# Nonideal Reactor Design using POLYMATH

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The latest version of POLYMATH is now available from the CACHE office. An order form is attached to this article. All users who have a continuing site license should have received this latest version. Please contact the CACHE office if you have not. There is also a special offer of a POLYMATH trial period for four months for an academic department before a site license needs to be purchased. Details are also at the end of this article.

A number of improved and enhanced feature are now provided. Polymath programs now include capabilities for

1. Simultaneous Ordinary Differential Equations
2. Simultaneous Nonlinear Equations
3. Simultaneous Linear Equations
4. Polynomial, Linear and Nonlinear Regressions

with the separate Linear Equation Solver being a new program.

## Number of Equations/Lines per Equation

Most experience users will appreciate that the **number of equations** has been increase to 31 and up to three **lines per equation** are now allowed in the first three of the POLYMATH programs. These capabilities will allow much more complicated problems to be solved.

## Logical Variables

An important new capability is the unlimited use of **logical variables** in the differential and nonlinear equations programs. This allows an IF, THEN, ELSE logic to specify changes in any of the program variables. A variety of operators can be used including >, <, >=, <=, == (equals), <> (does not equal), | (or), and & (and). Since nesting is allowed with logical variables, a great deal of flexibility is afforded by this functionality. This is discussed with a simple example later in this article.

## Intrinsic Functions (Consistency with Calculator)

A number of intrinsic functions have been added, and there is now consistency between the POLYMATH calculator and all of the POLYMATH programs. Now included are most of the trigonometric functions and their inverses, the hyperbolic functions and their inverses, plus more useful functions. These are discussed in the README.TXT file with the POLYMATH software, in the help sections, and in the manual.

## Improved Numerical Algorithms

The Differential Equations Solver now has improved integration algorithms. For nonstiff problems, the Runge-Kutta-Fehlberg (RKF) algorithm, with error estimation and step-size control, is used. There is no lower limit on the step size (other than machine

precision). The program will decrease the step size in order to achieve a relative and absolute error or $10^{-10}$ if possible. If the accuracy become less than $10^{-4}$, then the user can choose a "semi-implicit midpoint rule" which is an algorithm for stiff problems.

**Expanded Statistical Output for Regressions**

More statistical information is now provided in the various regressions involving polynomials, multiple linear functions and general nonlinear functions. This includes the matrix of correlation coefficients, the 95% confidence intervals for all parameters, and the overall variance. This can be quite useful in deciding which model should be retained and used to correlate data.

**Improved Graphical Output and Support for Printers, Plotters and Graphics Files**

Most of the graphical results can be edited to change the scales of the x and y axes, to label the x and y axes, and to title the graph. Normal printing is to a variety of some 30 standard printers and six plotters. Advanced printing options provide a variety of standard graphical file types for incorporation into documents.

**Example of Logical Variable Use - Non Ideal Reactor Design Using Residence Time Distribution Functions**

Non ideal reactor design for segregated flow involves the solution of

$$\bar{C}_A = \int_0^\infty E(t)C_A(t)dt \qquad (1)$$

where $E(t)$ is the residence time distribution function (RTD) and $C_A(t)$ is the

concentration from a batch reactor at time t. $\bar{C}_A$ is the calculated outlet concentration.

The above integral equation can be written in differential equation form as

$$\frac{d\bar{C}_A}{dt} = E(t)C_A(t) \qquad \text{I. C.} = 0 \text{ at } t = 0 \qquad (2)$$

for evaluation by POLYMATH when the $E(t)$ function is known. Integration is carried

out to large values of t where the resulting outlet concentration $\bar{C}_A$ no longer changes with time.

For a laminar flow reactor the RTD is given by $E(t) = \dfrac{\tau}{2t^3}$ when $t \geq \dfrac{\tau}{2}$ else it is

zero. Here $\tau$ (tau) is the mean residence time of the reactor given by $V/v_0$. The RTD function for laminar flow can be entered using the POLYMATH if, then, or else logical variable statement.

EoftLAMINAR = if (t) >= tau/2.) then (tau^2/(2.*t^3) else (0.0)

Let us consider a second order, irreversible, liquid phase reaction occurring within the laminar flow reactor using the RTD function. This can easily be handled in

POLYMATH by numerically solving the differential equation for the batch reactor given by

$$\frac{dC_A}{dt} = -kC_A{}^2 \qquad \text{I. C.} \quad C_A = 1.0 \text{ at } t = 0 \qquad (3)$$

during the during the simultaneous integration of the RTD differential equation (2) for $\overline{C}_A$. The initial condition (I. C.) on $C_A$ is considered to be 1.0

The POLYMATH equations for the case where $k = 0.2$ and tau=5.0 are shown below in Figure 1 as they appear on the screen prior to solution.

```
          RTD Treatment for a 2nd Order Reaction in a Laminar Flow Reactor
 Equations                                                        Initial values

   d(CABATCH)/d(t)=-k*CABATCH^2                                          1
   d(CALAMINAR)/d(t)=EoftLAMINAR*CABATCH                                 0
   k=.2
   tau=5.
   EoftLAMINAR=if(t)=tau/2.)then(tau^2/(2.*t^3))else(0.0)
→ t₀ = 0,     t_f = 30
```

Figure 1 - Polymath Code for Laminar Flow Reactor

The scaled and titled POLYMATH plot for the laminar flow reactor is shown in Figure 2. Note that the calculated concentration is approaching a constant value at $t = 30$.
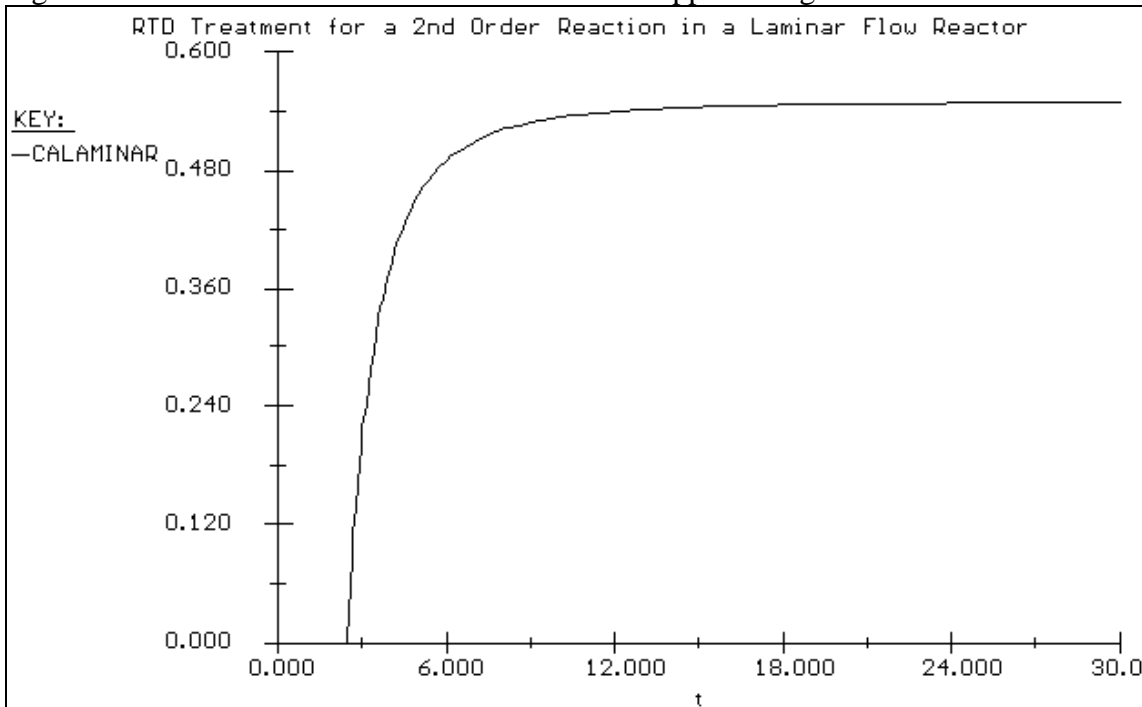


Figure 2 - Graphical Output of the Conversion for Laminar Flow Reactor

The RTD curve for the laminar flow reactor can also be plotted after the numerical solution has been obtained. This is shown in Figure 3 which nicely shows the breakthrough of the RTD curve at one half of the mean residence time where tau = 2.5.
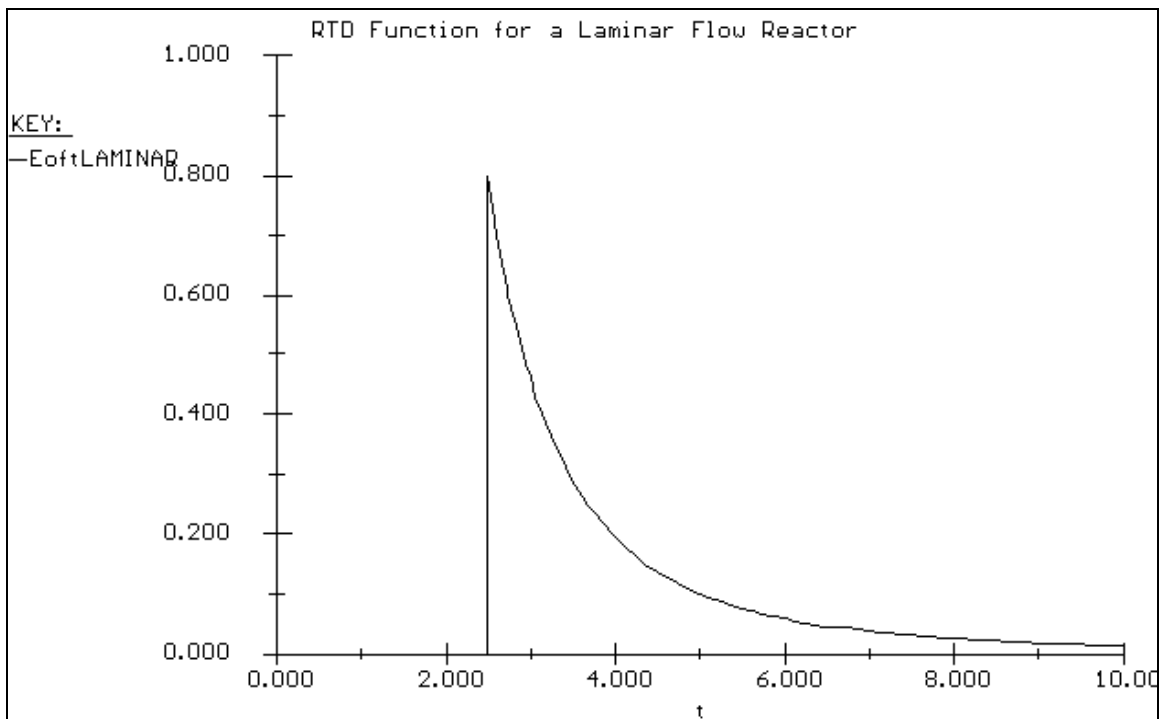
Figure 3 - RTD for Laminar Flow Reactor

This simple example shows the usefulness of the logical variable capability with POLYMATH. This problem involving segregated flow modeling can easily be expanded to include the RTD functions for various ideal reactors and experimental RTD's for real reactors as polynomial expressions. This is treated in the next section of this article.

**How to Compare Simulations Easily within POLYMATH**

The previous example can be extended to other reactors when the RTD functions are known or can be measured. Some of the commonly used ideal reactor RTD for the plug flow, CSTR and series of N CSTR's are given below:

EoftPLUG=if((t)=.99*tau)&(t<1.01*tau))then(1./(tau*2.*(1-.99)))else(0.0)
        where this function approaches a dirac delta function at tau = 1.

EoftCSTR=exp(-t/tau)/tau

EoftNCSTR=(t^(N-1)/tau^N/(N-1)!*exp(-t*N/tau)
        where N is number of CSTR's in series

The POLYMATH entry for all of the discussed RTD functions is shown in Figure 4 for the case where k = 0.2, tau = 5.0 and N = 10 to a time of t = 30.0.

```
        RTD 2nd Order Reaction for Plug Flow, CSTR, N-CSTR, Laminar Flow
 Equations                                                    Initial values

  d(CAPLUG)/d(t)=EoftPLUG*CABATCH                                  0
  d(CABATCH)/d(t)=-k*CABATCH^2                                     1
  d(CALAMINAR)/d(t)=EoftLAMINAR*CABATCH                            0
  d(CACSTR)/d(t)=EoftCSTR*CABATCH                                  0
  d(CANCSTR)/d(t)=EoftNCSTR*CABATCH                                0
  k=.2
  tau=5.
  N=10
  EoftPLUG=if((t>=.99*tau)&(t<1.01*tau))then(1./(tau*2.*(1.-.99)))else
     (0.0)
  EoftLAMINAR=if(t>=tau/2.)then(tau^2/(2.*t^3))else(0.0)
  EoftCSTR=exp(-t/tau)/tau
  EoftNCSTR=(t^(N-1)/tau^N)*N^N/(N-1)!*exp(-t*N/tau)
→ t_0 = 0,    t_f = 30
```

Figure 4 - RTD Treatment for Various Ideal Reactors with Second Order Reaction

The Partial Results Table from the POLYMATH solution shown in Figure 5 gives general information on various problem variables before the user is prompted for various plots or tabular output.

```
RTD 2nd Order Reaction for Plug Flow, CSTR, N-CSTR, Laminar Flow
Variable          Initial value      Maximum value       Minimum value       Final value
t                 0                  30                  0                   30
CAPLUG            0                  0.500004            0                   0.500004
CABATCH           1                  1                   0.142857            0.142857
CALAMINAR         0                  0.54862             0                   0.54862
CACSTR            0                  0.596033            0                   0.596033
CANCSTR           0                  0.512182            0                   0.512182
k                 0.2                0.2                 0.2                 0.2
tau               5                  5                   5                   5
N                 10                 10                  10                  10
EoftPLUG          0                  10                  0                   0
EoftLAMINAR       0                  0.8                 0                   0.000462963
EoftCSTR          0.2                0.2                 0.00049575          0.00049575
EoftNCSTR         0                  0.263511            0                   4.86362e-16
```

Figure 5 - Partial Results Table Generated by POLYMATH

The graphical results of all four reactors are presented in Figure 6 as generated directly by POLYMATH. Note that the solution does not change for times greater than 30 where the solution for each of the various reactors is asymptotically approached. Thus summarized values of the predicted outlet concentrations given in Figure 5 are reasonable. Of course, the integration could be continued to larger time to confirm this. As expected, the calculated concentrations decrease according to the reactor types - CSTR, Laminar Flow, N-CSTR, and Plug Flow. The conversion increase according to the same order. Note that the N-CSTR with $N = 10$ approaches that of the Plug Flow reactor. This could also be calculated with larger values of N by rerunning the POLYMATH program.
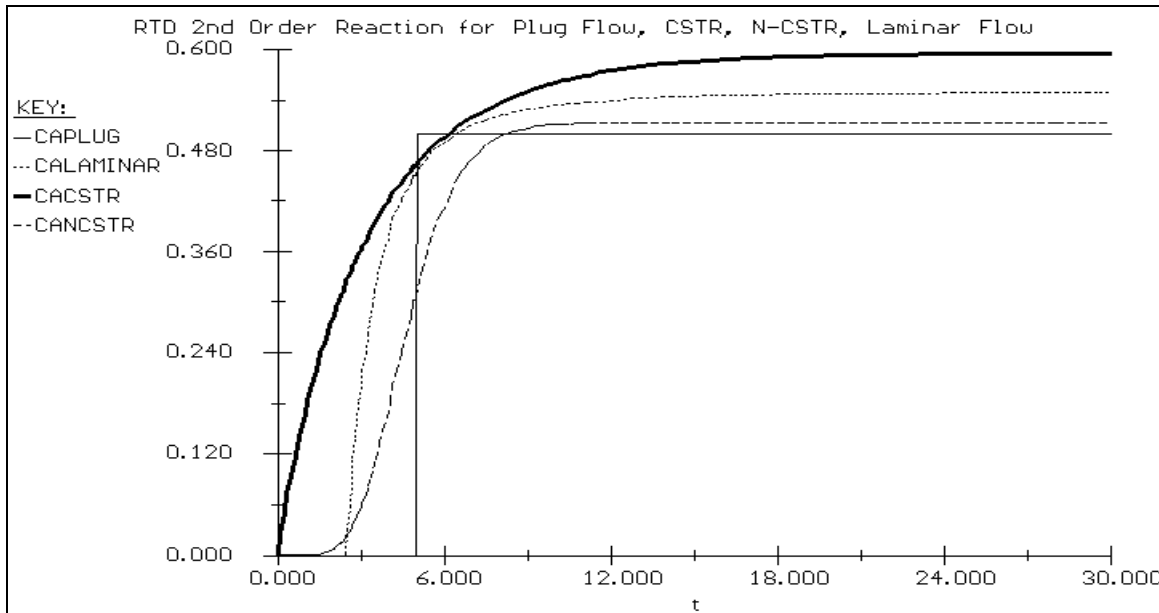
Figure 6 - RTD Solution for Average Concentrations Exiting Various Ideal Reactors

The RTD curves for the various reactors can also be plotted at the request of the user. These are shown in Figure 7 where the characteristics of the various reactors can easily be compared.
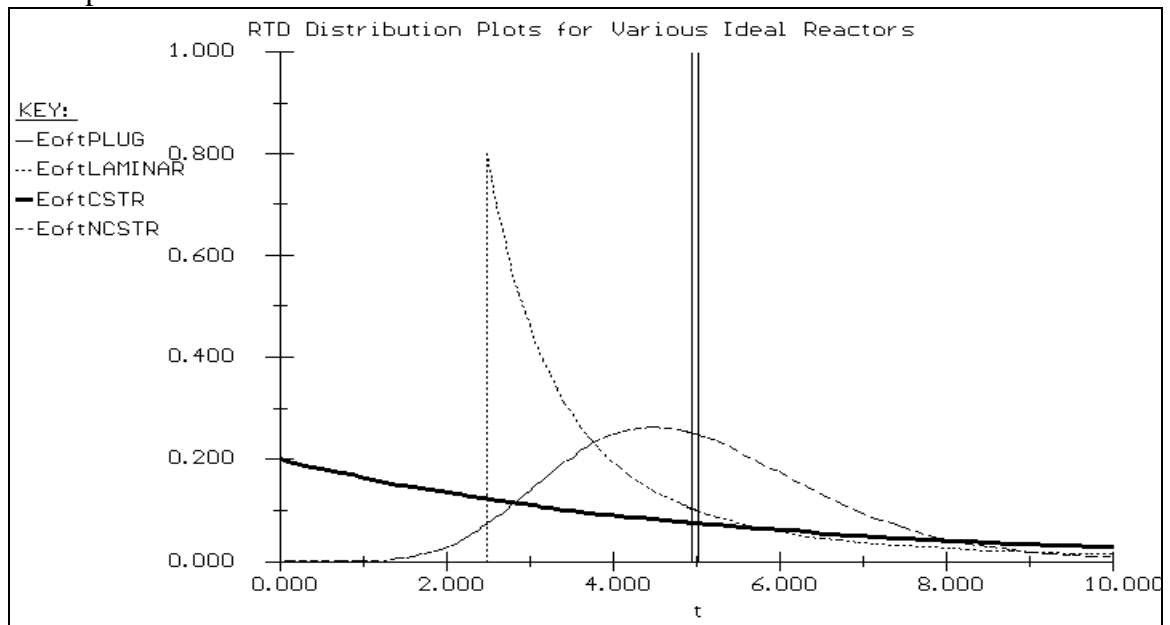


Figure 7 - RTD Functions for Various Ideal Reactors

In summary, the new version 4.0 of POLYMATH has new capabilities that greatly enhance the usefulness of the software. Student users find the software particularly easy to learn to use. There is no risk in evaluating this software. The inexpensive site license allows unlimited copying of the software for educational use by students, faculty and staff. and its use in Chemical Engineering.