RESIDENCE TIME DISTRIBUTION FUNCTIONS FOR

TUBULAR REACTORS IN TURBULENT FLOW

Jerald Linsley, Ph.D., P.E.
Associate Professor of Chemical Engineering
Florida Institute of Technology
Melbourne, Florida 32901

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ABSTRACT

To compliment the residence time distribution functions (RTD's) for the continuous stirred tank reactor (CSTR), the laminar flow reactor (LFR), and the plug flow reactor (PFR), a new residence time distribution function for the turbulent flow reactor (TFR) is developed. A review of the best available turbulent velocity profile data and turbulent velocity ratio data for pipe flow is performed. These data are used to evaluate the constants in a new empirical turbulent velocity profile correlation. This new correlation is then used to derive a new turbulent flow reactor residence time distribution. Additional work on an older TFR RTD using an older turbulent velocity profile correlation is also performed. The results of this study augment the available tools for the analysis and design of chemical reactors experiencing deviations from ideal flow conditions.

TURBULENT FLOW REACTOR

RESIDENCE TIME DISTRIBUTION

In the study of nonideal flow in chemical reactors, many reactor design texts present residence time distributions (RTD) for three types of reactors: the continuous stirred tank reactor (CSTR), the plug flow reactor (PFR), and the laminar flow reactor (LFR) (Carberry, 1976; Hill, 1977; Smith, 1981). The CSTR and PFR can be considered ideal tubular reactors at two extreme conditions of mixing___complete mixing in the CSTR and no mixing in the PFR. Figure 1 presents a schematic representation of the tubular reactor. Intermediate to these two extreme cases, is the LFR whose RTD represents the effects of the partial mixing which results from the radial variation of the axial velocity in laminar flow (the parabolic velocity profile). These three RTD's are expressed mathematically by equations (1), (2), and (3).

CSTR-RTD

(1) $$J(t) = 1 - e^{-t/\theta} \qquad t \geq 0$$

LFR-RTD

$$J(t) = 0 \qquad t < \theta/2$$

(2) $$J(t) = 1 - \left(\frac{\theta}{2t}\right)^2 \qquad t \geq \theta/2$$

PFR-RTD

(3) $$J(t) = u(t - \theta) \qquad t > 0$$

The utility of RTD's, both these ideal cases and other cases, is in the calculation of average conversions of chemical reactors by the expression

$$\overline{C}_A = \int_0^1 C_A(t)\, dJ(t) \qquad (4)$$

Further elaboration on the use of the RTD is beyond the scope of this project.

Intermediate to the LFR and the PFR is the turbulent flow reactor (TFR). The turbulent flow case is perhaps industrially more important than the laminar flow case. It is well known that, as the Reynolds number increases, i.e., as flow becomes more turbulent, the parabolic velocity profile of laminar flow approaches the flat velocity profile of plug flow. Use of the PFR model for turbulent flow is quite common.

Recently, we have performed some initial studies on the TFR (Linsley, 1986). Based upon a common empirical expression of the radial variation of the axial velocity for turbulent flow (the $1/n$ velocity distribution) an RTD for the TFR is derived and the resulting TFR RTD is depicted for a range of Reynolds numbers.

Consider the turbulent flow velocity distribution (Schlichting, 1968).

$$v_z(\xi) = \frac{\bar{v}_z}{C}(1-\xi)^{\frac{1}{n}} \qquad (4.)$$

Here C is the ratio of the mean velocity to the maximum centerline velocity (0.5 for laminar flow, 1.0 for plug flow). A relation between C and n is derived by calculating the average velocity.

$$(5.)\quad \bar{v}_z = \frac{\int_0^1 v_z(\xi)\,2\pi\xi\,d\xi}{\int_0^1 2\pi\xi\,d\xi}$$

The ratio between the mean and maximum velocity, C, is evaluated as:

$$(6.)\quad C = \frac{2n^2}{(n+1)(2n+1)}$$

This is also given in Schlichting.

Using the data of Nikuradse (Schlichting, 1968), n is given empirically as a function of the Reynolds number (Figure 2). Resulting velocity profiles are shown in Figure 3.

For the turbulent flow velocity distribution, the RTD is given, in general as:

$$J(t) = 0 \qquad t < C\theta$$

$$(7.)\quad J(t) = \frac{\int_0^{\xi} v_z(\phi)\,2\pi\phi\,d\phi}{\int_0^1 v_z(\phi)\,2\pi\phi\,d\phi} \qquad t \geq C\theta$$

with ξ and t related by:

$$(8)\quad v_z(\xi) = \frac{L}{t} = \frac{\bar{v}_z}{C}(1-\xi)^{\frac{1}{n}}$$

or, since $\theta = L/\bar{v}_z$

$$(9)\quad \left(\frac{C\theta}{t}\right) = (1-\xi)^{\frac{1}{n}}$$

The TFR RTD evalutes to:

$$J(t) = 0 \qquad t < \theta$$

(10.)

$$J(t) = \left\{1 - \left(\frac{1}{n}\right)\left(\frac{c\theta}{t}\right)^{1+n}\left[(2n+1) - (n+1)\left(\frac{c\theta}{t}\right)^{n}\right]\right\} \qquad t \geq \theta$$

Figure 4 shows the TFR RTD for various values of the Reynolds number as well as the CSTR, LFR, and PFR RTD's.

It is commonly stated and/or assumed that the LFR RTD evolves to the PFR RTD as $Re \rightarrow \infty$, i.e., as the flow becomes more turbulent and that the PFR RTD can be used for turbulent flow conditions. While the evolution of the LFR RTD to the PFR RTD is not contra-indicated here, we note that, for a practical Reynolds number range $(10^4 < Re < 10^8)$, the TFR RTD varies over a rather small region of the RTD graph. We, therefore, conclude that the use of a single TFR RTD curve at a particular Reynolds number (we suggest $Re = 10^8$) for the TFR RTD should be justified and should provide an improvement over the use of the PFR RTD for turbulent flow reactors. This, we think, establishes the desirability for further study of the TFR RTD.

One major shortcoming of the above work is that the turbulent velocity profile and the resulting RTD do not reduce to the laminar case as the Re decreases to the laminar region (2100). We propose to eliminate this shortcoming by the result of this project. We propose a new empirical turbulent velocity profile of the form:

$$(11.) \qquad V_z(\xi) = \frac{\bar{V}_z}{C}\left(1 - \xi^2\right)^{\frac{1}{m}}$$

Here C has the same interpretation as in previous equations____the ratio of the average velocity to the maximum or centerline velocity.

Substitution of equation (11) into equation (5) results in the following relationship between C and m.

$$C = \frac{m}{1+m} \tag{12.}$$

or

$$m = \frac{C}{1-C} \tag{13.}$$

For laminar flow, $C = 0.5$ and m becomes unity; i.e., equation (11) reduces to the laminar flow form. For the PFR case, $C = 1.0$, and $m \rightarrow \infty$ or $1/m = 0$ and equation (11) reduces to the PFR form (constant). Substitution of equation (11) into equation (7) gives a new, simpler TFR RTD.

$$J(t) = 0 \qquad t < C\theta$$

$$J(t) = 1 - \left(\frac{C\theta}{t}\right)^{1+m} \qquad t \geq C\theta \tag{14.}$$

This form will reduce to the LFR RTD as the flow reduces from turbulent to laminar.

Another approach to relating C and m of equation (11) is possible. In fact, this approach could have been used to relate C and n of equation (4). What we have, in effect, done is use experimental turbulent velocity profile data to evaluate n (this was already done in Schlichting) and then use equations (5) and (6) to evaluate C. We propose to perform analogous work with the new empirical velocity profile. The other approach is to use experimental data for the velocity ratio, C versus Reynolds number (Perry, 1984;

Rothfus, 1957) and then use equations (5), (6) and (13) to evaluate n and m as a function of c.

At this point the question arises: "Does the world really need a new empirical turbulent velocity profile and, if so, why hasn't it been proposed previously?" We surmise that previous empirical turbulent velocity profiles such as the $1/n$ velocity profile presented above or the so called universal velocity profile (Faust, 1980) have been proposed to explain momentum transport. For this problem, the largest momentum fluxes (forces) occur at the wall of the pipe rather than in the turbulent core. Hence, the emphasis has been on accuracy near the pipe wall. For residence time distributions, the largest effect will be that of the turbulent core and inaccuracies in the profile near the tube wall will have less effect on the RTD. We believe that this different purpose, the explanation of RTD's, justifies the formulation of a new empirical turbulent velocity profile.

Finally, as background, we note that it is commonly known that Nickuradse fudged some data (Churchill, 1983). The graphs of $(v_z/V)^n$ vs $(1-\xi)$ attributed to Nickuradse (Schlichting, 1968) do not pass through the point $(v_z/V)=1$ at $\xi=0$. This could be either an instance of the data fudging or merely an attempt to emphasize accuracy near the pipe wall. In either case, this makes the velocity distribution, using Nichuradse's n vs Re determination, less accurate in the turbulent core. Thus the RTD's calculated using this data (Figure 2) will be less accurate. So, for the sake of completeness, it would seem prudent to reevaluate n vs Re for the $1/n$ velocity distribution.

NOMENCLATURE

C - ratio of the average velocity, $\bar{v}_z$, to the maximum (centerline) velocity V.

C_A - concentration of component A

$\bar{C}_A$ - average concentration of component A

D - diameter of tubular reactor $(2R)$

e - base of natural logarithm, 2.718...

J - residence time distribution function

L - length of tubular reactor

m - reciprocal exponent in turbulent velocity profile, equation (11)

n - reciprocal exponent in turbulent velocity profile, equation (4.).

r - radial coordinate

R - radius of tubular reactor $(D/2)$

Re - Reynolds number $(D \bar{v}_z \rho / \mu)$

t - time

u - unit step function

v_z - axial velocity

$\bar{v}_z$ - average axial velocity

V - maximum axial velocity

z - axial coordinate

ξ - dimensionless radius, r/R

θ - PFR residence time, $L/\bar{v}_z$

μ - viscosity

ρ - density

φ - dummy variable of integration

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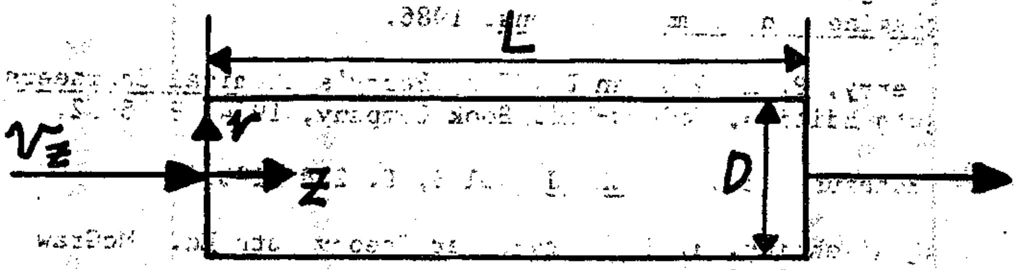


FIGURE 1 SCHEMATIC REPRESENTATION OF A TUBULAR REACTOR

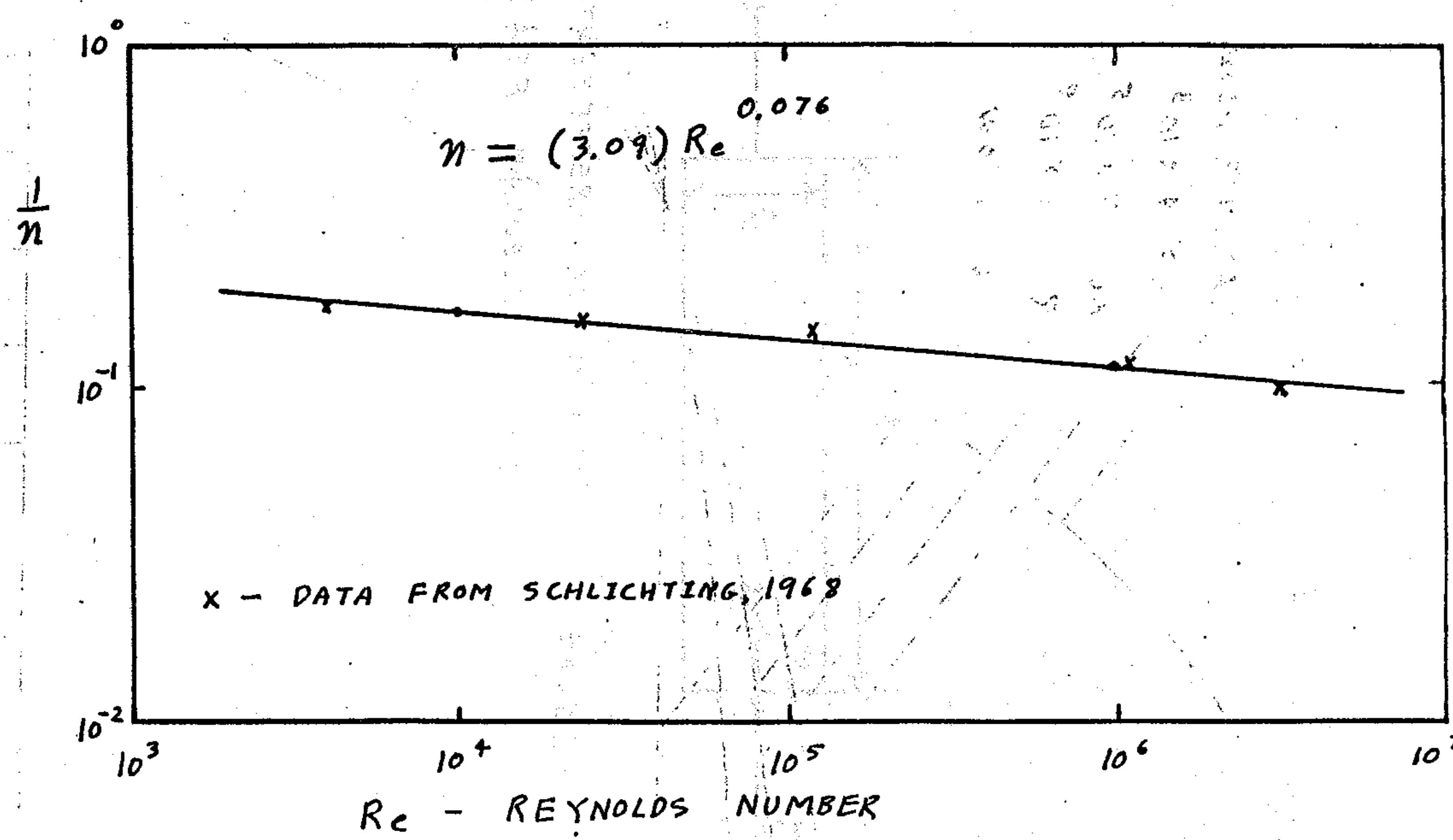
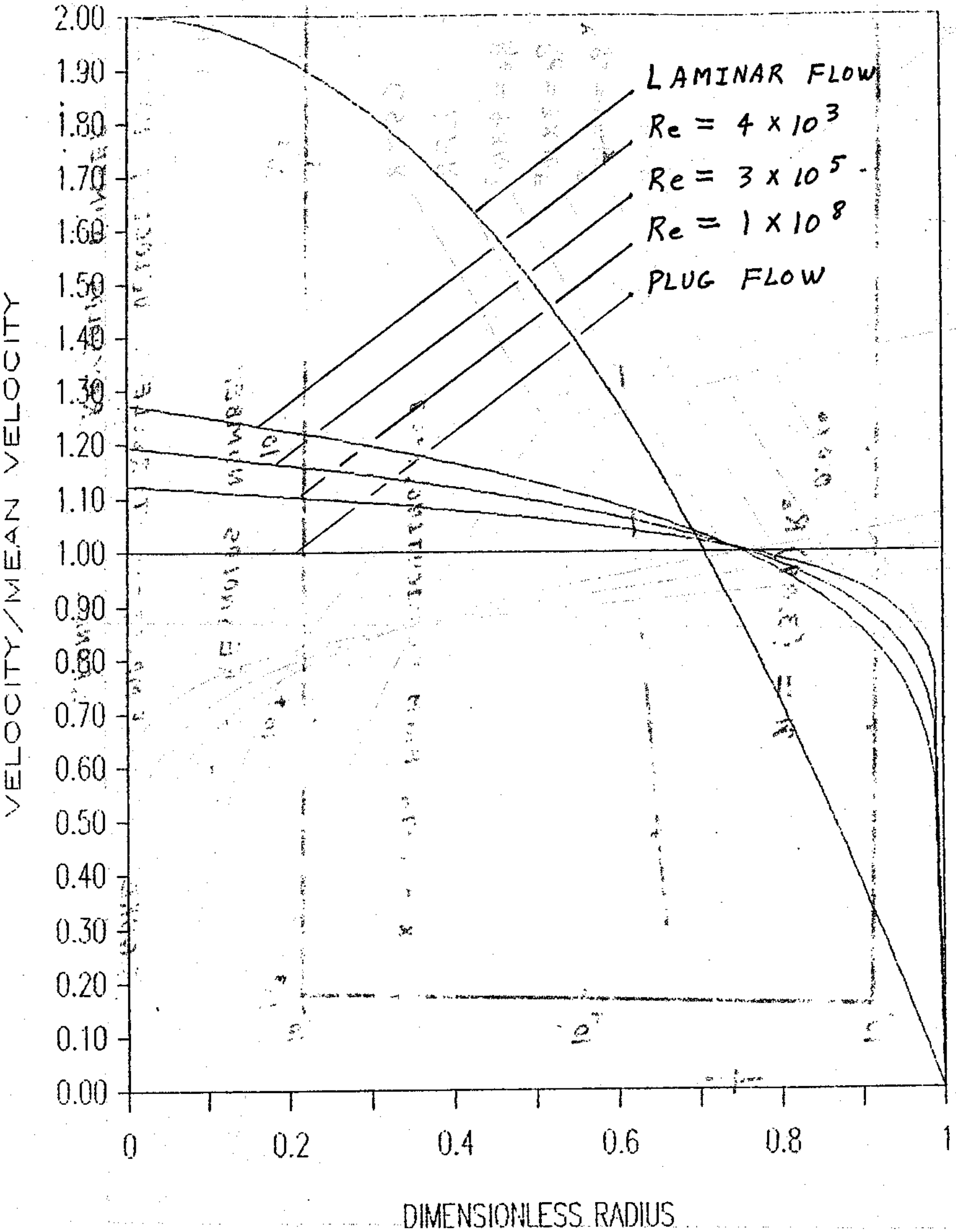


FIGURE 2 - EMPIRICAL TURBULENT VELOCITY PROFILE EXPONENT VS. REYNOLDS NUMBER



LAMINAR FLOW
Re = 4 x 10^3
Re = 3 x 10^5
Re = 1 x 10^8
PLUG FLOW
VELOCITY/MEAN VELOCITY
2.00
1.90
1.80
1.70
1.60
1.50
1.40
1.30
1.20
1.10
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
0
0.2
0.4
0.6
0.8
1
DIMENSIONLESS RADIUS

FIGURE 3

RESIDENCE TIME DISTRIBUTION

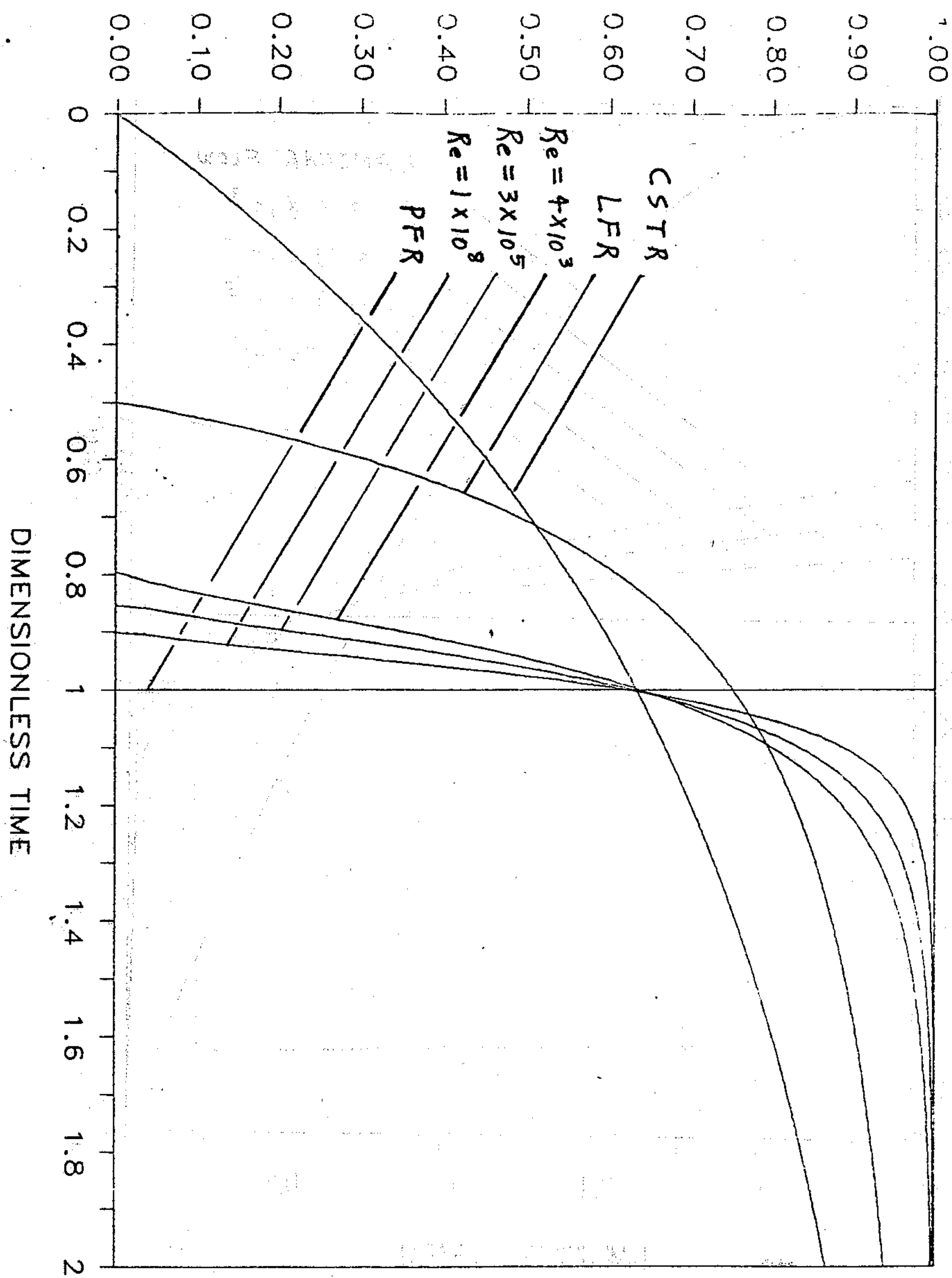


FIGURE 4