'
behavior was estimated for those cases where the power-law
failed to interpret the shear stress-shear rate
relations.

Homsy and Strohman (13) extended the theoretical
treatment of the problem involving an irreversible, first-
order chemical reaction in an isothermal, laminar flow,
tubular reactor to include the flow of non-Newtonian

fluids. They used zero-order Bessel's function as their trial solution for Galerkin's method in solving the Sturm-Liouville characteristic ordinary differential equation, which was derived after the separation of variables of the continuity equation. Both Ostwald-de Waele and Prandtl-Eyring models were used to describe non-Newtonian fluid behavior. The curves they obtained relating the logarithm of bulk average concentration C with the Damkohler Group I, $Kz/\langle v \rangle$, show a slight deviation from linearity for the various non-Newtonian fluids. In fact, they are all bracketed by envelope bounded by Poiseuille flow , for which s=1.0, and plug flow, for which s=0. It was also found that near the center of the tube the concentration of reactant decreases with increasing pseudoplasticity, while near the wall the situation is reversed.

Mihail and Tausch (14) also dealt with non-Newtonian fluids neglecting diffusional effects. They derived three integrals and used a numerical method (Simpson's rule) to evaluate the average concentrations for first-order chemical reactions. These were categorized into irreversible, reversible and consecutive reactions.

To partially eliminate the difficulties involved in the calculation of chemical conversions in laminar flow tubular reactors, the axial dispersion model is often used. The axial dispersion model with radial and longitudinal mixing effects are incorporated into a single effective axial dispersion coefficient. This approach has

the advantage of allowing the actual two dimensional complex system to be approximated by a simple one-dimensional system.   The effect is to reduce a partial differential equation to an ordinary differential equation.   Though simple, it has certain limitations, because the model gives some kind of cross sectionally averaged description of the reaction without precise two-dimensional calculations.   It is obvious that this model will not predict concentration over a extended range of variables.   For this reason, most of the efforts using axial dispersion model have also been primarily concerned on specifying quantitatively the region in which the model will accurately describe the actual process.

Workers (15)-(18) before Mashelkor (19) have concentrated their efforts on laminar flow tubular reactors handling Newtonian liquids only.   Mashelker applied the axial dispersion model to power-law fluids flowing through tubular reactor, in which the flowing reactant undergoes a first-order chemical reaction.   A linear second-order ordinary differential equation was solved and the average concentrations were examined with the exact values for both Newtonian and non-Newtonian fluids to obtain the range in which the axial dispersion model is applicable.

In spite of so much work which has been done on this topic, no one seems to have attempted to make a general analysis for non-Newtonian fluids with any order of

chemical reaction. This is what has been sought in this study.

CHAPTER III

REVIEW OF BASIC THEORY

The concept of bulk contact time loses meaning for
isothermal chemical reaction in the liquid phase in a
tubular reactor in the laminar flow region. There is a
distribution of contact or residence times brought about
by the velocity profile. A radial concentration gradient
is caused by the velocity profile, i.e. the distribution
of contact time. The concentration gradient then in turn
tends to be smoothed by molecular diffusion. Thus
chemical reaction, flow regime, and diffusional effects
are interrelated.

Review of non-Newtonian Fluids

A Newtonian fluid is one for which a linear relation
exists between stress and the spatial variation of
velocity. If changes in fluid density are not important,
the constant of proportionality is the viscosity, a
characteristic constant of the material at a given
temperature and pressure. Non-Newtonian fluids are those
for which the linear relation does not exist. The non-
Newtonian fluids classification covers an extremely wide
range of different materials. The only common features

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are fluidity and a failure to obey Newton's law of
friction.

Consider a shear force acting on a fluid in a certain
plane as shown in Figure 1. The velocity gradient or
shear rate, dv/dy, is directly proportional to the shear
stress, τ_{yx}, where the proportionality constant μ is the
viscosity. The viscosity is independent of shear rate and
affected only by temperature for a given fluid system. A
plot of shear stress τ_{yx} against shear rate dv/dy in
laminar flow is known as a 'flow curve'. Typical flow
curves are shown in Figure 2.

All fluids for which the flow curve is not linear and
through the origin at a given temperature and pressure are
said to be non-Newtonian. These materials can be divided
into three genera groups: time-independent; time-
dependent, and viscoelastic fluids. Here we will discuss
a little about time-independent non-Newtonian fluids. In
this class, a convenient preliminary classification may be
made into those which exhibit a yield stress and those
which do not.

Fluids with a yield stress

Fluids in this category are capable of preventing
movement for values of shear stress less than the yield
value. Some of the empirical models which have been
proposed for relating shear stress to shear rate in these
substances are given in Table II. Among these models, the
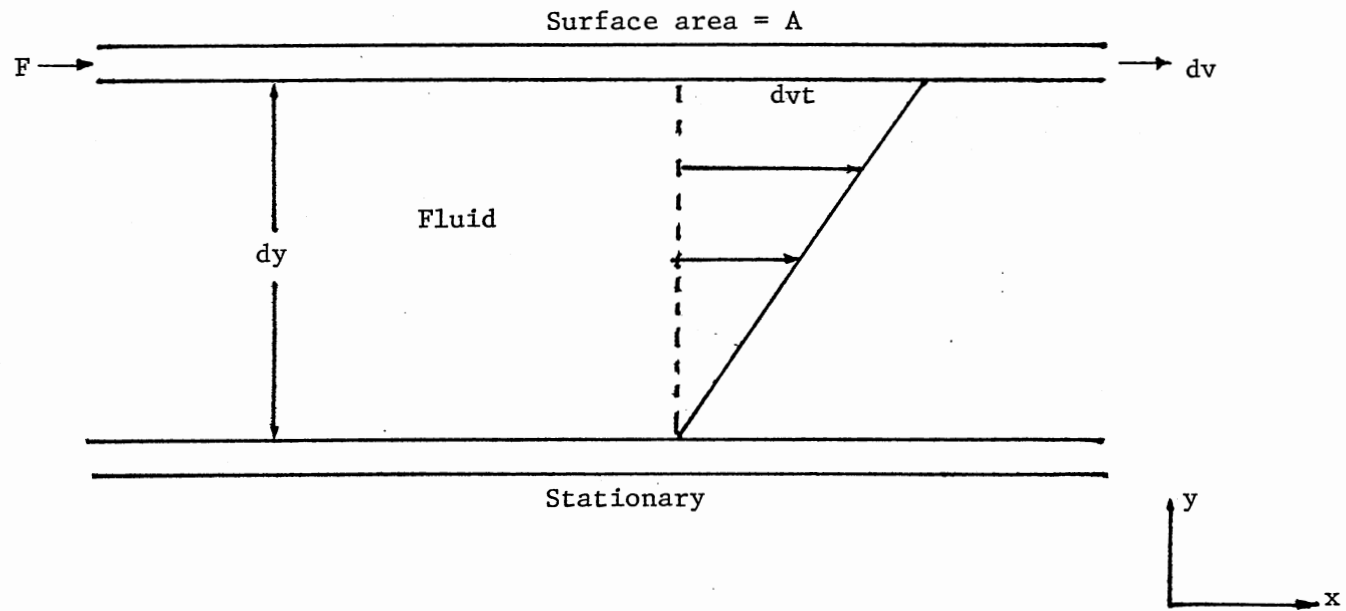
Figure 1.   Steady Laminar Shearing Motion Between Two Parallel Plates.
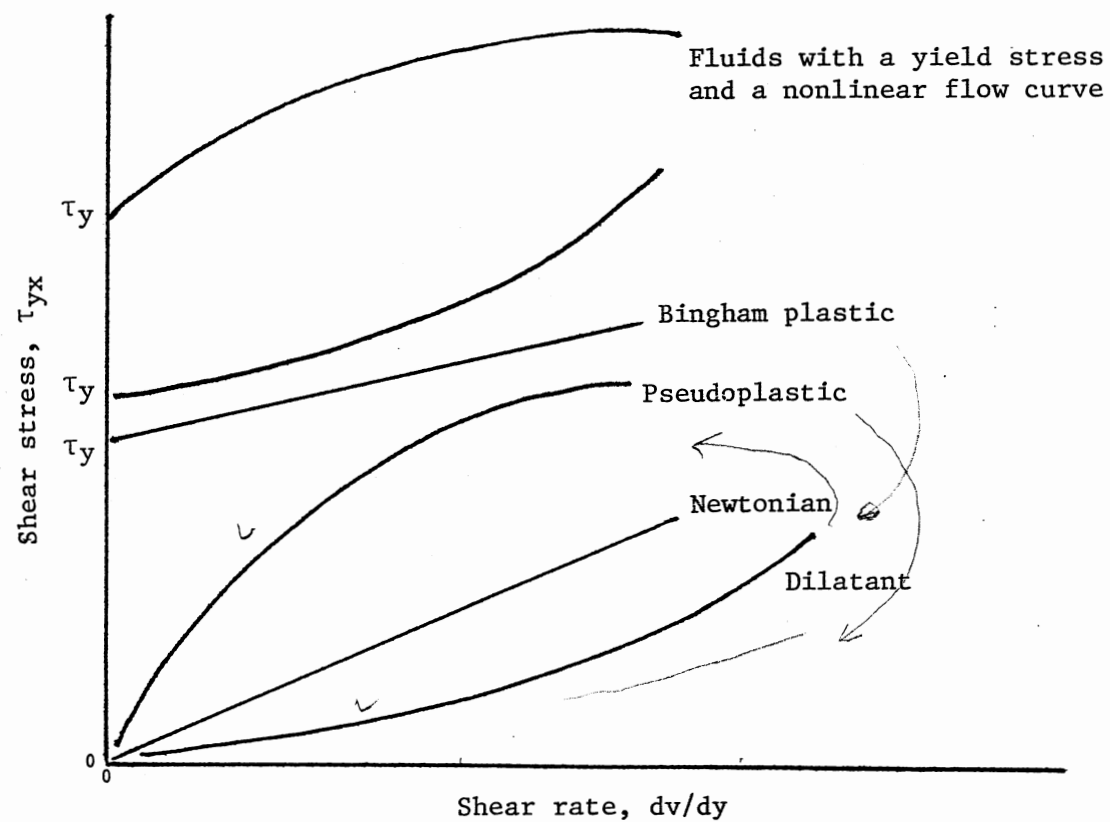
Figure 2. Flow Curves on Arithmetic Coordinates for
Various Types of Time-Independent Fluids

TABLE II

MODELS RELATING τ_{yx} TO dv/dy FOR FLLUIDS
WITH A YIELD STRESS

Model	Form(for $\tau_{yx} > \tau_y$) (dv/dy=0 for $\tau_{yx} < \tau_y$)	Empirical Constants
Bingham plastic	$\tau_{yx} - \tau_y = (\eta/g)(dv/dy)$	τ_y lbf/ft^2 η lbm/ft sec
I. Herschel-Bulkley	$\tau_{yx} - \tau_y = [(\eta/g)(dv/dy)]^{1/m}$	τ_y lbf/ft^2 η'(lbf)$^{m-1}$lbm ft^{1-2m}sec^{-1} m dimensionless
II.	$\tau_{yx} - \tau_y = \dfrac{\eta_0/g}{1+C(\tau_{yx} - \tau_y)^n}(dv/dy)$	τ_y lbf/ft^2 η_0 lbm/ft sec C (lbf/ft^2)$^{-n}$ n dimensionless

Bingham plastic model describes a linear flow curve with positive intercept, and has been widely used for its simplicity and negligible departure from real fluids.

Fluids without a Yield Stress

Pseudoplastic fluids. The majority of non-Newtonian materials are found in this category. The flow curve is sketched in Figure 2 and is characterized by linearity at very low and very high shear rates. Some of the empirical models which have been proposed for relating shear stress to shear rate in pseudopastic fluids are listed in Table III. Usually a logarithmic plot of shear stress versus shear rate for these materials is found to be linear over a wide range of shear rate. This accounts for the widespread use of the power law model to characterize fluids of this type. The 'flow behavior index', s, is the slope of this logarithmic plot. Values of s range from unity towards zero with increasing pseudoplasticity. The 'consistency index', K, is calculated from the intercept on the shear stress axis at unit shear rate. Examples of pseudoplastic fluid behavior are usually found in the following materials: rubber solutions, adhesives, polymer solutions or melts, greased, starch suspensions, soap, detergent slurries, paper pulp, napalm, paints,dispersion media in certain pharmaceuticals, biological fluids.

Dilatant fluids. The flow curve for dilatant fluids, Figure 2, is characterized by zero yield stress and may

TABLE III

MODELS RELATING τ_{yx} TO dv/dy FOR FLUIDS WITHOUT A YIELD STRESS

Model	Form	Empirical Constants
Power law or Ostwald-deWaele	$\tau_{yx}=(K/g)(dv/dy)^n$	K lbm $sec^{n-2}ft^{-1}$ n dimensionless
Ellis	$\tau_{yx}=\dfrac{1}{A+B\tau_{yx}^{\alpha-1}}(dv/dy)$	α dimensionless A $ft^2 sec^{-1}lbf^{-1}$ B $ft^2 sec^{-1}lbf$
DeHaven	$\tau_{yx}=\dfrac{\mu_0/g}{1+C\tau_{yx}^n}(dv/dy)$	μ_0 lbm/ft sec C $(lbf/ft^2)^{-n}$ n dimensionless
Prandl-Eyring	$\tau_{yx}=A\ sinh^{-1}[\dfrac{1}{B}(dv/dy)]$	A lbf/ft^2 B sec^{-1}
Powell-Eyring	$\tau_{yx}=C(dv/dy)+(1/B)$ $sinh^{-1}[(1/A)(dv/dy)]$	A sec^{-1} B ft^2/lbf C $lbf\ sec/ft^2$
Sisko	$\tau_{yx}=A(dv/dy)+B(dv/dy)^n$	A $lbf\ sec/ft^2$ B $lbf\ sec^n/ft^2$ n dimensionless

usually be fitted by one of the models in Table III. The power law is often applicable, but with s greater than unity.

Velocity Profile

The velocity profile for a power-law fluid flowing inside a circular tube in the laminar flow region can be derived from a momentum balance (APPENDIX A) and expressed as:

$$v_z = v_o[1 - (r/R)^{(s+1)/s}] \qquad (3.1)$$

and

$$v_o = [(3s+1)/(s+1)]\langle v \rangle \qquad (3.2)$$

where v_z is the axial velocity, $\langle v \rangle$ is the average velocity, v_o is the velocity at the center line, i.e. the maximum axial velocity.

Figure 3 shows the limiting velocity profiles for several extreme s values.

Derivation of Differential Equation

The derivation of a general model for a laminar flow, isothermal, tubular chemical reactor starts with the assumptions of steady state and axial symmetry. The material balance equation for each components contains radial diffusion and reaction terms and models concentration changes with respect to axial and radial
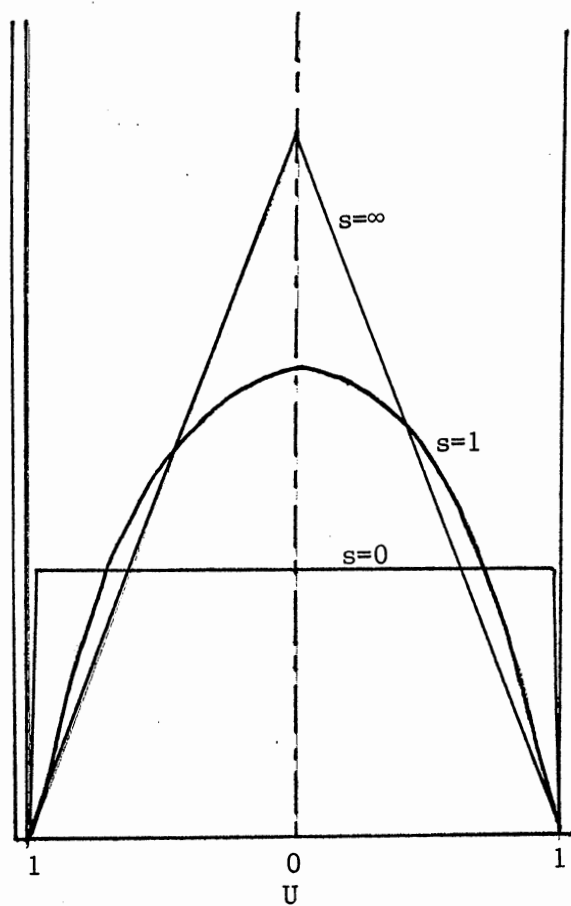
Figure 3. Velocity Profiles in a
Circular Tube for
Non-Newtonian Fluids

position:

$$-v_z\left(\frac{\partial c_i}{\partial z}\right)+D_i\left(\frac{\partial^2 c_i}{\partial r^2} + \frac{1}{r}\frac{\partial c_i}{\partial r} + \frac{\partial^2 c_i}{\partial z^2}\right) - Rn_i = 0 \quad (3.3)$$

with boundary conditions:

$$z=0, \quad c_i = c_{io} \tag{3.3-1}$$

$$r=R, \quad \frac{\partial c_i}{\partial r} = 0 \tag{3.3-2}$$

If axial diffusion is negligible compared with radial diffusion, and the velocity profile is replaced by Equation (3.1), then Equation (3.3) becomes:

$$-v_o\left[1-\left(\frac{r}{R}\right)^{(s+1)/s}\right]\frac{\partial c_i}{\partial z} + D_i\left(\frac{\partial^2 c_i}{\partial r^2} + \frac{1}{r}\frac{\partial c_i}{\partial r}\right) - Rn_i = 0$$

$$(3.4)$$

Further, if the chemical reaction rate, Rn_i, is replaced by Kc_i^n, the equation is:

$$-v_o\left[1-\left(\frac{r}{R}\right)^{(s+1)/s}\right]\frac{\partial c_i}{\partial z} + D_i\left(\frac{\partial^2 c_i}{\partial r^2} + \frac{1}{r}\frac{\partial c_i}{\partial r}\right) - Kc_i^n = 0$$

$$(3.5)$$

For convenience the subscript i is dropped and Equation (3.5) can be transformed to dimensionless form

$$-(1-U^{(s+1)/s})\frac{\partial C}{\partial Z} + A\left(\frac{\partial^2 C}{\partial U^2} + \frac{1}{U}\frac{\partial C}{\partial U}\right) - C^n = 0 \quad (3.6)$$

where:

$$Z = \frac{Kzc_o^{n-1}}{v_o} \qquad (3.7)$$

$$C = \frac{c}{c_o} \qquad (3.8)$$

$$A = \frac{D}{Kc_o^{n-1}R^2} \qquad (3.9)$$

$$U = \frac{r}{R} \qquad (3.10)$$

with boundary conditions also be translated to:

$$Z = 0, \quad C = 1 \qquad (3.6\text{-}1)$$

$$U = 1, \quad \frac{\partial C}{\partial U} = 0 \qquad (3.6\text{-}2)$$

Equation (3.6), (3.6-1) and (3.6-2) are the characteristic equations solved in later chapters.

CHAPTER IV

REVIEW AND EXTENSION OF NUMERICAL METHOD THEORY

There are many numerical methods for solving partial differential equations . Of these, only one stands out as being universally appplicable to both linear and nonlinear problems, this is the method of finite differences. In this work, only the finite difference method will be considered. Since, the partial differential equation derived in last chapter is characterized as a parabolic partial differential equation, the methods which are considered will naturally be restricted in this category.

The approach to solving a parabolic partial differential equation by a numerical method is to replace the partial derivatives by finite-difference approximations. The simplest form for the approximations are:

$$\frac{\partial C}{\partial Z} \cong \frac{C(U, Z+\Delta Z) - C(U, Z)}{\Delta Z} \tag{4.1}$$

$$\frac{\partial C}{\partial U} \cong \frac{C(U+\Delta U, Z) - C(U, Z)}{\Delta U} \tag{4.2}$$

$$\frac{\partial^2 C}{\partial U^2} = \frac{C(U+\Delta U, Z) - 2C(U, Z) + C(U-\Delta U, Z)}{(\Delta U)^2} \qquad (4.3)$$

If these expressions are substituted into differential equation (3.6) and the boundary values specified in Equations (3.6-1) and (3.6-2) are applied, the values of C at the grid points $Z=Z$, $Z=Z+\Delta Z$, ..., can be successively calculated provided $\Delta Z/(\Delta U)^2$ is less than or equal to one half. If $\Delta Z/(\Delta U)^2$ is greater than one half, the difference equation becomes unstable. The method presented here is an explicit method because concentration at a new position can be immediately calculated from quantities that are already known (either from boundary conditions or previous calculations). It is a simple and economical method of calculation, but has a severely limited upper value for the ratio $\Delta Z/(\Delta U)^2$. Note that a mixed order of errors was involved in Equation (4.1) to Equation (4.3) , a forward difference was used to approximate $\partial C/\partial Z$ and $\partial C/\partial U$ while a central difference was used for the second derivative $\partial^2 C/\partial U^2$. This restriction forces the computer to use very small steps in the Z direction. There is therefore, considerable interest in the so-called implicit difference methods, where stability for all $\Delta Z/(\Delta U)^2$ greater than zero is ensured, but at the price of greater computational complexity. Such implicit methods seem to have been used for the first time by Crank and Nicolson in 1974. The

method is briefly illustrated below.

If the second derivative with respect to U is replaced by the second difference quotient, not at the level Z as in Equation (4.3) , but at $Z+\Delta Z/2$. Then the second derivative with respect to U can be approximated by averaging the difference quotient at the beginning and at the end of the Z-step.

$$\frac{\partial^2 C}{\partial U^2} \cong \frac{1}{2} \left[\frac{C(U+\Delta U,Z)-2C(U,Z)+C(U-\Delta U,Z)}{(\Delta U)^2} + \right.$$

$$\left. \frac{C(U+\Delta U,Z+\Delta Z)-2C(U,Z+\Delta Z)+C(U-\Delta U,Z+\Delta Z)}{(\Delta U)^2} \right] \quad (4.4)$$

In that case, we do consider the difference expression Equation (4.1) as a central difference approximation.

Similarly, Equation (4.2) must be replaced by

$$\frac{\partial C}{\partial U} \cong \frac{1}{2} \left[\frac{C(U+\Delta U,Z)-C(U-\Delta U,Z)}{2\Delta U} + \right.$$

$$\left. \frac{C(U+\Delta U.Z+\Delta Z)-C(U-\Delta U,Z+\Delta Z)}{2\Delta U} \right] \quad (4.5)$$

to show central difference approximation.

After substituting these expressions [Equation (4.1) (4.4) and (4.5)] into the differential equation (3.6), it is seen that the unknowns can no longer be solved for explicitly. This is unsuitable for problems in which

infinite U-regions appear. But for problems with a finite
U-interval, like what we have in this work, can be handled
by means of an implicit method. To that end, we can
write the difference equation for each grid point and
interpret them as a system of simultaneous algebraic
equations. The number of unknowns will be equal to the
number of equations, which is equal to the number of grid
points in each Z-step. If values of C at the grid points
of the level Z are already known, the values for Z+ ΔZ can
be found by solving this algebraic system, provided the
determinant is not equal to zero. The numerical solution
of systems of algebraic equations is a large and widely
studied subject and will not be discussed here.

Fortunately, the system of equations created by this
implicit difference method is such that the matrix of the
system has zeros everywhere except on the main diagonal
and on the two diagonals parellel to it on either side.
Such a matrix is sometimes called tridiagonal. This
special situation saves a great deal of computation work
when solving the equation set.

The convergence of the solution $C(U,Z)$ of the
implicit difference equation can be proved by the Fourier
series method under reasonably weak hypotheses.

Another central topic of numerical techniques is the
question as to how well a solution of a difference
equation approximates the solution of a related
differential equation problem. The appraisals obtained

have usually been either uniformly valid for all values of
U and Z in the domain under consideration or at least
uniformly with respect to U, when Z is given. Since a
full description of the ideas and results of this topic
would require too much space. Readers are recommended to
refer to Lax and Richtmyer (20).

Calculational Procedures

The grids obtained by dividing in both U and Z
dimensions (radial and axial respectively) for this
derivation are shown in Figure 4. The difference equation
is derived by substituting the following expressions into
the partial differential equation (3.6):

$$\frac{\partial C}{\partial Z} \cong \frac{C_{j,k+1} - C_{j,k}}{\Delta Z} \qquad (4.6)$$

$$\frac{\partial C}{\partial U} \cong \frac{1}{2} \left(\frac{C_{j+1,k} - C_{j-1,k}}{2\Delta U} + \frac{C_{j+1,k+1} - C_{j-1,k+1}}{2\,\Delta U} \right) \qquad (4.7)$$

$$\frac{\partial^2 C}{\partial U^2} \cong \frac{1}{2} \left(\frac{C_{j+1,k} - 2C_{j,k} + C_{j-1,k}}{(\Delta U)^2} + \right.$$

$$\left. \frac{C_{j+1,k+1} - C_{j,k+1} + C_{j-1,k+1}}{(\Delta U)^2} \right) \qquad (4.8)$$

where the first subscript denotes radial position, and the
second the axial position. This is the so called Crank-
Nicolson method, which is not only unconditionally stable
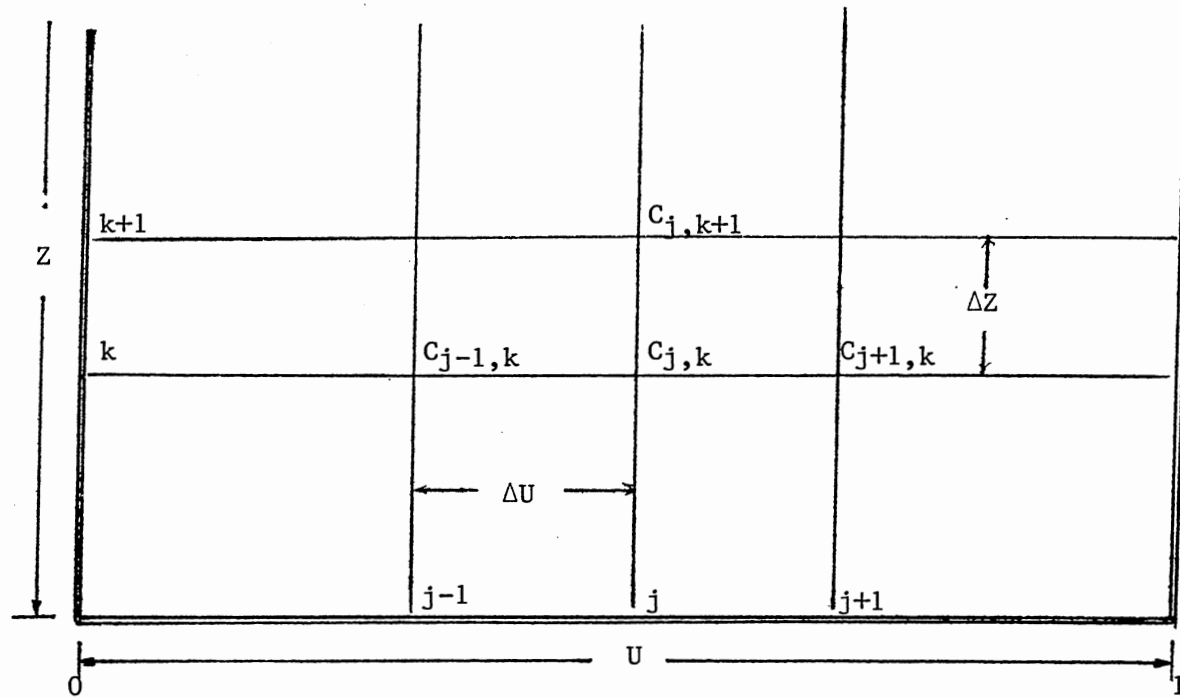
Figure 4. Reference Grid for Difference-Equation Derivation.

but also second order correct.

The difference equation becomes:

$$\frac{(1-U_j^{(S+1)/S})(C_{j,k+1}-C_{j,k})}{\Delta Z} =$$

$$A[\frac{C_{j+1,k+1}+C_{j-1,k+1}-2C_{j,k+1}+C_{j+1,k}+C_{j-1,k}-2C_{j,k}}{2(\Delta U)^2} +$$

$$\frac{1}{4U_j\Delta U}(C_{j+1,k+1}-C_{j-1,k+1}+C_{j+1,k}-C_{j-1,k})] -(\frac{C_{j,k+1}+C_{j,k}}{2})^n$$

(4.9)

with boundary conditions:

$$Z = 0, \quad C_{j,k} = 0 \qquad\qquad (4.9-1)$$

(i.e. for all j when k=0)

$$U = 1, \quad \frac{\partial C}{\partial U} = 0 \qquad\qquad (4.9-2)$$

Equation (4.9-2) is equivalent to:

$$\frac{1}{2\Delta U}(C_{j,k+1}-C_{j-1,k+1}+C_{j,k}-C_{j-1,k}) = 0 \qquad (4.9-3)$$

At the centerline we can use dC/dU=0 as the boundary condition equation and get our difference equation by forward differencing instead of backward differencing, or we can follow Cleland's (2) approach by substituting the $(1/U)(\partial C/\partial U)$ term in Equation (3.6) with $\partial^2 C/\partial U^2$ (applying

L'Hospital's rule as U->0). After substituting the approximation expressions for each term and incorporating the relationship that concentration distribution is symmetric about the tube axis, the following equation is derived:

$$\frac{C_{o,k+1} - C_{o,k}}{\Delta Z} = \frac{2A}{(\Delta U)^2}(C_{1,k+1} - C_{o,k+1} + C_{1,k} - C_{o,k}) - (\frac{C_{o,k+1} + C_{o,k}}{2})n \qquad (4.10)$$

Applying the Crank-Nicolson's method requires us to solve a set of simultaneous nonlinear algebraic equations at each Z-step progress. A Newton-Raphson's iteration is applied to solve these equations because an explicit expression for the Jacobian can be derived. As a matter of fact, the derivatives for the difference equations will also form a tridiagonal matrix.

If $\vec{C}$ denotes the solution vector with dimensionless concentration as its elements, and f_j are the scalar functions set up from the difference equations at each grid nodes and form a vector $\vec{F}(\vec{C})$, then:

$$f_o(\vec{C}) = \frac{C_{o,k+1} - C_{o,k}}{\Delta Z} - \frac{2A}{(\Delta U)^2}(C_{1,k+1} - C_{o,k+1} + C_{1,k} - C_{o,k}) + (\frac{C_{o,k+1} + C_{o,k}}{2})n \qquad (4.11)$$

$$f_j(\vec{C}) = \frac{(1-U^{(s+1)/s})(C_{j,k+1}-C_{j,k})}{\Delta Z} -$$

$$A[\frac{C_{j+1,k+1}+C_{j-1,k+1}-2C_{j,k+1}+C_{j+1,k}+C_{j-1,k}-2C_{j,k}}{2(\Delta U)^2} +$$

$$\frac{1}{4U_j \Delta U}(C_{j+1,k+1}-C_{j-1,k+1}+C_{j+1,k}-C_{j-1,k})+(\frac{C_{j,k+1}+C_{j,k}}{2})^n$$

$$(j = 1, 2,..., N-1) \tag{4.12}$$

$$f_N(\vec{C}) = [1/(2\Delta U)](C_{N,k+1}-C_{N-1,k+1}+C_{N,k}-C_{N-1,k}) \tag{4.13}$$

Note : C(k+1)'s are unknowns, while C(k)'s are known from boundary conditions or previous results.

Let:

$$\vec{F}(\vec{C})=[f_0(\vec{C})\ f_1(\vec{C})....f_N(\vec{C})]^T \tag{4.14}$$

If a matrix $J(\vec{C})$ is introduced whose determinant is the Jacobian of the functions $f_j(\vec{C})$, where j = 0,1,.. N. then:

$$
F'(\vec{C}) = \begin{pmatrix}
\dfrac{\partial f_0}{\partial C_{0,k+1}} & \dfrac{\partial f_0}{\partial C_{1,k+1}} & \cdots\cdots\cdots & \dfrac{\partial f_0}{\partial C_{N,k+1}} \\[2em]
\dfrac{\partial f_1}{\partial C_{0,k+1}} & \dfrac{\partial f_1}{\partial C_{1,k+1}} & \cdots\cdots\cdots & \dfrac{\partial f_1}{\partial C_{N,k+1}} \\[2em]
\vdots & \vdots & \vdots & \vdots \\[2em]
\dfrac{\partial f_N}{\partial C_{0,k+1}} & \cdots\cdots\cdots\cdots & & \dfrac{\partial f_N}{\partial C_{N,k+1}}
\end{pmatrix}
$$

$$(4.15)$$

Here $F'(\vec{C})$ is a tridiagonal matrix since there are at most three consecutive variables in each difference equation.

Let H be the correction vector of each iteration so that

$$\vec{C}(m+1) = \vec{C}(m) + \vec{H} \tag{4.16}$$

$$\vec{H} = -[F'(\vec{C})]^{-1}\ \vec{F}(\vec{C}) \tag{4.17}$$

In this problem, it is almost impossible to have initial guesses that are close enough to the roots to get convergence in each iteration. A damped method is thus introduced to force, or at least encourage, convergence. This is accomplished by testing norms in each pseudo progress to decide if the progress is too much. An exponential power index, I, is chosen to decide how far to

go in each step. The integer I must satisfy the following criteria:

$$I = \min \{j, \ 0 <= j, \ ||\vec{F}(\vec{C}_m + \vec{H}/2^j)|| \ < \ ||\vec{F}(\vec{C}m)||\}$$

$$(4.18)$$

The successful correction for every iteration will be $\vec{H}/2^j$.

To conserve storage usage in the computer, the tridiagonal matrix of coefficients $F'(\vec{C})$ is compressed, together with the constant terms $\vec{F}(\vec{C})$, into an N x 4 matrix. Column 1 holds the coefficients to the left of the diagonal, column two holds the diagonal terms, column three holds the coefficient to the right of the diagonal, and column four holds the constant terms. The j and (j-1) rows of the compressed matrix corresponding to elements in the uncompressed matrix are shown:

$$
\begin{vmatrix}
*** & *** & 0 & 0 & \cdots \cdots \cdots \cdots \\
*** & *** & *** & 0 & \cdots \cdots \cdots \cdots \\
0 & *** & *** & *** & 0 \cdots \cdots \cdots \\
& \vdots & & & \\
& \vdots & & & \\
0 \cdots \dfrac{\partial f_{j-1}}{\partial C_{j-2,k+1}} & \dfrac{\partial f_{j-1}}{\partial C_{j-1,k+1}} & \dfrac{\partial f_{j-1}}{\partial C_{j,k+1}} & 0 \cdots & \\
0 \cdots \cdots \cdots 0 & \dfrac{\partial f_{j}}{\partial C_{j-1,k+1}} & \dfrac{\partial f_{j}}{\partial C_{j,k+1}} & \dfrac{\partial f_{j}}{\partial C_{j+1,k+1}} & \\
& & \vdots & & \\
& & \vdots & & \\
& \cdots & 0 & *** & *** \quad *** \\
& & \cdots 0 & *** & ***
\end{vmatrix}
\begin{vmatrix}
\\ \\ \\ \\ \\ f_{j-1} \\ \\ \\ f_{j} \\ \\ \\ \\
\end{vmatrix}
$$

We can eliminate $\partial f_j / \partial C_{j-1,k+1}$ by subtraction of $(\partial f_j / \partial C_{j-1,k+1})/(\partial f_{i-1} / \partial C_{j-1,k+1})$ times the (j-1) row from the j row. Since we know a zero will replace $\partial f_j / \partial C_{j-1,k+1}$ we don't need actually to perform the arithmetic. The values of $\partial f_j / \partial C_{j,k+1}$ and f_j change as follows:

$$\frac{\partial f_j}{\partial C_{j,k+1}} = \frac{\partial f_j}{\partial C_{j,k+1}} - \frac{\partial f_j / \partial C_{j-1,k+1}}{\partial f_{j-1} / \partial C_{j-1,k+1}} * \frac{\partial f_{j-1}}{\partial C_{j,k+1}}$$

$$(4.19)$$

$$f_j = f_j - \frac{\partial f_j / \partial C_{j-1,k+1}}{\partial f_{j-1} / \partial C_{j-1,k+1}} \times f_{j-1} \qquad (4.20)$$

When the j row is reduced, $\partial f_j / \partial C_{j+1,k+1}$ is unaffected because there is a zero above it. After reduction, a backsubstitution is performed. The elements of the solution vector replace the constant vector in the fourth column of the matrix.

The equations for back substitution are:

$$f_N = f_N / \left(\frac{\partial f_N}{\partial C_{N,k+1}}\right) \qquad (4.21)$$

$$f_j = \left[f_j - f_{j+1}\left(\frac{\partial f_j}{\partial C_{j+1,k+1}}\right)\right] / \left(\frac{\partial f_j}{\partial C_{j,k+1}}\right) \qquad (4.22)$$

where j=N-1, N-2,...., 1, 0

In addition to the concentration distribution the bulk average concentration is desired which can be derived

by an integral expression.

$$\bar{C} = \frac{\int_o^R 2\pi rvCdr}{\int_o^R 2\pi rvdr}$$

$$= \frac{6s+2}{s+1} \int_o^1 U(1-U^{(s+1)/s})CdU \qquad (4.23)$$

Simpson's rule is used to evaluate the integral.

An interactive Fortran program was developed to execute the above numerical jobs. The package is designed to run on IBM personal computers which are inexpensive and widely available. The results are presented in next Chapter.

CHAPTER V

RESULTS AND DISCUSSION

Numerical solutions for concentrations of reacting species under a certain set of conditions was obtained as function of position in a circular tube, both axial and radial.

It is necessary to discuss the accuracy of the numerical results that have been obtained. The error incurred in a finite difference method depends upon both the grid sizes in axial and radial directions, and the tolerance specified in computer iterations. The price for accuracy is computer calculation time.

Comparisons of the dimensionless bulk concentration along the axial direction and dimensionless axial concentration profiles for Newtonian fluids undergoing first order chemical reaction were made with the results obtained by Cleland and Wilhelm (2).

Tabulated concentrations, $\bar{C}$, for analytical and numerical solutions derived by Cleland and Wilhelm (2) are compared in Table IV with results of this work with A=0 (a value of A=0 means no diffusion is considered). The data in the fourth column was derived by specifying an axial grid number of fifty, an axial increment size, Z, of 0.02

TABLE IV

COMPARISON OF AVERAGE CONCENTRATIONS, $\bar{C}$, FROM
NUMERICAL AND ANALYTICAL INTEGRATIONS
FOR $A = 0$

Z	Analytical Solution $\bar{C}$	Numerical Solutions	
		Ref.(2) $\bar{C}$	Current Model $\bar{C}$
0.01	0.9806	0.9810	0.9807
0.05	0.9098	0.9105	0.9098
0.20	0.7039	0.7037	0.7036
1.00	0.2194	0.2194	0.2195
2.00	0.0603	0.0603	0.0603

or 0.01 and a dimensionless concentration tolerance of
0.0001. (Refer to Appendix C.) A very slight deviation
from analytical solution was observed when Z=0.20 and
1.00. The rest of the results show even better estimation
than that of Cleland and Wilhelm. Specifying stricter
calculating conditions will certainly result in closer
solutions, however, Table IV shows crudly how close we can
get with a fixed degree of specification.

Table V and Table VI list the theoretical and
calculated values of $\bar{C}$ as a function of Z for various
values of A, based on the work of Cleland and Wilhelm.
Agreement to the fourth significant figure is apparent.

Theoretical radial concentration profiles for A=0.1
along the tube axis (different Z values) are shown in
Figures 5 - 7. The bulk dimensionless concentration
profiles along Z with A as a parameter are illustrated in
Figure 8. The curve for plug flow (A=∞) is not shown on
the same graph, but obviously that the curves for A=0 and
A= ∞ form the upper and lower boundary of the curve band.
The fraction unconverted is highest when radial diffusion
is negligibe and lowest when A approaches infinity.

Concentration profiles for various A values at a
definite axial position are shown in Figure 9. This plot
demonstrates that the concentration profiles are
"straightened" by the effect of radial diffusion.

In the case of non-Newtonian fluids an additional
parameter, s, is introduced. The dimensionless group Z

TABLE V

THEORETICAL VALUES OF $\bar{C}$ AS A FUNCTION OF Z FOR
VARIOUS VALUES OF A, REF(2)

Z	A=0	A=.01	A=.1
.00	1.0000	1.0000	1.0000
.01	.9810	.9800	.9806
.02	.9625	.9608	.9615
.03	.9447	.9424	.9428
.04	.9273	.9246	.9247
.05	.9105	.9073	.9071
.07	.8780	.8743	.8731
.10	.8328	.8282	.8251
.15	.7645	.7585	.7520
.20	.7037	.6965	.6963
.25	.6491	.6409	.6270
.30	.5999	.5906	.5733
.40	.5145	.5037	.4803
.50	.4432	.4316	.4033
.60	.3831	.3711	.3392
.70	.3321	.3201	.2856
.80	.2887	.2768	.2407
.90	.2514	.2397	.2030
1.00	.2194	.2082	.1709
1.10	.1918	.1809	.1446
1.20	.1679	.1576	.1222
1.30	.1472	.1372	.1031
1.40	.1211	.1199	.0871
1.60	.0998	.0917	.0621
1.80	.0774	.0702	.0443
2.00	.0603	.0540	.0316

TABLE VI

MODELED VALUES OF $\bar{C}$ AS A FUNCTION OF Z FOR VARIOUS VALUES OF A

Z	A=0	A=.01	A=.1
.00	1.0000	1.0000	1.0000
.01	.9807	.9805	.9809
.02	.9621	.9621	.9619
.03	.9441	.9442	.9435
.04	.9267	.9268	.9259
.05	.9098	.9095	.9083
.07	.8776	.8764	.8748
.10	.8325	.8298	.8266
.15	.7645	.7610	.7530
.20	.7036	.6983	.6968
.25	.6492	.6427	.6273
.30	.6000	.5928	.5734
.40	.5145	.5040	.4838
.50	.4432	.4316	.4069
.60	.3831	.3711	.3427
.70	.3322	.3199	.2888
.80	.2887	.2765	.2436
.90	.2515	.2395	.2055
1.00	.2195	.2078	.1736
1.10	.1918	.1806	.1466
1.20	.1679	.1572	.1238
1.30	.1472	.1370	.1047
1.40	.1292	.1195	.0884
1.60	.0998	.0913	.0631
1.80	.0775	.0699	.0451
2.00	.0603	.0537	.0322
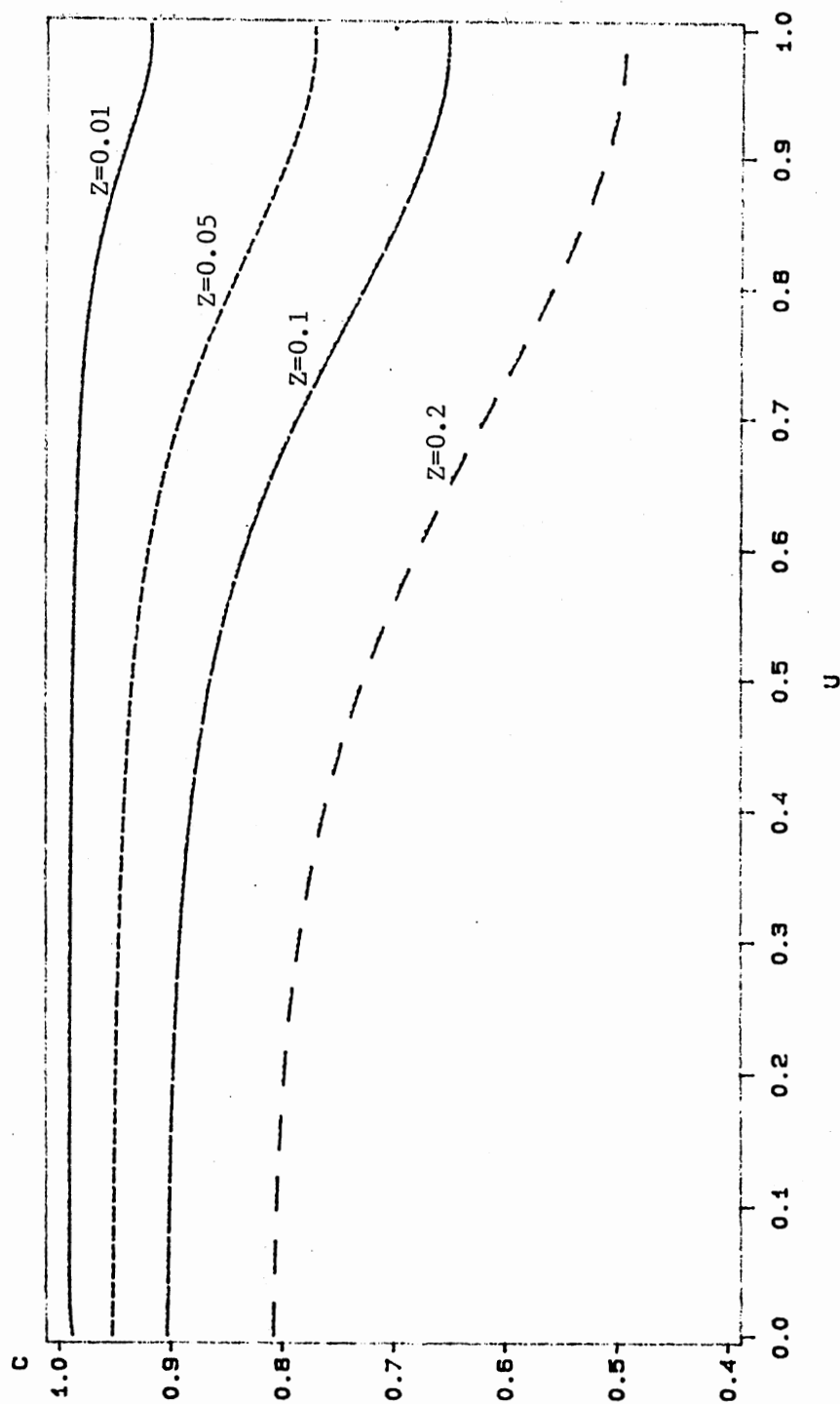
Figure 5. Radial Concentration Profiles for Z=0.01 to Z=0.2 at A=0.1
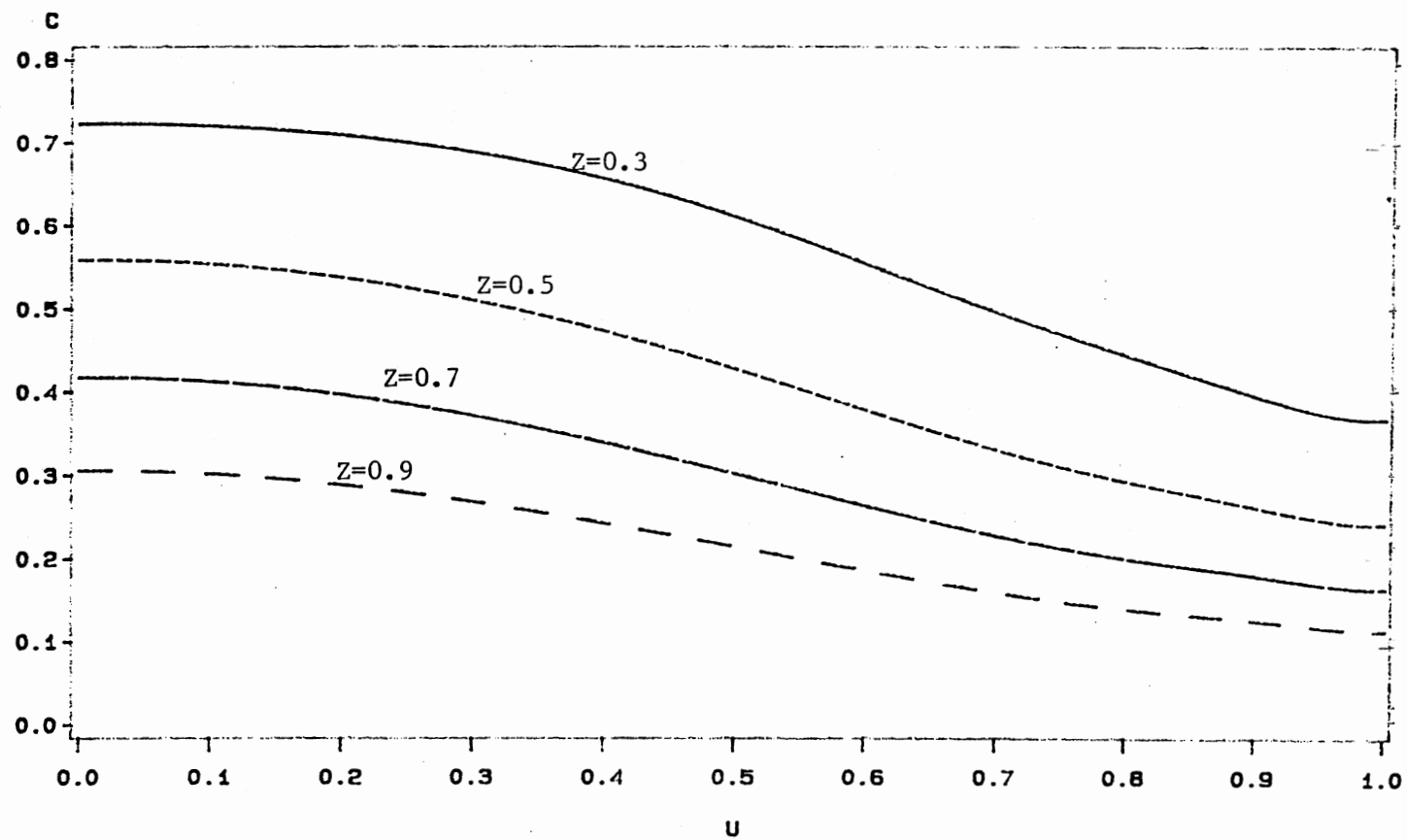
Figure 6. Radial Concentration Profiles for Z=0.3 to Z=0.9 at A=0.1
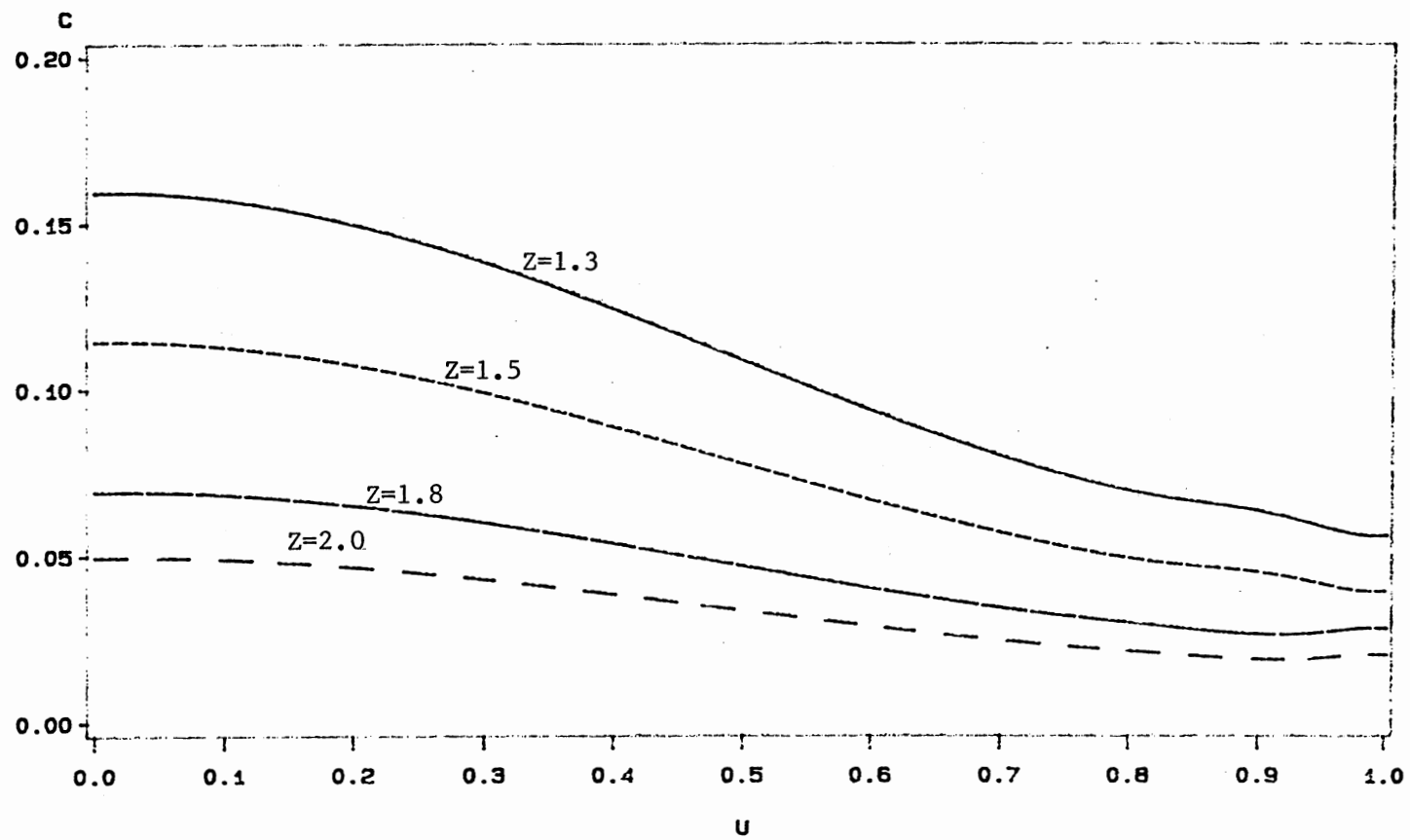
Figure 7. Radial Concentration Profiles for Z=1.3 to Z=2.0 at A=0.1
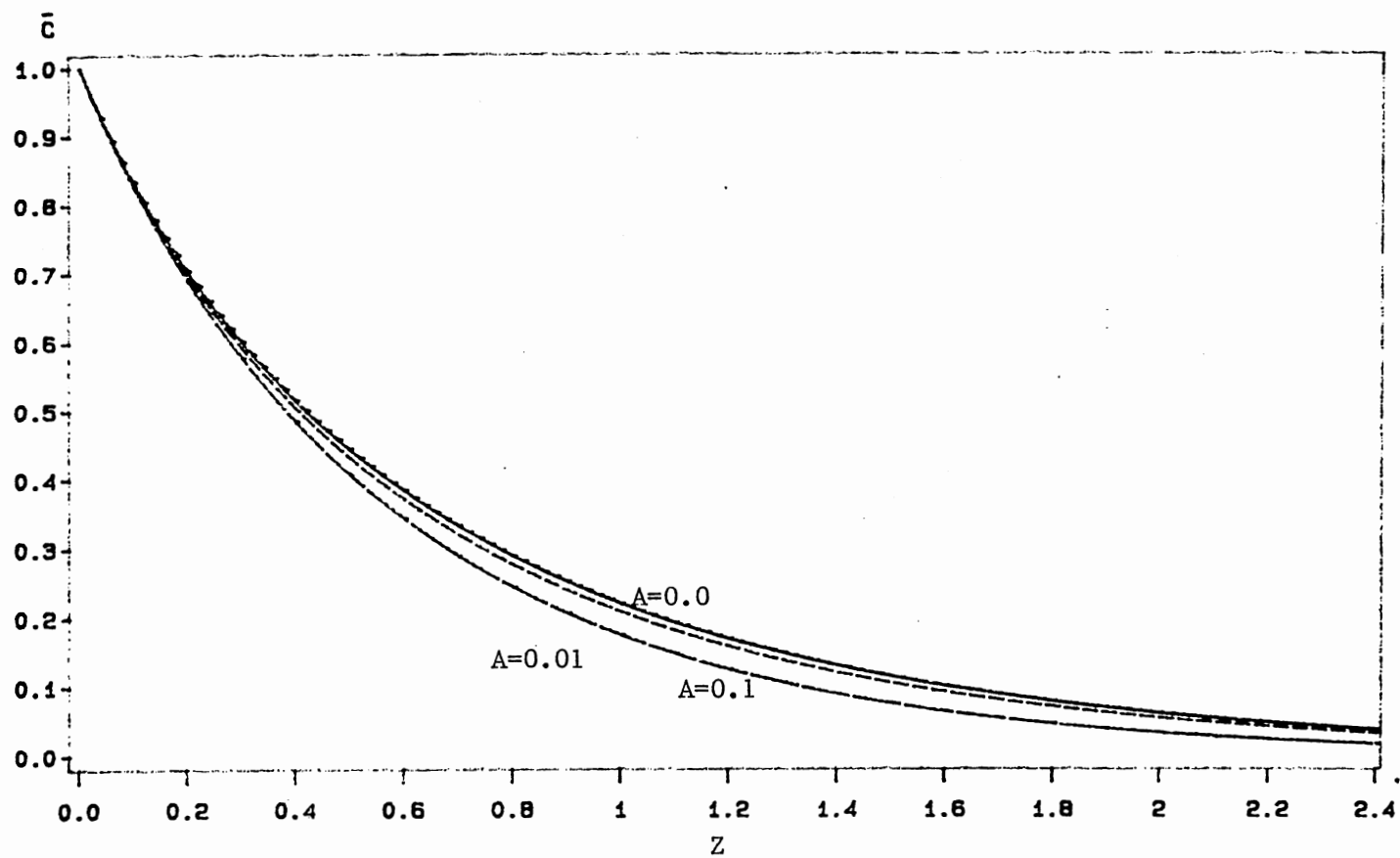
Figure 8. Calculated Curves of $\bar{C}$ vs. Z with A as a Parameter.
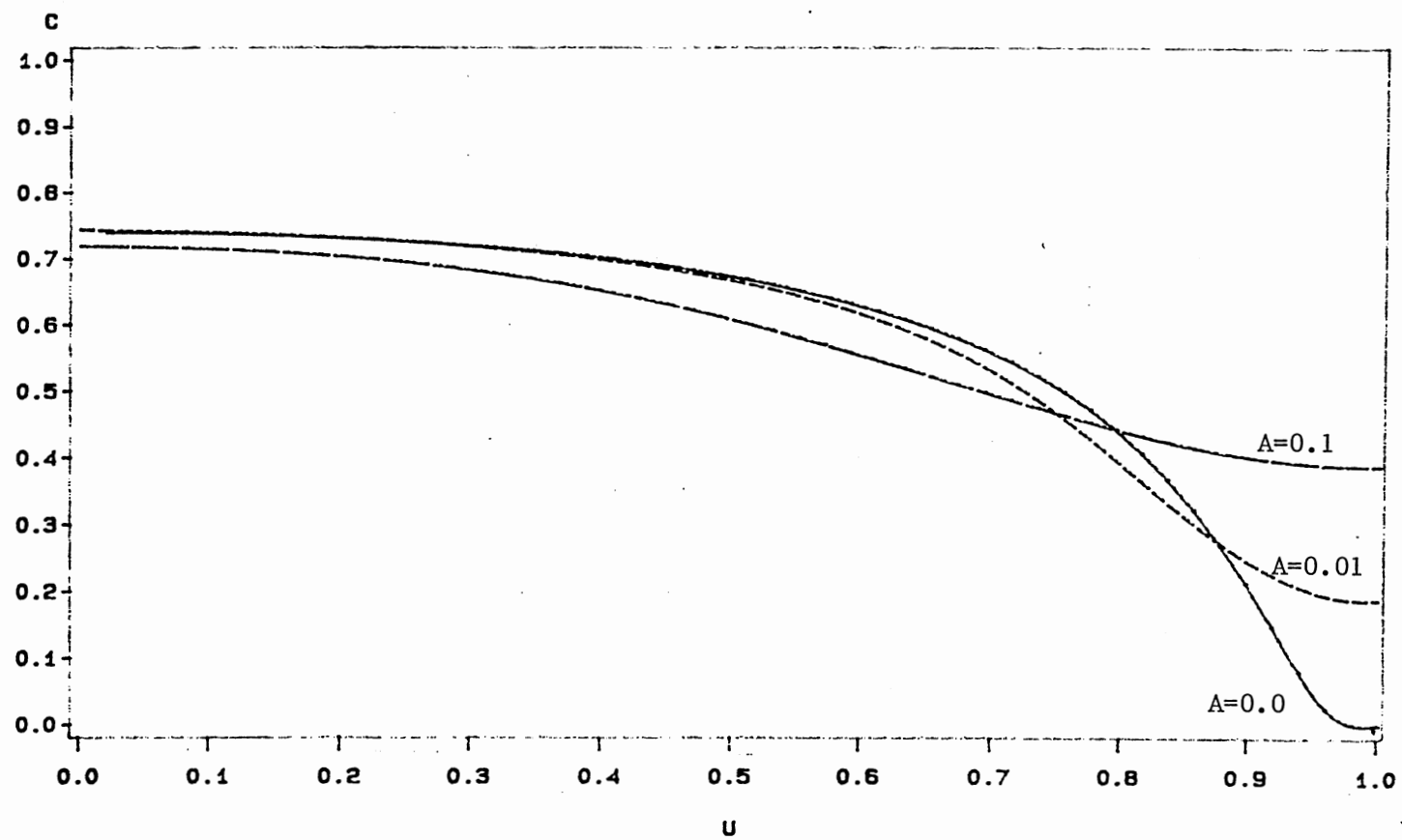
Figure 9. Concentration Profiles for Various Values of A with Z=0.3

when dealing with Newtonian fluids does not have much physical meaning if applied in non-Newtonian systems. A similar dimensionless group Z' can be defined for reacting systems with non-Newtonian fluids as flowing media.

$$Z' = \frac{kzc_o{}^{n-1}}{\langle v \rangle}$$

Note that there is a relationship between Z and Z' which is:

$$Z' = \frac{3s+1}{s+1} Z$$

Figure 10 shows the concentration profiles for A=0.01 and Z'=5.0 for Ostwald-de Waele fluids with different rheology index values. It is apparent that the concentration is a maximum at the center, as expected, and decreases with increasing pseudoplasticity. However, a reversed situation occurs near the wall.

The effect of different order kinetics is shown in Figure 11.

Figure 5 shows that chemical conversion is initially radially distributed by differences in residence time. When the concentration profile is more profound, chemical reaction and diffusion effects predominate and tend to smooth out concentration differences as shown in Figure 6-7. Figure 11 shows the same trend. The higher conversion curve contributes to a deeper concentration bend near the
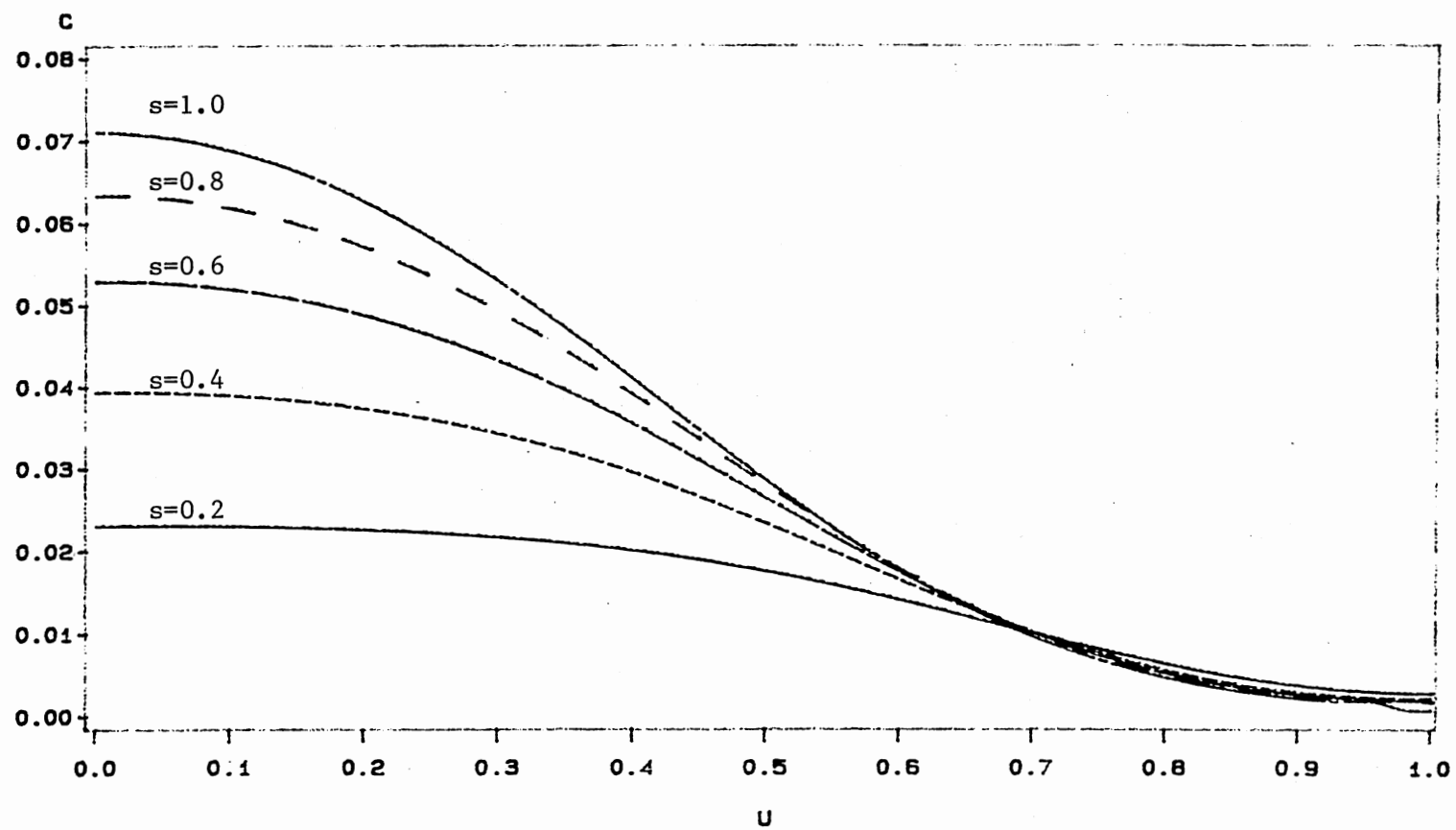
Figure 10.   Concentration Profiles for A=0.01, Z'=5.0 for
Ostwald-de Waele Fluids.
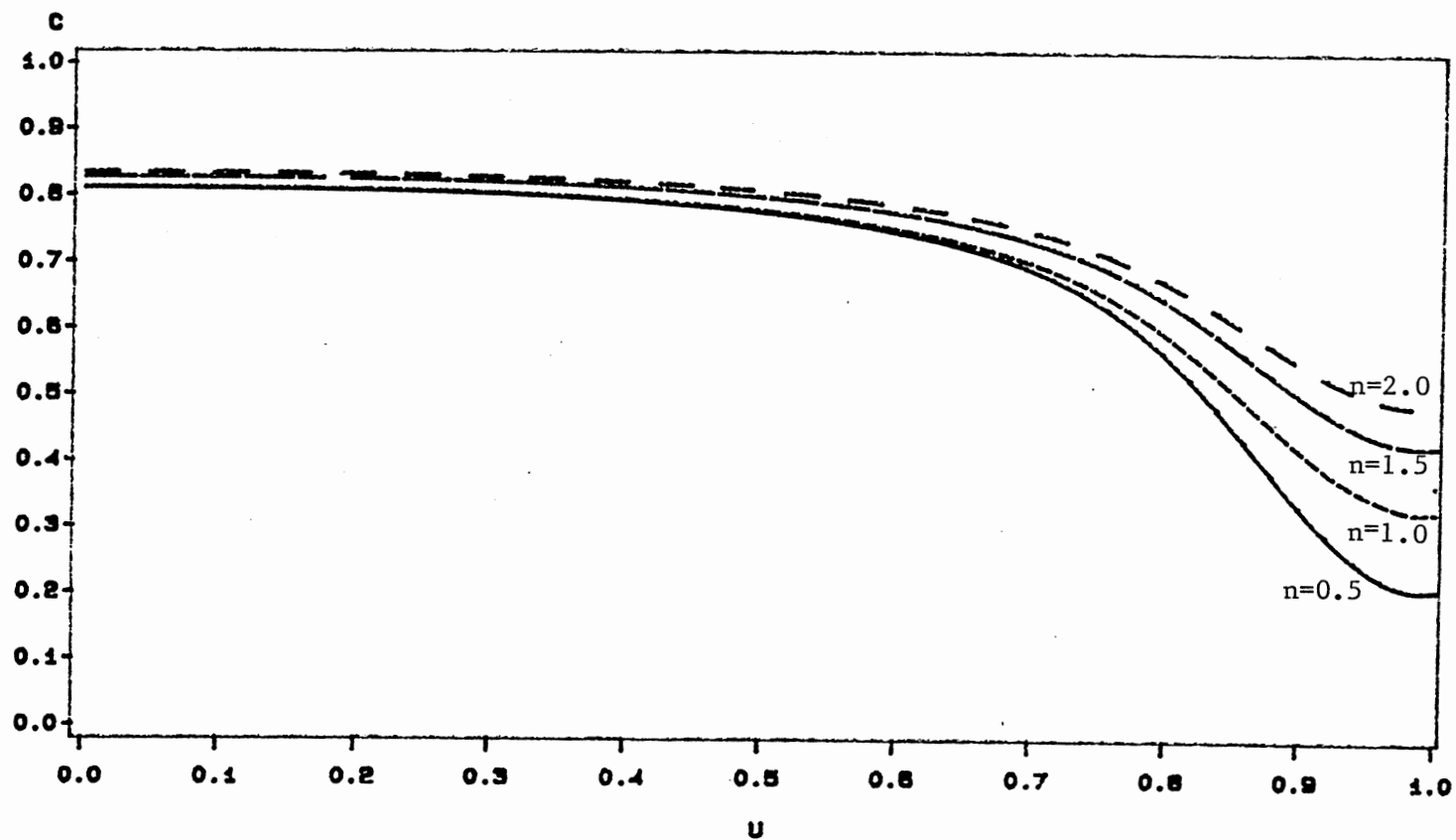
Figure 11. Concentration Profiles for A=0.01, Z'=0.35, s=0.6 with
Different Chemical Reaction Orders.

tube wall in the beginning of the reaction.

Table VII lists the criterion for neglecting the effects of radial diffusion. Radial diffusion can be neglected when the unconverted fraction is less than one percent lower than it would be in the absence of diffusion. The product of Z' and A was not found to be constant for non-Newtonian fluids as it was for Newtonian fluids.

TABLE VII

VALUES OF [D/(R<v>)]*(z/R) REQUIRED TO LOWER $\bar{C}$ BY 1%

s	Z'	$\bar{C}$ at A=0	A when C=.99*(C at A=0)	A*Z'= [D/(R<v>)]*(z/R)
0.2	0.2	0.8262	----	----
	0.4	0.6881	0.0837	0.0335
	0.6	0.5756	0.0108	0.00648
	0.8	0.4831	0.00552	0.00442
	1.0	0.4064	0.00342	0.00342
	1.6	0.2444	0.000986	0.00158
	2.0	0.1752	0.000754	0.00151
0.4	0.2	0.8260	----	----
	0.4	0.6904	0.0387	0.0158
	0.6	0.5885	0.00803	0.00478
	0.8	0.4972	0.00498	0.00399
	1.0	0.4215	0.00354	0.00356
	1.6	0.2639	0.00165	0.00265
	2.0	0.1956	0.00121	0.00242
0.6	0.2	0.8363	----	----
	0.4	0.6980	----	----
	0.6	0.5958	0.00786	0.00468
	0.8	0.5039	0.00499	0.00403
	1.0	0.4337	0.00372	0.00372
	1.6	0.2773	0.00228	0.00363
	2.0	0.2069	0.00197	0.00393
0.8	0.2	0.8262	----	----
	0.4	0.7040	0.0329	0.0131
	0.6	0.5952	0.00746	0.00451
	0.8	0.5137	0.00490	0.00389
	1.0	0.4387	0.00357	0.00357
	1.6	0.2825	0.00204	0.00328
	2.0	0.2139	0.00169	0.00338
	3.0	0.1088	0.000930	0.00279

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

The program derived in this work is interactive and
user friendly. It provides a solution for chemical
conversion problems for laminar flow in a tubular reactor.
Non-Newtonian fluids and non-first order reactions have
been taken into account in one single program. A
concentration profile or an area average concentration can
be displayed and saved in data files to produce
demonstrative graphs, if numerical data are not
illustrative enough. The accuracy of the results can be
specified by the user in advance depending on the users
requirements. The results are precise to at least the
fourth significant figure (chemical conversion) under
reasonable accuracy specifications. Tedious quasi-
analytical solutions are eliminated by using this program.

Overall, the program is simple and user friendly. It
can be used as an effective design tool to predict the
concentration distribution for an existing tubular reactor
or for a future design. The accuracy of the results it
generates and the wide range of availability make it one

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of the few powerful and economical tools available for tubular reactor design.

Recommendations

There are always limitations implied when assumptions are made. The same is true for this work. The following recommendations are listed to improve the power of this program if one desired.

1. If an energy balance equation is incorporated and solved simultaneously, the utility of the program can be extended to solve problems for a non-isothermal system.

2. Replacing the concentration of one specific reactant in the characteristic equation by a chemical reaction coordinate (reaction extent) can make this program applicable for any kinetic expression.

3. The boundary condition on the tube wall does not have to be $\partial C/\partial r=0$ as used traditionally. If C=0 is used instead, the predicted results will be more close to the actual conditions, considering that fluid is 'adhered' to the tube wall and has infinite residence time.

4. The maximum of the radial grid number in this program, N, is limited to fifty due to the consideration of saving array memory usage for Personal Computers. If more accurate results are desired, the user can either increase the grid density near the tube wall region by decreasing the density near the center or change the array declaration at the beginning of the program.

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APPENDIXES

APPENDIX A

MOMENTUM BALANCE DERIVATION

Select a cylindrical shell of thickness Δr and length L as the system (see Figure 12), the momentum balance in the z-direction is listed below:

(rate of momentum in across cylindrical surface at r) –
(rate of momentum out across cylindrical surface at r+Δr)
+ (rate of momentum in across annular surface at z=0) –
(rate of momentum out across annular surface at z=L) +
(gravity force acting on cylindrical shell) +
(pressure force acting on annular surface at z=0) –
(pressure force acting on annular surface at z=L) = 0
That is:

$$(2\pi r L \tau_{rz})_r - (2\pi r L \tau_{rz})_{r+\Delta r} + (2\pi r \Delta r \rho v^2)_{z=0} - (2\pi r \Delta r \rho v^2)_{z=L} +$$

$$2\pi r \Delta r L \rho g + 2\pi r \Delta r (p_0 - p_L) = 0 \qquad\qquad (AA-1)$$

Because the fluid is assumed to be incompressible, v is the same at z=0 and z=L, hence the third and fourth terms cancel one another. Divide Equation (AA-1) by $2\pi L \Delta r$ and take the limit as Δr goes to zero; this gives

$$\lim_{\Delta r \to 0} \left[\frac{(r\tau_{rz})_{r+\Delta r} - (r\tau_{rz})_r}{\Delta r}\right] = \left(\frac{P_0 - P_L}{L} + \rho g\right)r \qquad (AA-2)$$

$$\frac{d}{dr}(r\tau_{rz}) = \left(\frac{P_0 - P_L}{L}\right)r \qquad\qquad (AA-3)$$

in which $P = p - \rho g z$. Equation (AA-3) may be integrated to give:
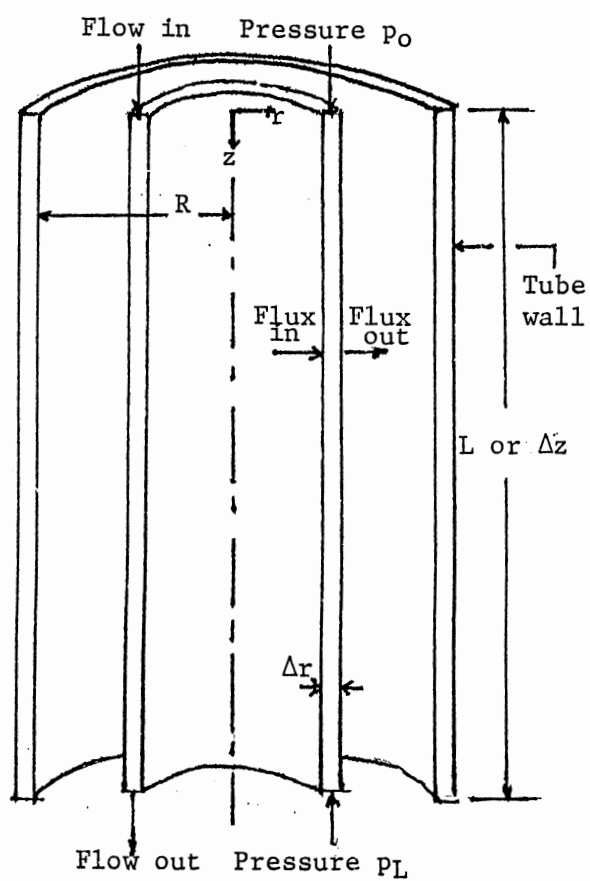
Figure 12. Cylindrical Shell of
Fluid

$$\tau_{rz} = (\frac{P_o - P_L}{2L})r + \frac{C1}{r} \tag{AA-4}$$

The constant C1 must be zero if the momentum flux is not to be infinite at r=0. Hence the momentum flux distribution is

$$\tau_{rz} = (\frac{P_o - P_L}{2L})r \tag{AA-5}$$

Power-law of shear-stress and shear-rate for this situation is

$$\tau_{rz} = -\kappa(\frac{dv}{dr})^s \tag{AA-6}$$

$$\frac{dv}{dr} = (\frac{P_L - P_o}{2\kappa L})^{1/s}\, r^{1/s} \tag{AA-7}$$

Integration of this and application of boundary condition that v=0 at r=R give

$$v = \frac{s}{s+1}\ \frac{P_o - P_L}{2L\kappa}\ R^{(s+1)/s}\ [1-(\frac{r}{R})^{(s+1)/s}] \tag{AA-8}$$

The maximum velocity v_o occurs at r=0 and has the value

$$v_o = \frac{s}{s+1}\ \frac{P_o - P_L}{2L\kappa}\ R^{(s+1)/s} \tag{AA-9}$$

The average velocity <v> is calculated by summing up all the velocities over a cross section and then dividing by

the cross-sectional area:

$$\langle v \rangle = \frac{\int_o^R 2\pi r v\, dr}{\int_o^R 2\pi r\, dr}$$

$$= \frac{s}{3s+1} \frac{P_o - P_L}{2LK} R^{(s+1)/s} \qquad (AA-10)$$

Compare with Equation (AA-10)

$$v_o = \frac{3s+1}{s+1} \langle v \rangle \qquad (AA-11)$$

Combine Equation (AA-8) through (AA-11) and change into dimensionless form

$$v/v_o = [1-U^{(s+1)/s}] \qquad (AA-12)$$

APPENDIX B

DERIVATION OF CONTINUITY EQUATION

Referring to the same annular shell shown in Figure 12 we can make a material balance with respect to component i under following conditions and assumptions:

1. Laminar flow in axial direction only, i.e. z-direction.
2. Neglect axial diffusion.
3. Undergoing an n-th order chemical reaction w.r.t. component i.

(component i flow in across annular surface at z=z) − (component i flow out across annular surface at z=z+Δz) +(component i diffuses in across cylindrical surface at r) −(component i diffuses out across cylindrical surface at r+Δr) − (component i consumed due to chemical reaction)=0

That is:

$$(c_i \rho v \, 2\pi r \Delta r|_z) - (c_i \rho v \, 2\pi r \Delta r|_{z+\Delta z}) + 2\pi r \Delta z (-D\frac{\partial c_i}{\partial r}\Big|_r + D\frac{\partial c_i}{\partial r}\Big|_{r+\Delta r})$$

$$-2\pi r \Delta r \Delta z K c_i^n = 0 \qquad\qquad\qquad (AB-1)$$

Divide above equation by $2\pi \Delta r \Delta z$ and take the limit as Δr and Δz go to zero; this gives

$$-rv\frac{\partial c_i}{\partial z} + D\frac{\partial}{\partial r}(r\frac{\partial c_i}{\partial r}) - rKc_i^n = 0 \qquad\qquad (AB-2)$$

Rearrange above equation and substitute into the velocity profile derived in Appendix A and dimensionless variables, Equation (AB-2) becomes

$$-(1-U^{(s+1)/s})\frac{\partial C}{\partial Z} + A(\frac{\partial^2 C}{\partial U^2} + \frac{1}{U}\frac{\partial C}{\partial U}) - C^n = 0 \qquad \text{(AB-3)}$$

APPENDIX C

INPUT SPECIFICATIONS USED IN MACHINE CALCULATIONS

INPUT SPECIFICATIONS

	n	s	N	A	Xtol	dlamda
TABLE IV						
Z < 0.20	1	1	50	0.	0.001	0.01
Z => 0.20	1	1	50	0.	0.0001	0.02
TABLE VI						
Z <= 0.25	1	1	50	0.	0.001	0.01
Z > 0.25	1	1	50	0.	0.0001	0.02
Z <= 0.30	1	1	50	0.1 (0.01)	0.001	0.01
Z > 0.30	1	1	50	0.1 (0.01)	0.0001	0.02
TABLE VII	1	(.2-.8)	50	0. (0.0001) (0.001) (0.01) (0.1)	0.0001	0.01*
Figure 5	1	1	50	0.1	0.001	0.01
Figure 6,7	1	1	50	0.1	0.001	0.1
Figure 8,9	1	1	50	0.	0.0001	0.02
	1	1	50	0.1 (0.01)	0.001	0.1
Figure 10	1	1	50	0.01	0.001	0.1
	1	(.2-.8)	50	0.01	0.00001	0.03*
Figure 11	1	0.6	50	0.01	0.00001	0.03*
	0.5 (1.5) (2.0)	0.6	50	0.01	0.0001	0.02*

* Converted to Z': $Z'=[(3s+1)/(s+1)](dlamda)$

APPENDIX D

LISTING OF FORTRAN PROGRAM

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                     C
C                                                     C
C    NOMENCLATURE                                     C
C                                                     C
C        A(50,4)    : Compressed Matrix               C
C        ALPHA      : Diffusion Parameter             C
C        C(50,2)    : Concentration                   C
C        COLD(50,2) : Temporary Concentration         C
C        DLAMDA     : Step Size in Axial dir.         C
C        F(50)      : Function Values of Difference   C
C                         Equations                   C
C        FOLD(50)   : Temporary Function Values of    C
C                         Difference Equations        C
C        FP(50,50)  : Jacobian Matrix                 C
C                                                     C
C        GUESS      : Initial Guess of Concentration  C
C                         at the tube center          C
C        H(50)      : Progress in Newton-Raphson's    C
C                         Iterations                  C
C        I,II,J,JJ  : Do Loop Index                   C
C        L          : Axial Step Number,              C
C                       Tube Length=L*DLAMDA          C
C        LAMDA      : Axial Coordinate                C
C                                                     C
C        N          : Number of Grid Nodes in Radial  C
C                         Derection                   C
C        ORDER      : Chemical Reaction Order         C
C        S          : Rheology Index                  C
C        U(50)      : Radial Position                 C
C        XTOL       : Tolerance of Concentration      C
C                                                     C
C                                                     C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


        PROGRAM THESIS
        DIMENSION FOLD(50),COLD(50,2)
        COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
       -ORDER
        DATA GUESS/.95/


C READ INPUT DATA FROM KEYBOARD OR ANY DEFAULT DEVICE
        WRITE (*,*) 'Rxn Order ='
        READ (*,*) ORDER
        WRITE (*,*) 'Rheology Index ?'
        READ (*,*) S
        WRITE (*,*) 'Subdivided into N Grid, N=?'
        READ (*,*) N
        WRITE (*,*) 'ALPHA = ?'
        READ (*,*) ALPHA
        WRITE (*,*) 'Xtolerence=?'
```

```
      READ (*,*) XTOL
      WRITE (*,*)'dlamda'
      READ (*,*) DLAMDA
      WRITE (*,*) 'LENGTH NEEDED (LENGTH=L*DLAMDA)?'
      READ (*,*) L
C END OF INPUT

      OPEN (6, FILE='PLOT.DAT', STATUS='NEW')

C BOUNDARY (INITIAL) CONDITION
C SET INLET DIMENSIONLESS CONC. TO BE UNIFORM,1.
      DO 10 I=1,N
      C(I,0)=1.
  10  CONTINUE


      DO 100 K=0, L
C 'K' IS AXIAL STEP INDEX

C INITIAL GUESS:
C A LINEAR CONC. PROFILE IS OBTAINED FOR THE FIRST STEP.
C FOR THE REST AXIAL STEPS, PREVIOUS CONC. PROFILE IS
C USED AS THE INITIAL RADIAL CONC. PROFILE.
      IF (K .EQ. 0) THEN
        DO 20 I=1,N
          C(I,1)=GUESS-I*.001
  20    CONTINUE
      ELSE
        DO 60 I=1,N
          C(I,0)=C(I,1)
  60    CONTINUE
      ENDIF

      GOTO 41

C TEST IF TOLERANCE IS MET
  40  ITEST=0
      DO 25 I=1,N
        IF (ABS(H(I)/(2**jj)) .GT. XTOL) ITEST=ITEST+1
  25  CONTINUE
      IF (ITEST .EQ. 0) GOTO 150

C EVALUATE FUNCTION VALUES OF EACH DIFFERENCE EQN.
  41  CALL FCNVALUE (N,K,DLAMDA,S,ALPHA)

C EVALUATE EACH PARTIAL DERIVATIVE OF EVERY FUNCTION
C W.R.T. EVERY INDEPENDENT VARIABLE, I.E. JACOBIAN.
      CALL DERIVATIVE (N,K,DLAMDA,S,ALPHA)

C COMPRESS JACOBIAN MATRIX, FP, AND FUNCTION VALUE
C VECTOR, F, INTO AN N x 4 MATRIX
      CALL FPTOA (N)
```

```
C SOLVE FOR H VECTOR, THE PROGRESS STEP
      CALL TRIDG (N)

C EVALUATE THE NORM FOR OLD CONC. PROFILE
      CALL NORM (N,FNORM)
      FONORM=FNORM

C SAVE RESULTS BEFORE MAKING PROGRESS
      DO 27 I=1,N
         COLD(I,1)=C(I,1)
         FOLD(I)=F(I)
   27 CONTINUE

C TEST IF THERE IS ANY NEGATIVE VALUE OF CONC. PRESENT
C AFTER PROGRESSING
      JJ=0
   31 IJTEST=0
      DO 30 I=1,N
         C(I,1)=COLD(I,1)-H(I)/(2**JJ)
         IF (C(I,1) .LT. 0.) THEN
           IJTEST=IJTEST+1
         ELSE
         ENDIF
   30 CONTINUE
C CHECK THE TEST RESULT
      IF (IJTEST .NE. 0) THEN
         JJ=JJ+1
         GOTO 31
      ELSE
      ENDIF

C REEVALUATE FUNCTION VALUES AND NORM USING NON-NEGATIVE
C SOLUTION
      CALL FCNVALUE (N,K,DLAMDA,S,ALPHA)
      CALL NORM (N,FNORM)

C DECIDE IF THIS IS AN DESIRED PROGRESS BY CHECKING
C NORMS
      IF (FONORM .LT. FNORM) THEN
         IF (JJ .LT. 100) THEN
            JJ=JJ+1
            GOTO 31
         ELSE
            WRITE (*,*) 'SUA',JJ
            STOP
         ENDIF
      ELSE
         GOTO 40
      ENDIF

C PRINT OUT THE RESULTS
  150 DO 50 I=1,N
         LAMDA=(K+1)*DLAMDA
```

```fortran
        U(I)=(I-1.)/(N-1.)
        WRITE (6,1000) LAMDA,U(I),C(I,1),ORDER,S,ALPHA
1000    FORMAT (1X,F6.2,2F10.6,2F6.2,F8.4))
  50    CONTINUE

C CALCULATE THE AREA AVERAGE CONC. BY SIMPSON'S
C METHOD
        CALL SIMPSON (N,S,K,TOT)
C MAKE A FLAG MARK IN OUTPUT TO IDENTIFY AVERAGE
C CONC. FROM OTHER RADIAL CONC. PROFILE
        FLAG=2.0
        WRITE (6,1000) LAMDA,FLAG,TOT,ORDER,S,ALPHA

 100    CONTINUE

        END



        SUBROUTINE FCNVALUE(N,K,DLAMDA,S,ALPHA)
        COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
       -ORDER
        DU=1./(N-1.)
        F(1)=(C(1,1)-C(1,0))/DLAMDA-2.*ALPHA*(C(2,1)-C(1,1
       -1)+C(2,0)-C(1,0))/DU**2+((C(1,1)+C(1,0))/2)**ORDER
        DO 10 I=2,N-1
          U(I)=(I-1.)/(N-1)
          FIRST=(1-U(I)**((S+1)/S))*(C(I,1)-C(I,0))/DLAMDA
          SECOND=(C(I+1,1)+C(I-1,1)-2*C(I,1)+C(I+1,0)+C(I
       --1,0)-2*C(I,0))/(2*DU**2)
          THIRD=(C(I+1,1)-C(I-1,1)+C(I+1,0)-C(I-1,0))/(4*
       -U(I)*DU)
          FOURTH=((C(I,1)+C(I,0))/2)**ORDER
          F(I)=FIRST-ALPHA*(SECOND+THIRD)+FOURTH
  10    CONTINUE
        F(N)=(C(N,1)-C(N-1,1)+C(N,0)-C(N-1,0))/(2*DU)
        RETURN
        END


        SUBROUTINE DERIVATIVE (N,K,DLAMDA,S,ALPHA)
        COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
       -ORDER
        DU=1./(N-1)
        FP(1,1)=1./DLAMDA+(2*ALPHA)/DU**2+(ORDER/2.)*((
       -C(1,1)+C(1,0))/2)**(ORDER-1)
        FP(1,2)=(-2*ALPHA)/DU**2
        DO 10 I=2,N-1
          U(I)=(I-1.)/(N-1)
          FP(I,I-1)=-ALPHA/(2*DU**2)+ALPHA/(4*U(I)*DU)
          FP(I,I)=(1-U(I)**((S+1)/S))+ALPHA/DU**2+ORDER*
       -0.5*((C(I,1)+C(I,0))/2)**(ORDER-1)
          FP(I,I+1)=-ALPHA/(2*DU**2)-ALPHA/(4*U(I)*DU)
```

```
10   CONTINUE
     FP(N,N-1)=-1./(2*DU)
     FP(N,N)=1./(2*DU)
     RETURN
     END



     SUBROUTINE FPTOA (N)
     COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
    -ORDER
     A(1,2)=FP(1,1)
     A(1,3)=FP(1,2)
     A(1,4)=F(1)
     DO 10 I=2,N
        DO 20 J=1,3
           A(I,J)=FP(I,I+J-2)
20      CONTINUE
        A(I,4)=F(I)
10   CONTINUE
     A(N,1)=-1.
     A(N,2)=1.
     A(N,4)=F(N)
     RETURN
     END



     SUBROUTINE TRIDG (N)
     COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
    -ORDER
     DO 10 I=2,N
        A(I,1)=A(I,1)/A(I-1,2)
        A(I,2)=A(I,2)-A(I,1)*A(I-1,3)
        A(I,4)=A(I,4)-A(I,1)*A(I-1,4)
10   CONTINUE

C BACK SUBSTITUTING

     NM1=N-1
     A(N,4)=A(N,4)/A(N,2)
     DO 20 I=NM1,1,-1

C THE INDEX M WILL COUNT UP THE ROWS

        A(I,4)=(A(I,4)-A(I,3)*A(I+1,4))/A(I,2)
20   CONTINUE
     DO 30 I=1,N
        H(I)=A(I,4)
30   CONTINUE
     RETURN
     END
```

```
      SUBROUTINE NORM (N,FNORM)
      COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
     -ORDER
      FNORM=0
      DO 10 I=1,N
      FNORM=FNORM+F(I)**2
10    CONTINUE
      RETURN
      END


      SUBROUTINE SIMPSON (N,S,K,TOT)
      COMMON C(50,2),F(50),A(50,4),H(50),U(50),FP(50,50),
     -ORDER
      DIMENSION VF(50)
      COE=(6*S+2)/(S+1)
      DU=1./(N-1)
      TOT=0.
      DO 10 I=1,N
        VF(I)=U(I)*(1-U(I)**((S+1)/S))*C(I,1)
10    CONTINUE
      MA=MOD(N,2)
      IF (MA .EQ. 0) THEN
        DO 20 I=1,N-5,2
          TOT=TOT+(DU/3)*(VF(I)+4*VF(I+1)+VF(I+2))
20      CONTINUE
      TOT=TOT+(3*DU/8)*(VF(N-3)+3*VF(N-2)+3*VF(N-1)+
     -VF(N))
      ELSE
        DO 30 I=1,N-2,2
          TOT=TOT+(DU/3)*(VF(I)+4*VF(I+1)+VF(I+2))
30      CONTINUE
      ENDIF
        TOT=COE*TOT
      RETURN
      END
```

APPENDIX E

BRIEF LITERATURE SURVEY

```
                                              ┌─Bosworth (1)
                                              │
                                              ├─Cleland &
                                     ┌─Diff.   │ Wilhelm (2)
                          1-st       │        ├─Walker (7) ────────┐
                          order      │        │                    │
                          Homo. R.───┤        └─Soloman & ─────────┤
                                     │          Hudson (8)         │
            Newtonian               └─No Diff. ──┐                │
            Fluids                               │                │─1-st
                                            Johnson               │ order
                                                 │                │ Heter.
                                      ┌─No Diff. ─┘               │ Rxn.
                          non-1st     │                          │
                          order ──────┤        ┌─Krongelb (6)────┘
                          Homo. R.    └─Diff.──┤
                                               └─Vignes (5)

TUBULAR
REACTOR
                                     ┌─Diff.──Homsy &
                                     │         Strohman (13)
                          1-st       │
                          order ─────┼─No Diff.──Mihail &
                          Homo. R.   │            Tausch (14)
            non-                     │
            Newtonian                │  Axial
            Fluids                   └─Dispersion - Mashelkar (19)
                                        Model

                          non-1st
                          order
                          Homo. R.
```
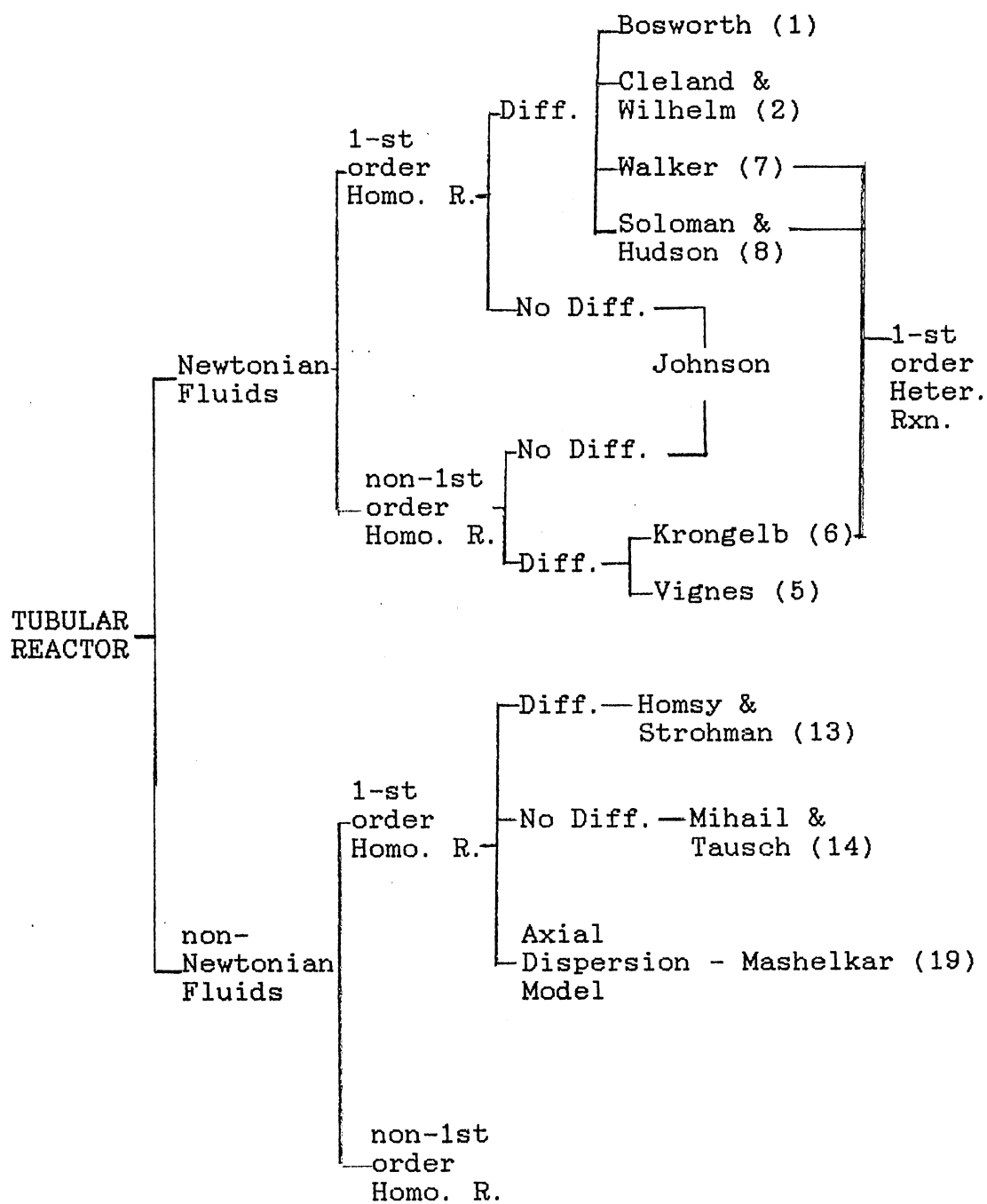
APPENDIX F

INSTRUCTIONS FOR PROGRAM INPUTS AND OUTPUTS

PROGRAM INPUT

C> THE2
Rxn Order =

--

[Input order of chemical reaction, e.g. 0, .5, 1, etc.]

Rheology Index ?

--

[Input rheology index 's' for power-law fluids

  0.< s < 1. ==> pseudoplastic non-Newtonian fluids
  s = 1.0   ==> Newtonian fluids
  s > 1.0   ==> dilatant non-Newtonian fluids]

Subdivided into N Grid, N=?

--

[Input the number of nodes along radial direction, i.e.
 from tube center to tube wall.
 Maximum is 50]

ALPHA = ?

--

[Input the dimensionless diffusion parameter 'A'.

 For A = 0 ==> Neglecting radial diffusion effect]

xtolerence=?

[Input dimensionless potential concentration tolerance,
 e.g. .001, .0001, etc.]

dlamda

--

[Input the step length in tube axial direction, Z.
 For example, .1, .01, etc.]

LENGTH NEEDED (LENGTH=L*DLAMDA)?

--

[Input the number of steps needed in tube axial
 direction. Tube length is equal to the product of Z
 and the number of steps specified here.
 e.g. 10, 50, 200, etc.]

PROGRAM OUTPUT

(SAMPLE)

```
.01    .000000    .988121   1.00   1.00    .1000
.01    .020408    .990125   1.00   1.00    .1000
.01    .040816    .990364   1.00   1.00    .1000
.01    .061224    .990368   1.00   1.00    .1000
.01    .081633    .990326   1.00   1.00    .1000
.01    .102041    .990277   1.00   1.00    .1000
.01    .122449    .990225   1.00   1.00    .1000
.01    .142857    .990168   1.00   1.00    .1000
.01    .163265    .990102   1.00   1.00    .1000

                        :
                        :
                        :
                        :

.01   2.00000    .980024   1.00   1.00    .1000
```

The output data will be saved in an automatically created
file named PLOT.DAT. Each column shows different
information as follows:

Column 1 : Shows Z values

Column 2 : Dimensionless radial position, U values.

Column 3 : Dimensionless concentration, C values.
Note that when U > 1.0, this column shows
the average dimensionless concentration
at a specified Z in stead of potential
concentration.

Column 4 : The order of chemical reaction.

Column 5 : Rheology Index

Column 6 : Dimensionless diffusion parameter 'A'.

VITA

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