# TRANSIENTS IN PLUG FLOW SYSTEMS

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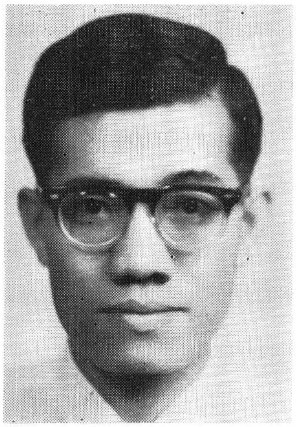
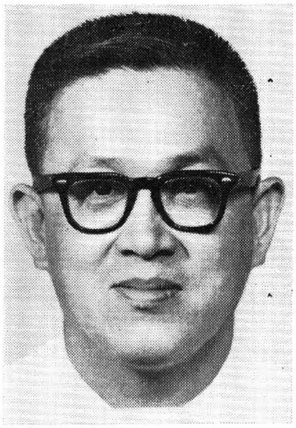
THE PLUG FLOW MODEL, along with the completely stirred tank model, may be one of the most basic or elementary flow models in chemical engineering. This is hardly surprising because of the tubular nature of many of the equipment employed in a variety of continuous chemical systems and processes such as chemical reactors, heat exchangers, gas adsorption, extraction, and adsorption. Many steady state design equations for these processes are based on the plug flow model (e.g. see Perry and Chilton, 1973).





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These processes as well as other chemical processes, are often operated under transient or unsteady conditions during start-up and shut-down. They are also constantly subject to environmental disturbances and changes in feed conditions.

It appears that, in spite of its importance, the elementary analysis of transient characteristics of processes represented by the plug flow model has seen only limited coverage in undergraduate textbooks in process dynamics and control, reaction engineering, transport phenomena, and process design. This contrasts sharply to the situation for processes described by the completely stirred tank model.

The deterministic mathematical representation of a plug flow process under transient conditions is a first order, one-dimensional partial differential equation (hyperbolic PDE) or a set of such equations. This note contains tutorial material for solution of a first order partial differential equation by means of a well-known technique, namely the method of characteristics (Abbott, 1966; Acrivos, 1956; Aris and Amundson, 1973; Courant, 1962; Lapidus, 1962; Liu, Aris, and Amundson, 1962), which is suitable for presentation to undergraduate classes.

## BASIC PRINCIPLE

THE GENERAL EXPRESSION for a first-order, one-dimensional partial differential equation can be written as

$$A(T, t, x)\frac{\partial T}{\partial t} + B(T, t, x)\frac{\partial T}{\partial x} = R(T, t, x) \quad (1)$$

subject to

$$T = T_o(x) \text{ at } t = 0, x \geq 0 \quad (2)$$

$$T = T_1(t) \text{ at } t > 0, x = 0 \quad (3)$$

in which T denotes the dependent variable, t the time variable, x the space variable, and R(T, t, x) the source or sink term. A(T, t, x) and B(T, t, x) represent arbitrary functions of T, t and x or a constant,

As indicated by Eq. (1), the solution for T can be expressed in terms of t and x; hence, the total differential of T can be written as

$$\frac{\partial T}{\partial t}dt + \frac{\partial T}{\partial x}dx = dT \qquad (4)$$

Since the solution of Eq. (1) should also satisfy Eq. (4), there exists a parameter $\alpha$ such that $A(T,t,x) = \alpha dt$, $B(T,t,x) = \alpha dx$, $R(T,t,x) = \alpha dT$ or

$$\frac{dt}{A(T,t,x)} = \frac{dx}{B(T,t,x)} = \frac{dT}{R(T,t,x)} = \frac{1}{\alpha} \qquad (5)$$

Equation (5) can be rewritten as

$$\frac{dx}{dt} = \frac{B(T,t,x)}{A(T,t,x)} \qquad (6)$$

and

$$\frac{dT}{dt} = \frac{R(T,t,x)}{A(T,t,x)} \qquad (7)$$

Equations (6) and (7) should satisfy the conditions given by Eqs. (2) and (3).

The original partial differential equation, Eq. (1), now is transformed into two ordinary differential equations, Eqs. (6) and (7). The first, Eq. (6), represents the so-called characteristic lines along which the second, Eq. (7), is integrated. Both Eqs. (6) and (7) can be integrated either analytically or numerically. It should be noted that a set of these two equations is not an approximation to the original partial differential equation. However, approximate or exact solutions can be obtained for these two equations depending on their complexities.

The integration of Eqs. (6) and (7) subject to the appropriate conditions can be graphically interpreted by Fig. 1. In this figure, the independent variables, t and x, are chosen as two coordinates, and the magnitude of T, if shown, will appear as a line segment perpendicular to the (t — x) plane. The curves, i.e., characteristic lines, originating from the t-axis or the x-axis represent the (t — x) relation determined by integrating Eq. (6). The characteristic line passing through the origin divides the (t — x) plane into two regions: the upper left region, and the lower right region. In the upper left region the dependent variable, T, can be obtained by integrating Eq. (7) and by using the condition given by Eq. (3). Therefore, starting from a certain point on the t-axis, the values T can be determined for every point along the corresponding characteristic line. Similarly the values of T on the lower right region can be obtained by integrating Eq. (7) with the condition given by Eq. (2). Note that there exists a discontinuity in the values of T along the characteristic line passing the origin if $T_1(0) \neq T_o(0)$.

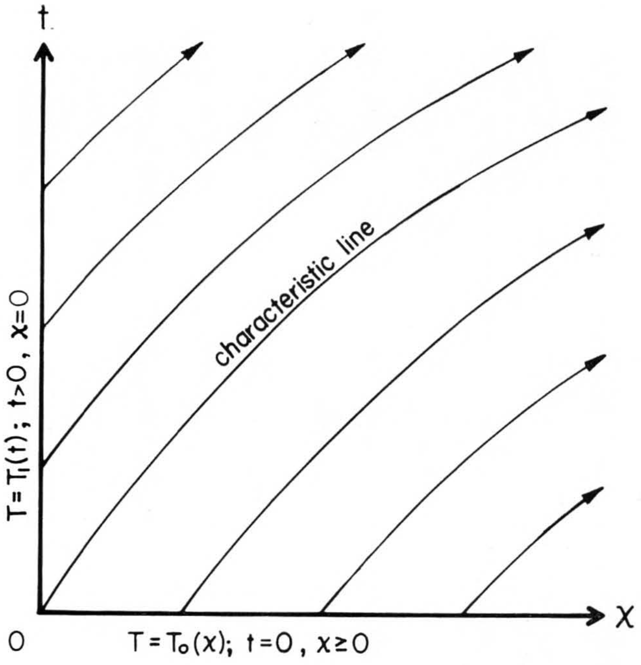

FIGURE 1. Representation of the characteristic lines in the (t—x) plane.

The characteristic lines shown in Fig. 1 are projections down from the three-dimensional space. They are plotted parallel to each other in this figure for clarity. In reality, the characteristic lines may not be so simple especially when A and B are strongly nonlinear functions of T, t, and x. They may become twisted as the value of T changes, and projections of them down from the three dimensional space to the (t — x) plane may lead to their crossing.

## EXAMPLES

TWO EXAMPLES ARE GIVEN here for illustration. Consider the linear partial differention equation

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = -kC \qquad (8)$$

subject to

$$C = 0 \text{ at } t = 0, x \geq 0 \qquad (9)$$

$$C = C_o \text{ at } t > 0, x = 0 \qquad (10)$$

Equation (8) represents the start-up of an isothermal plug flow reactor, with a first order chemical reaction. The reactor contains no reactant initially and is then fed with a reactant with a fixed concentration of $C_o$. In reality, performance equations of numerous processes such as ion exchange, gas adsorption and heat transfer which take place in a long tubular system can be

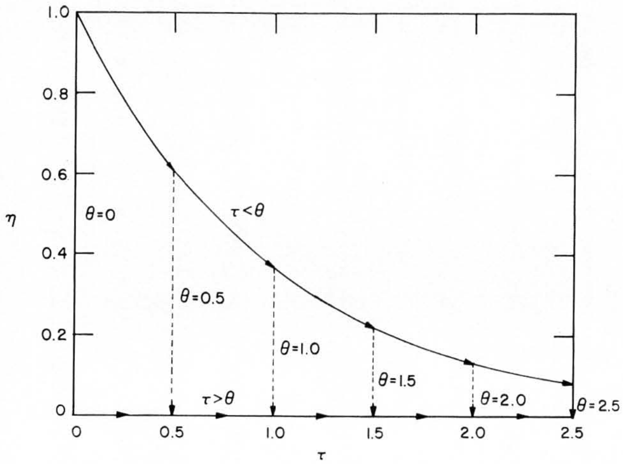

FIGURE 2. Concentration vs. distance for the first example.

transformed into the form represented by Eq. (8) by simple linear transformation.

For simplicity, the following dimensionless groups* are introduced:

$$\eta = \frac{C}{C_o}, \theta = kt, \tau = \frac{xk}{U}$$

Then Eqs. (8), (9) and (10) can be rewritten as

$$\frac{\partial \eta}{\partial \theta} + \frac{\partial \eta}{\partial \tau} = -\eta \tag{11}$$

subject to

$$\eta = 0 \text{ at } \theta = 0, \tau \geq 0 \tag{12}$$

$$\eta = 1 \text{ at } \theta > 0, \tau = 0 \tag{13}$$

According to Eq. (5), one can write

$$\frac{d\theta}{1} = \frac{d\tau}{1} = \frac{d\eta}{-\eta} \tag{14}$$

This expression can be rewritten into the following two parts;

$$\frac{d\tau}{d\theta} = 1 \text{ with } \theta \geq 0, \tau \geq 0 \tag{15}$$

and

$$\frac{d\eta}{d\tau} = -\eta \tag{16}$$

$$\eta = \frac{C}{C_o}, \theta = kt, l = \frac{x}{L}$$

with

$$\eta = 0 \text{ at } \theta = 0, \tau \geq 0 \tag{17}$$

$$\eta = 1 \text{ at } \theta > 0, \tau = 0 \tag{18}$$

Integration of Eqs. (15) and (16) yields, respectively,

$$\tau = \theta + \triangle\theta \tag{19}$$

$$\eta = Ae^{-\tau} \tag{20}$$

where $\triangle\theta$ and A are integration constants to be determined.

For the condition of $\theta = 0$ and $\tau \geq 0$ which appears in Eq. (17), Eq. (19) gives

$$\triangle\theta \geq 0$$

which implies that

$$\tau \geq \theta$$

because $\tau = \theta + \triangle\theta$. Therefore, the solution obtained by using the condition of Eq. (17) is applicable when $\tau \geq \theta$. Thus from Eq. (20), one obtains $A = 0$ and

$$\eta = 0, \tau \geq \theta \tag{21}$$

Similarly, for the condition of $\theta > 0$ and $\tau = 0$, which appears in Eq. (18), Eq. (19) gives

$$\triangle\theta < 0$$

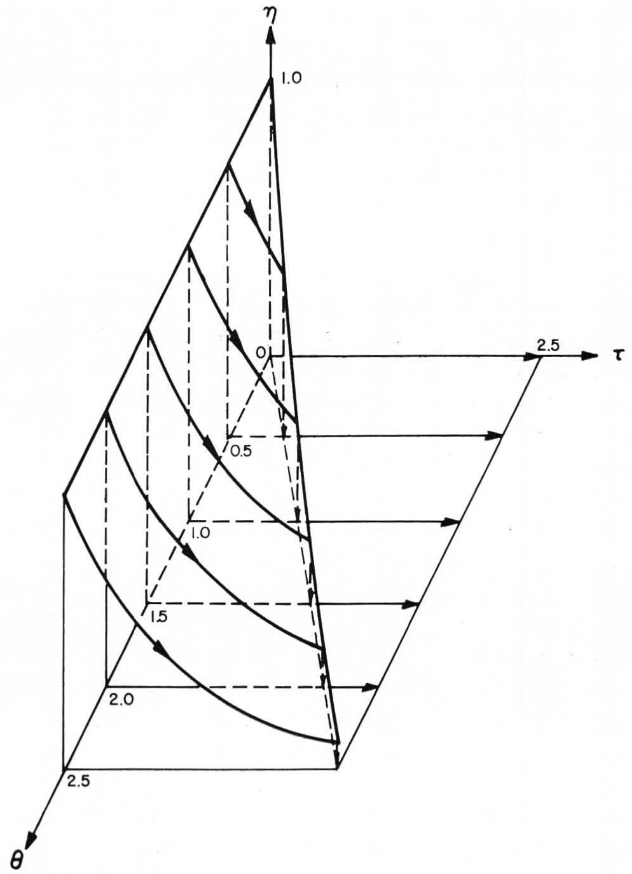

FIGURE 3. Three-dimensional concentration plot for the first example.

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*The dimensionless groups used here are not necessarily unique. For example, the following dimensionless groups can also be employed in many cases.

which is equivalent to

$$\tau < \theta$$

because $\tau = \theta + \Delta\theta$. Hence, the solution obtained by using the condition, Eq. (18), is valid in the region $\tau < \theta$. The solution obtained by applying Eq. (18) to Eq. (20) is

$$\eta = e^{-\tau}, \tau < \theta \tag{22}$$

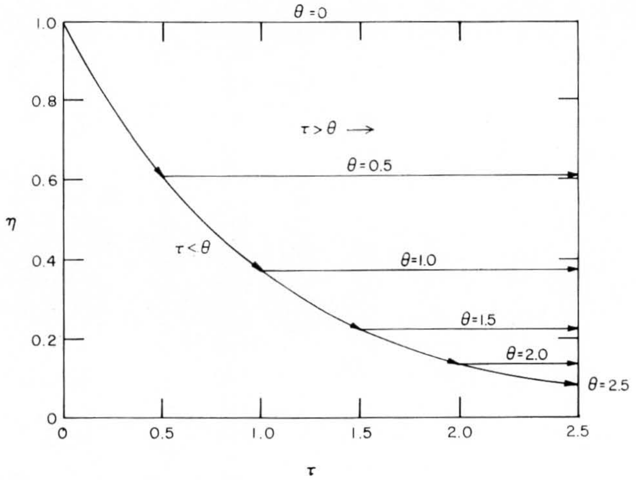

FIGURE 4. Concentration vs. distance for the second example.

Equations (21) and (22) constitute the complete solution of Eq. (11) subject to Eqs. (12) and (13).

Figures 2 and 3, respectively, show the two- and three-dimensional concentration distributions. It can be seen in Fig. 3 that there is a discontinuity in the concentration surface along the characteristic line passing the origin.

Consider a second example which is governed by the same partial differential equation, Eq. (11), but subject to the following conditions;

$$C = C_o \text{ at } t = 0, x \geq 0, \text{ or } \eta = 1 \text{ at } \theta = 0, \tau \geq 0 \tag{23}$$

$$C = C_o \text{ at } t > 0, x = 0, \text{ or } \eta = 1 \text{ at } \theta > 0, \tau = 0 \tag{24}$$

These conditions imply that the reactor is originally filled with a reactant having the concentration of the feed. Obviously, Eqs. (19) and (20) are still applicable.

From Eqs. (19), (20) and (23), one has

$$\tau \geq \theta$$

and

$$1 = A\, e^{-\Delta\theta} \tag{25}$$

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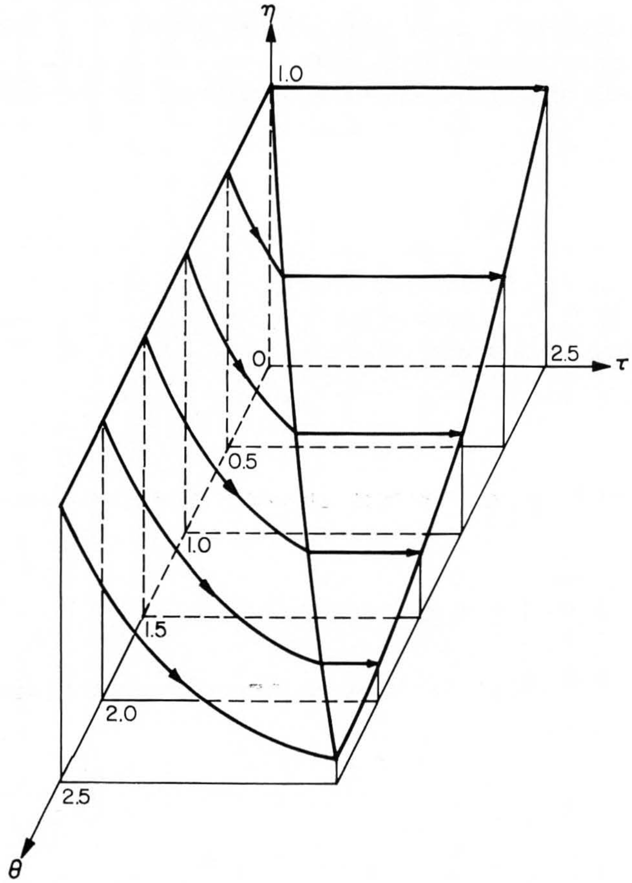

FIGURE 5. Three-dimensional concentration plot for the second example.

Elimination of A from Eqs. (20) and (25) leads to

$$\eta = e^{-(\tau - \Delta\theta)} = e^{-\theta}, \tau \geq \theta \quad (26)$$

Similarly, application of Eq. (24) to Eqs. (19) and (20) yields

$$\tau < \theta$$

and

$$1 = A\, e^{0} = A$$

Hence,

$$\eta = e^{-\tau}, \tau < \theta \quad (27)$$

The concentration distributions represented by Eqs. (26) and (27) are graphically shown in Figs. 4 and 5. In all the figures, the numerical values are given up to an arbitrary dimensionless time and length of 2.5.

### CONCLUDING REMARKS

IT CAN BE SEEN THAT for relatively simple linear systems, the solution procedure by means of the method of characteristics is straightforward, and the graphical interpretation of the numerical results can be very instructive. If the original first order partial differential equation is nonlinear, or if one has a set of simultaneous first order partial differential equations in hand, the analytical solution as illustrated by the two simple examples may become impossible, and more often than not, one must resort to numerical solution. Even under such a situation, numerical integration of the ordinary differential equations resulting from the application of the method of characteristics, i.e., Eqs. (6) and (7), may be more desirable than direct numerical solution of the original partial differential equation. There are two reasons for this. The first is that most of the undergraduates are sufficiently familiar only with the solution of ordinary differential operations. The second is that the numerical solutions of ordinary differential equations can always be made stable in contrast to those of partial differential equations. Many easily accessible packaged computer subroutines, e.g. CSMP, are available for the numerical solution of ordinary differential equations.

Those who are interested in the mathematical foundation and other applications of the method of characteristics should consult the references cited. □

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