Process Modelling

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Summary:

The general balance rate equation for an arbitrary physical process is discussed. Of primary importance is the physical meaning of the rate equation, its link to mathematics and how it can be used to estimate how a process variable evolves in time. The concepts in this chapter are simple but fundamentally important to developing a facility with modeling physically processes.

Table of Contents

List of Figures

1 Introduction

1.1 Overview

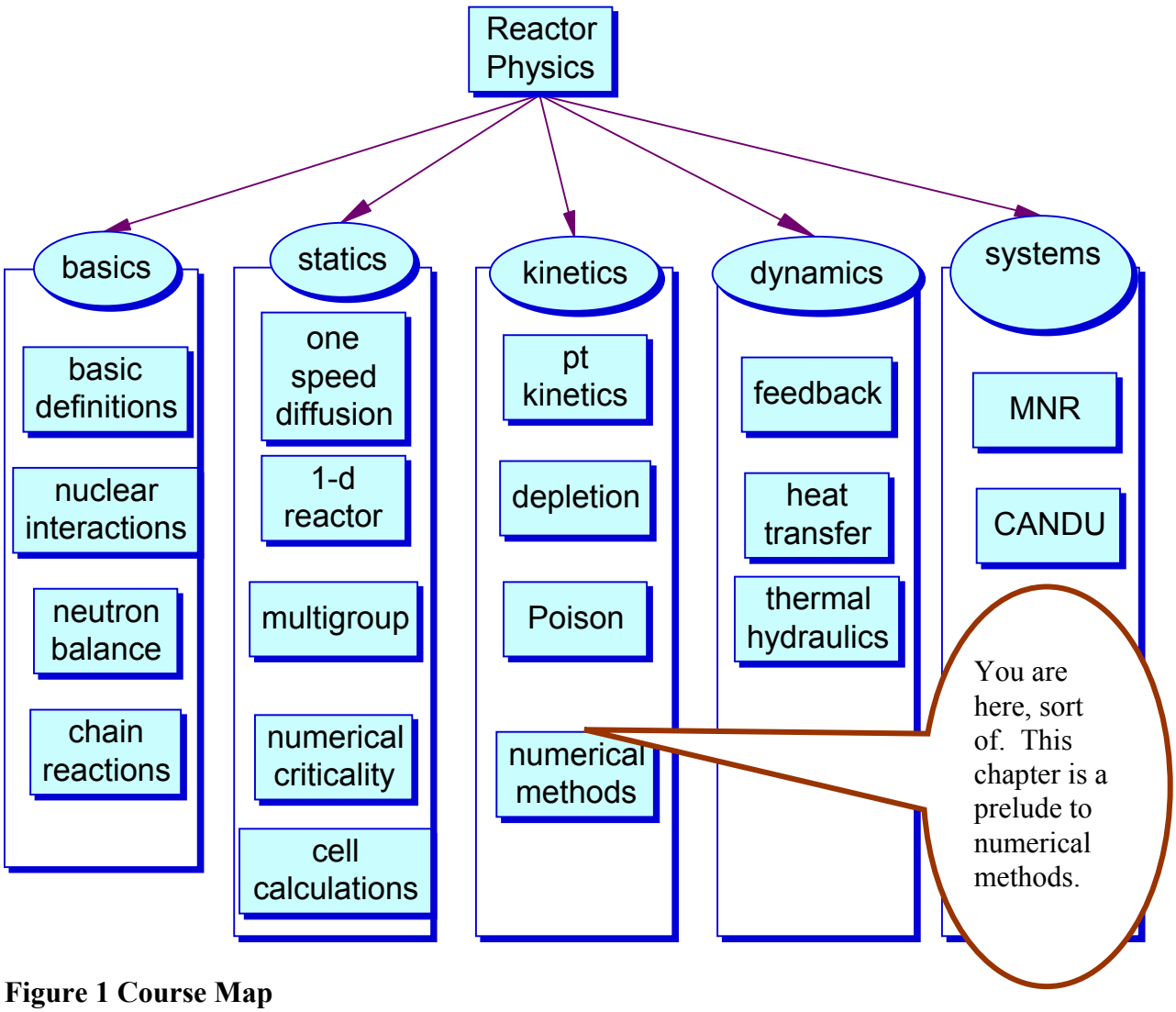

Figure 1 Course Map

- We will consider modeling a physical process.
- Itinerary:
  - Parameter values and slopes
  - Process rate equations

1.2 Learning Outcomes

The goal of this chapter is for the student to understand:

- The dynamic nature of physical processes
- How rate equations are used to give the evolution of process parameters over time (and space).
- How the rate equations can be altered to make the solution more effective without introducing excessive errors.

2 Estimating a parameter from its current value and its slope

Just about everything in life is a dynamic process, else it could hardly be called life! Things change; it's a fact of life. Even processes that appear static from the overall point of view are often dynamic on the local level. For instance, the steady flow in a river is, at the local level, a dynamic flow of water through an area. This can be also viewed as a flow into and out of an arbitrary volume. So in general, we consider a parameter, Y, which could represent, temperature, pressure, density (of molecules, neutrons, …), etc., which in general is a function of time, t. Over some time Δt, the property Y may change from Y(t) to Y(t+Δt). This change is denoted ΔY:

$$\Delta Y = Y(t+\Delta t) - Y(t) \tag{2.1}$$

We estimate the rate of change of Y to be:

$$\frac{\Delta Y}{\Delta t} = \frac{Y(t+\Delta t) - Y(t)}{\Delta t} \tag{2.2}$$

This is illustrated graphically in figure 2.

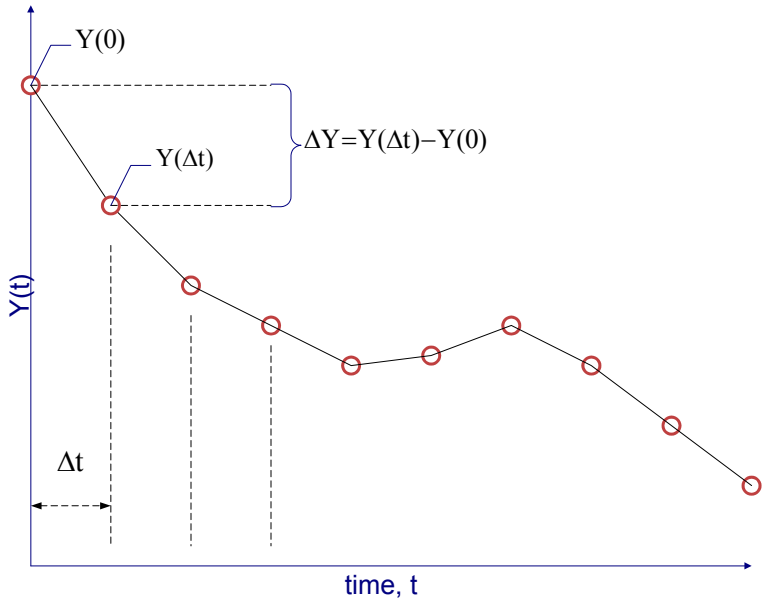

Figure 2 Y vs. t.

Of course, if Δt is small enough, we can consider the change to be infinitesimal, denoted dt. Thus

$$\left.\frac{\Delta Y}{\Delta t}\right|_{\lim \Delta t \to 0} \to \frac{dY}{dt} = \frac{Y(t+dt) - Y(t)}{dt} \tag{2.3}$$

On the assumption that we will take incrementally small time steps, dt, we can rewrite equation 2.3 to give the future value of Y(t+dt) in terms of the current value, Y(t), and the slope, dY/dt:

$$Y(t+dt) = Y(t) + \left(\frac{dY}{dt}\right) \cdot dt \tag{2.4}$$

You should recognize this as a truncated Taylor's Series:

$$Y(t+dt) = Y(t) + \left(\frac{dY}{dt}\right) \cdot dt + \frac{1}{2!}\left(\frac{d^2Y}{dt^2}\right) \cdot (dt)^2 + \ldots + \frac{1}{k!}\left(\frac{d^kY}{dt^k}\right) \cdot (dt)^k + \ldots \tag{2.5}$$

where the higher order terms can be dropped for sufficiently small dt. So what we need now is the slope, dY/dt.

3 Rate equations

In general, we can write that the rate of change of a variable is equal to the net sum of all the sink and source rates for that variable, ie:

$$\frac{dY}{dt} = \sum \text{sources} - \sum \text{sinks} \tag{3.1}$$

Basically, this is just a statement of the fact that the change in a variable in a volume over time is just the net of what goes in and what goes out. Here we have not explicitly stated what the sinks and sources are or what the specific dependencies of Y are. In general, Y is a function of space and time but there could be other independent variables as well. For example, in the case of neutrons, we often consider energy and angle as additional independent variables. For the sake of the current discussion, however, we will limit ourselves to a single independent variable, e.g. time, only.

Often, the sinks and sources are functions of Y and it is quite common for there to be systems of equations like equation 6 that are interdependent.

A simple example of a rate equation is that for radioactive decay:

$$\frac{dN(t)}{dt} = -\lambda N(t) \tag{3.2}$$

where N is the nuclide concentration and λ is the decay constant.

A more complicated example would be the case of a radioactive decay chain:

$$\frac{dN_A(t)}{dt} = -\lambda_A N_A(t)$$
$$\frac{dN_B(t)}{dt} = +\lambda_A N_A(t) - \lambda_B N_B(t) \qquad (3.3)$$
$$\frac{dN_C(t)}{dt} = +\lambda_B N_B(t) - \lambda_C N_C(t)$$

Another example is particle beam attenuation:

$$\frac{dI(x)}{dx} = -\Sigma(x)I(x) \qquad (3.4)$$

where I is the beam intensity, x is distance and Σ is the cross section, typically a function of x.

An example that involves space and time would be the one speed neutron balance equation:

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} \equiv \frac{1}{v}\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = S(\mathbf{r}, t) - \Sigma_a \phi(\mathbf{r}, t) - \nabla \bullet \mathbf{J}(\mathbf{r}, t) \qquad (3.5)$$

as defined in *Reactor Physics: Basic Definitions and Perspectives, Section 8*.

For the moment, though, only one point needs to be made clear:

- ***Whatever the details of the governing rate equations, they all look like equation 6 in general form. If we can estimate the values of the sinks and sources, we have directly an estimate of the rate of change of the variable in question. And from that estimate, we can update the value of Y at a future time.***

So the calculational procedure is quite straightforward (in principle):

- Estimate the sinks and sources
- Calculate dY/dt (equation 3.1)
- Calculate Y(t+dt) from equation 2.4 or 2.5.

What could be easier? Well, the devil is in the details, as they say. Typically, the equation sets that we obtain when we model a physical process can only be solved analytically for special, simple cases. We usually resort to a numerical process to generate the answers we are looking for. But no matter what technique we use to solve the problem at hand, it is important to keep the physical process model clearly in mind when you are mired in the mathematics. And that physical process is invariably a form of the rate equation, i.e. equation 6, which is nothing more than a statement of the fact that the change in a variable in a volume over time is just the net of what goes in and what goes out.

4 Steady state

A special case of the above that is encountered quite often is the steady state wherein dY/dt = 0. Because the steady state is such an important case, the model derivation is often developed from the steady state. Consequently, it is often difficult to see the rate form that is implicit in the

model. But it is there and the reader would be wise to seek it out even when it is not evident since solution schemes often present themselves when a steady state process is viewed as a transient process that comes to a steady state. An example of this is the solution to the steady state neutron diffusion equation, equation 3.5. As we shall see, the iterative solution to that equation is less intuitive than solving the transient form.

5 Stiff Systems

Systems of equations that have vastly different time constants (or eigenvalues, if you wish to be use a more mathematical term) are called stiff. They are stiff in the sense that the equations with the longer time constants will not change hardly at all (ie are stiff) in the time it takes the other, less stiff, equations to change drastically, perhaps by orders of magnitude. Obviously, if you want to capture the full solution details, you would need to use a small Δt to capture the rapidly changing variations of the equations with short time constants, and you would need to simulate for a long time (many iterations) to capture the slow change in the equations with the long time constants. The usual mathematical approach to mitigate this problem is to use an implicit numerical algorithm (see the chapter on *Numerical Methods*). This permits the use of large Δt's for stiff systems but it comes at the expense of having to invert matrices. Of course, any method that uses large Δt's will not see the fine detail in the time evolution of the equations with the short time constants, but if you are only interested in the long term behaviour, that is of no consequence. With the simple explicit approach, you are forced to calculate the fine structure, whether you want it or not!

5.1 Altering Reality

There is an alternative to taking a mathematical approach to mitigate the stiffness problem. Why not change the problem to be solved into one that is easier to handle? By way of an example, let's say that you need to solve the following two equations:

$$\frac{dy_1}{dt} = 10\left(-y_1 + y_2\right) \equiv \frac{y_2 - y_1}{\tau_1}, \text{ ie } \tau_1 \text{ is 0.1 sec}$$

$$\frac{dy_2}{dt} = -0.1y_2 \equiv -\frac{y_2}{\tau_2}, \text{ ie } \tau_2 \text{ is 10 sec}$$

Initial conditions: (5.1)

$$y_1(0) = 0$$

$$y_2(0) = 1$$

Variable y_2 has a time constant that is 100 times linger than y_1 so you would expect y_1 to change much more rapidly than y_2. Solving this system numerically with a $\Delta t = 0.01$ sec gives a solution as shown in figure 3.

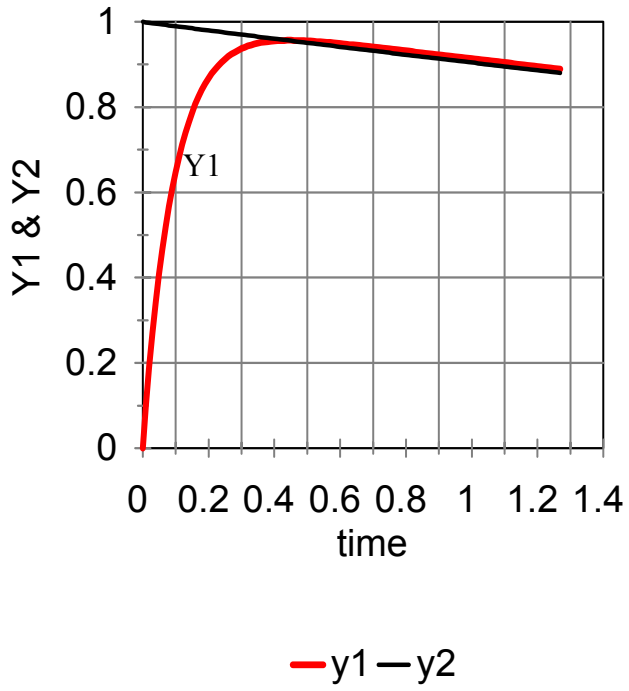

Figure 3 Stiff system example.

Notice how y_1, with its shorter time constant, rapidly evolves while y_2, with its longer time constant, evolves much more slowly. In this simple example, y_2 is simply decaying away and is a source for y_1. Variable y_1 goes in quickly and settles down to a pseudo steady state, ie a state that is in equilibrium with its environment but is not quite steady because its boundary conditions are changing. In this case y_2 represents a boundary or external influence on y_1.

The fast moving y_1 forces us to take small Δt's. But if we are only interested in the long term behaviour, ie, are not interested in the initial "growing in" period, we can safely adjust τ_1 to something closer to τ_2 without affecting the long term solution. This is true because, once y_1 has "grown in",

$$\frac{dy_1}{dt} \approx 0 = 10\left(-y_1 + y_2\right) \Rightarrow y_1 \approx y_2 \tag{5.2}$$

so the value of τ_1 is not in the long term solution to y_1, leaving us free to "fudge" the problem definition to make it more amenable to solution. Prudence dictates that we adjust τ_1 to be $\tau_2/10$ so that it y_1 is still significantly faster than y_2 but not so fast as to force us to use a Δt that is much smaller than the Δt needed to get a reasonable solution to y_2.

A physical example, to set the idea firmly, would be that of placing a solid object in your outstretched hand, palm up, and then raising your hand. The differential equation for the object's motion would involve a force balance in which your hand is providing the boundary condition. The object's motion will be identical to that of your hand, except for the detailed

motion involving the compression of your skin. If we were not interested in this detailed motion, then we could safely use a crude model for the compression (say with a time constant just faster than the time constant of the overall motion) or ignore the compression altogether (equivalent to setting $y_1=y_2$ in the above).

No, it is not mathematically elegant; but elegance can take on many forms and, to an engineer, this has a touch of elegance since it gives an acceptably good solution at very low cost, numerically. We'll use this notion to efficiently and effectively solve the neutron diffusion equations developed in other chapters.

5.2 The Fudge Factor Approach Applied to Systems

Consider a systems of coupled equations with different time constants, such as:

$$\frac{d\underline{Y}}{dt} = \underline{\underline{A}}\,\underline{Y} + \underline{B} \tag{5.3}$$

where, for a 3x3 system:

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \tag{5.4}$$

where, perhaps

$$\begin{aligned} y_1 &= \phi_1 \\ y_2 &= \phi_2 \\ y_1 &= C \Leftarrow \text{precursor concentration} \end{aligned} \tag{5.5}$$

or

$$\begin{aligned} y_1 &= \phi_1 \\ y_2 &= \phi_2 \\ y_1 &= N \Leftarrow \text{fuel concentration} \end{aligned} \tag{5.6}$$

The coefficients a_{ij} determine the rates of change of y_i. For the flux, the a_{ij} contain velocity factors; for C, the a_{ij} terms contain λ's, etc.

Note that it is the dy/dt on the L.H.S. that contains the reference to the time scale within the dt portion of the term. It is here that we can stretch and shrink the time scale, if we so desire, to slow down a fast transient or speed up a slow one. Note that the steady state, ie, when the rate terms on the L.H.S. $\rightarrow 0$, ie:

$$0 = \underline{\underline{A}}\,\underline{Y} + \underline{B} \tag{5.7}$$

would not be altered if fudge factors were introduced into the L.H.S. of equation 5.3 as follows:

$$\underline{\underline{F}}\,\frac{d\underline{Y}}{dt} = \underline{\underline{A}}\,\underline{Y} + \underline{B} \tag{5.8}$$

or

$$\begin{bmatrix} F_1 & 0 & 0 \\ 0 & F_2 & 0 \\ 0 & 0 & F_3 \end{bmatrix} \begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \tag{5.9}$$

The F factors are our time scale adjustment factors.

A specific example might be the one speed, one dimensional, homogeneous, transient neutron diffusion equation in finite difference form:

$$\frac{F}{v}\frac{\left(\phi_p^{\,t+\Delta t} - \phi_p^{\,t}\right)}{\Delta t} = \frac{D}{\Delta^2}\phi_w - \frac{2D}{\Delta^2}\phi_p + \frac{D}{\Delta^2}\phi_E - \Sigma_a \phi_p + S_p \tag{5.10}$$

where $v\Delta t$ has been replaced by $v\Delta t/F$. In terms of the unknown flux using the semi-implicit algorithm:

$$\phi_p^{\,t+\Delta t} = \frac{\phi_p^{\,t} + \frac{v\Delta t}{F}\left[\frac{D}{\Delta^2}\phi_w^{\,t+\Delta t} + \frac{D}{\Delta^2}\phi_E^{\,t} + S_p\right]}{\left[1 + \frac{v\Delta t}{F}\left(\frac{2D}{\Delta^2} + \Sigma_a\right)\right]} \tag{5.11}$$

If we were to choose F = v, this would be equivalent to setting v = 1, ie, we would be making things change more slowly. Effectively, dy/dt is reduced by a factor F, making it less "twitchy". This is okay if you don't want to track the details of dy/dt and you just want the steady state, or pseudo steady state solution.

So if you were solving the multigroup equations, you'd have:

$$\begin{bmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{d\phi_3}{dt} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \tag{5.12}$$

For a slightly sub-critical reactor, ϕ_1, representing the fast neutrons, would decay quickly until it was in balance with its source, which is the thermal fission ($\alpha\ \phi_3$). Since ϕ_3 is moving much more slowly, you'd waste a lot of CPU grinding along at a Δt such that

$$v_1\Delta t\left(\frac{2D_1}{\Delta^2} + \Sigma_{a1}\right) \le 0.1 \text{ (to stay stable)} \tag{5.13}$$

If you set $v_1 = v_2 \simeq 10v_3$, you'd get just as accurate decay profile once you got past the initial adjustment. So set

$$F_1 = \frac{v_1}{v_3} \cdot \frac{1}{10} \Rightarrow v_1 = 10 v_3$$
$$F_2 = \frac{v_2}{v_3} \cdot \frac{1}{10} \Rightarrow v_2 = 10 v_3 \qquad (5.14)$$
$$F_3 = 1 \qquad \Rightarrow v_3 = v_3$$

Use the same reasoning when you are dealing with the precursor equations, fuel depletion, or, indeed, any stiff system.

Using equation 5.3 as a specific example, we have a fast and thermal flux and delayed precursors that are far slower:

$$\begin{bmatrix} F_1 & 0 & 0 \\ 0 & F_2 & 0 \\ 0 & 0 & F_3 \end{bmatrix} \begin{bmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{dC}{dt} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ C \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \qquad (5.15)$$

Let's say that we are interested in the precursor transient. Set $F_3 = 1$ for that equation since you want accuracy in time. Set the time step size, Δt, for stability and accuracy, such that, say

$$\Delta t(\cdots) \le 0.01 \text{ for the precursor equation.} \qquad (5.16)$$

Set F_1 and F_2 as follows:

$$F_1 = \frac{1}{10} \cdot \frac{a_{11}}{a_{33}}$$
$$F_2 = \frac{1}{10} \cdot \frac{a_{22}}{a_{33}} \qquad (5.17)$$

so that the flux equations will be moving much slower than is the true physical case but about 10 times faster than the precursor equation. This should be fast enough that the fluxes are in pseudo steady state and are presenting themselves appropriately to the precursor equation. In each particular case, you should experiment with various F factors because the off diagonal terms and non-linearities may have a large effect on system dynamics.

If there were other equations in the system that were even slower moving that the precursor equations (fuel depletion, for example), then you can leave those equations alone (ie, set their F's = 1) or even just use their steady state solution since they will not be changing significantly in the time that the precursors are changing. You might recalculate the slower equations on an infrequent basis, say every 100 Δt steps or so, depending on the speed of those slow equations and the cost of recalculation.

Use your engineering judgment. You will be amazed at how effective a simply written code using only straight forward rate equations can be for solving a wide range of problems in an effective manner.

6 Final words

The above probably is self evident to you and not particularly profound. What is surprising, though, is how infrequently common sense is uttered. The above may be simple. But it is no less essential and fundamental for all that.

7 Exercises

7.1 Simple decay question

Consider the process of equation 3.2. Solve for N(t) analytically given N(0). Write a pseudo-code for solving equation 7 numerically.

7.2 Decay chain question

Consider the process of equation 3.3. The analytical solution is messy but if we can assume that process has reached a pseudo-steady state, the solution is easy. What is it? Also, write a pseudo-code for solving equation 8 numerically.

7.3 Simple attenuation question

Consider the process of equation 3.4. Solve for I(x) analytically given I(0), stating clearly what simplification must be made to do so. Write a pseudo-code for solving equation 9 numerically.

About this document:

back to page 1

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