



RTD Studies in Plug Flow Reactor and its Simulation with Comparing Non Ideal Reactors

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Abstract

This paper proposes RTD studies in plug flow reactor and comparison of non-ideal reactors using residence time distribution function. The model also gives a prediction of the number of ideal continuous stirred tank reactors (CSTR) that could represent the non-ideal plug flow reactor (PFR) in question. Simulated results reveal that 10 numbers of ideal stirred tanks in series would represent the non-ideal plug flow reactor under study. The graphical result of all four reactors is generated directly by polymath.

Most of the chemical reactors in the industries have non-ideal regime. The non-ideal plug flow reactor (PFR) is one whose attributes deviate from that of the ideal plug flow reactors. Therefore, an in-depth knowledge of the residence time distribution (RTD) of components in the reactor is necessary for its analysis. The residence time distribution indicates how much time each fraction of a charged material spends in the vessel. The residence time distribution of reactants or tracers in a flow vessel is a key datum for determining reactor performance.

Key words: Plug flow reactor, nCSTR, polymath, simulation, RTD.

Introduction

The knowledge of RTD is directly useful in vessel design, improvement in performance and for the first order kinetics conversion calculations. Detailed knowledge of residence time distribution with the understanding of the overall flow pattern helps in development of a model of the system and this model can be used for the handling complicated kinetics. The choice of RTD characterizing parameters is often a matter of balancing complicity against the required degree of precision. In this regards, mixed model approach has gained importance in RTD understanding. According to this concept, a real reactor is considered as consisting of various flow regimes with known resistance time distribution (such as plug flow regions, perfectly mixed regions) and various types of flow.

To apply general equations for the RTD function of a complex system to the real system of volume V and overall flow rate Q , it is necessary to break V and Q into parts corresponding to regions of various kinds and to change their relative sizes until the calculated RTD function is the same as the real one. It is necessary to develop a simple model which fits reasonably well with the real RTD function and at same time is close to a physical flow situation anticipated from the geometry of the system and overall flow pattern in it.

Residence Time Distribution (RTD): The performance of reactor depends upon the residence time of material in the reactor. In case of plug flow reactor, the fluid or material

flow in an orderly manner and all the materials remains for equal time in the reactor. In batch reactor also all the fluid remains for equal time in the reactor. This time spent by the fluid in the reactor is called the residence time. Residence time distribution in a reactor is a characteristic of mixing that occurs in the chemical reactor. The RTD characteristics of plug flow reactor and CSTR are quite different because in PFR there is no axial mixing while in CSTR the content are uniformly mixed. RTD offers a clue to the type of mixing occurring in the reactor.

Need of RTD Studies and Modeling the Reactor: The time the atoms have spent in the reactor is called the residence time of the atom in the reactor. The residence time distribution (RTD) of a reactor is a characteristic of the mixing that occurs in the reactor. There is no axial mixing in plug flow reactor and this omission is reflected in the RTD that is exhibited by this class of reactors. The CSTR is thoroughly mixed and process a far different kind of RTD than the plug flow reactor. The RTD exhibited by a given reactor yields distinctive clues to the type of mixing occurring within it and one of the most informative characterization of the reactor.

There are many situations where the fluid in the reactor is neither well mixed nor approximately plug flow. Hence a reactor is modeled in a number of ways. The RTD tells us how long the various fluid elements have been in the reactor, but it does not specify the exchange of matter between the fluid elements. The mixing of reacting species is one of the

major factors controlling the behavior of chemical reactors. For the first order reactions knowledge of the length of time each molecule spends in the reactor is all needed to predict conversion.

Consequently mixing with the surrounding molecules is not important. Therefore once the RTD is determined we can predict the conversion that will be achieved in the real reactor provided that the specific reaction rate for the first order reaction is known. For reactions other than first order knowledge of RTD is not sufficient to predict conversion. In these cases the degree of mixing of molecules must be known in addition to how long each molecule spends in the reactor. Hence models are developed that account for the mixing of molecules inside the reactor.

Application of RTD Functions to the Prediction of Reactor Conversion: The application of the RTD to the prediction of reactor behavior is based on the assumption that each fluid element (assume constant density) behaves as a batch reactor, and that the total reactor conversion is then the average conversion of all the fluid elements. That is to say,

$$\left[\begin{array}{c} \text{mean conc. of} \\ \text{reactant in} \\ \text{reactor outlet} \end{array} \right] = \Sigma \left[\begin{array}{c} \text{conc. of reactant remaining} \\ \text{in a fluid element of age} \\ \text{between } t \text{ and } t + dt \end{array} \right] \left[\begin{array}{c} \text{fraction of exit stream} \\ \text{that consist of fluid} \\ \text{element of age between} \\ t \text{ and } t + dt \end{array} \right] \quad (1)$$

Where the summation is over all fluid elements in the reactor exit stream. This equation can be written analytically as,

$$C_A = \int_0^{\infty} C_A(\bar{t})E(\bar{t})d\bar{t} \quad (2)$$

Where $C_A(\bar{t})$ depends on the residence time of the element and is obtained from,

$$\frac{dC_A}{dt} = -v_A r(C_A) \quad \text{with, } C_A(0) = C_A^0 \quad (3)$$

For first order reaction

$$\frac{dC_A}{dt} = -kC_A \quad (4)$$

$$C_A = C_A^0 \exp(-kt) \quad (5)$$

Insertion of equation (5) in to equation (2) gives,

$$\langle C_A \rangle = \int_0^{\infty} C_A^0 \exp(-kt)E(\bar{t})d\bar{t} \quad (6)$$

Take for example the ideal CSTR. If the $E(t)$ -curve for the ideal CSTR is used in equation (6) the result is,

$$\langle C_A \rangle = \frac{C_A^0}{\tau} \int_0^{\infty} \exp(-k\bar{t}) \exp(-\bar{t}/\tau) d\bar{t} \quad (7)$$

$$\frac{\langle C_A \rangle}{C_A^0} = \frac{1}{\tau} \int_0^{\infty} \exp\left[-\left(k + \frac{1}{\tau}\right)\bar{t}\right] d\bar{t} \quad (8)$$

That gives after integration,

$$\frac{\langle C_A \rangle}{C_A^0} = \frac{1}{\tau} \left[-\left(\frac{1}{k + \frac{1}{\tau}}\right) \exp\left[-\left(k + \frac{1}{\tau}\right)t\right] \right]_0^{\infty} = \frac{1}{k\tau + 1} \quad (9)$$

Notice that the result shown in equation (9) is precisely that obtained from the material balance for an ideal CSTR accomplishing a first order reaction that is,

$$vC_A^0 = vC_A + V k C_A \quad (10)$$

$$\frac{C_A}{C_A^0} = \frac{1}{k\tau + 1} \quad (11)$$

Unfortunately, if the reaction rate is not first order, the RTD cannot be used so directly to obtain the conversion.

Importance of RTD: Residence time distribution has gained importance due to widespread acceptance of continuous process in chemical manufacture and processing. In order to understand the concept of residence time distribution, it is necessary to distinguish between “Macromixing” and “Micromixing” phenomena. RTD studies are quite useful for the understanding of “macromixing”. The reason is it is, difficult to exact the position of fluid elements during their residence in the system and it can't be extracted from residence time distribution function.

The knowledge of RTD is directly useful in vessel design, improvement in performance and for the first order kinetics conversion calculations. Detailed knowledge of residence time distribution with the understanding of the overall flow pattern helps in development of a model of the system and this model can be used for the handling complicated kinetics. The choice of RTD characterizing parameters is often a matter of balancing complicity against the required degree of precision. In this regards, mixed model approach has gained importance in RTD understanding. According to this concept, a real reactor is considered as consisting of various flow regimes with known resistance time distribution (such as plug flow regions, perfectly mixed regions) and various types of flow.

Scope of RTD for: Design of non-ideal reactors, Identify the possible deviations, Measurement of RTD, Quality of mixing, Models for mixing, Calculating the exit conversion in practical reactors

Reactor Modeling with the RTD: There are many situations where the fluid in the reactor is neither well mixed nor approximate plug flow. Hence reactor is modeled in a number of ways. In this report each model according to the number of adjustable parameters has been explained.

Models for predicting conversion from RTD data: (i) Zero adjustable parameter (a) Segregation model (b) Maximum mixedness model. (ii) One adjustable parameter (a) Tank in series model (b) Dispersion model. (iii) Two adjustable parameter (a) Real reactor modeled as combination of ideal reactor

The RTD tells us how long the various fluid elements have been in the reactor, but it does not specify the exchange of matter between the fluid elements. The mixing of reacting species is one of the major factors controlling the behavior of chemical reactors. For first order reaction knowledge of the length of time each molecule spends in the reactor is all needed to predict conversion.

Consequently mixing with the surrounding molecules is not important. Therefore once the RTD is determined we can predict the conversion that will be achieved in the real reactor provided that the specific reaction rate for the first order reaction is known. For reactions other than first order knowledge of RTD is not sufficient to predict conversion. In these cases the degree of mixing of molecules must be known in addition to how long each molecule spends in the reactor. Hence models are developed that account for the mixing of molecules inside the reactor.

Material and Methods

Tank in series model: In developing this model, let consider three equal sized ideal CSTRs in series. If a pulse tracer experiment is carried out on these three tanks in series, then from RTD function¹, the fraction of tracer material leaving the last tank between time t and t+Δt will be

$$E(t) = \frac{C_3(t)}{\int_0^{\infty} C_3(t)dt} \quad (1)$$

Where C_3 is the concentration of tracer material exiting the system (3rd tank); E(t) is the RTD function. The outlet concentration of tracer material, $C_3(t)$ as a function of time, can be obtained by carrying out material balance around each of the tanks. From the principle of conservation of mass; Input = Output + Disappearance + Accumulation (2) For a steady state system, there is no accumulation, therefore;

$$\text{Input} = \text{Output} + \text{Disappearance} \quad (3)$$

Equation (3) can be expressed in rate form. Taking a material balance around a continuous stirred tank;

$$v_{in}C_{in} = v_{out}C_{out} + V \frac{dC_{out}}{dt} \quad (4)$$

Where V is the volume of the tank; v is the volumetric flow rate and C is the tracer concentration. From the three identical tanks in series, the volumetric flow rate v_1 is constant i.e. $v_{in} = v_{out}$ for each of the tanks. The volume V of each of the tanks is also identical i.e. $V_1 = V_2 = V_i$. Therefore, the space time τ_1 of the individual reactors is also identical, since the space time for ideal CSTR is the ratio of volume to volumetric flow rate, i.e. $\tau_1 = \tau_2 = \tau_i$ Where the subscript 1, 2 and i represents the first, second and ith tank respectively. Taking the material balance around tank 1 (figure 1) gives

$$vC_0 = vC_1 + V \frac{dC_1}{dt} \quad (5)$$

Where, C_0 is the inlet concentration to tank 1; C_1 is the out let concentration from tank 1. For a pulse tracer experiment, C_0 as a function of time is zero. Therefore, equation (5) becomes

$$V_1 \frac{dC_1}{dt} = -vC_1 \quad (6)$$

$$C_1 = C_0 e^{-vt/v_1} \quad (7)$$

For ideal CSTR, the space time is given as;

$$\tau = V/v \quad \tau_1 = V_1/v \quad (8)$$

$$C_1 = C_0 e^{-t/\tau_1} \quad (9)$$

The material balance on tracer around tank 2 will be;

$$vC_1 = vC_2 + V_i \frac{dC_2}{dt} \quad (10)$$

Dividing through by V_i and then substituting equation (7) and (8) into equation (10) gives a first order ordinary differential equation;

$$\frac{dC_2}{dt} + \frac{C_2}{\tau_i} = \frac{C_0}{\tau_i} e^{-t/\tau_i} \quad (11)$$

Using an integrating factor, e^{-t/τ_i} along with the initial condition $C_2 = 0$ and $t = 0$ gives;

$$C_2 = \frac{tC_0}{\tau_i} e^{-t/\tau_i} \quad (12)$$

By taking material balance on tracer around tank 3, we have

$$vC_2 = vC_3 + V_i \frac{dC_3}{dt} \quad (13)$$

$$\frac{dC_3}{dt} + \frac{C_3}{\tau_i} = \frac{C_0}{\tau_i^2} e^{-t/\tau_i} \quad (14)$$

$$C_3 = \frac{t^2 C_0}{2\tau_i^2} e^{-t/\tau_i} \quad (15)$$

Substituting equation (15) into (1) we obtain

$$E(t) = \frac{\frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i}}{\int_0^{\infty} C_0 \frac{t^2}{2\tau_i^2} e^{-t/\tau_i}} \quad (16a)$$

$$E(t) = \frac{t^2 e^{-t/\tau_i}}{\int_0^{\infty} t^2 e^{-t/\tau_i} dt} \quad (16b)$$

By applying integration by part (Stroud 1995), equation (16b) becomes;

$$E(t) = \frac{t^2}{2\tau_i^3} e^{-t/\tau_i} \quad (17)$$

This is the RTD function for three tanks in series. Generalizing this method for a series of n CSTR gives the RTD function as;

$$E(t) = \frac{t^{n-1}}{(n-1)!\tau_i^n} e^{-t/\tau_i} \quad (18)$$

The RTD function can be normalized by expressing in dimensionless time scale as^{1,2}

$$\theta = t / \tau \quad (19)$$

Equation (18) becomes;

$$E(t) = \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta} \quad (20)$$

The variance, σ^2 of the RTD data from tracer experiment is given by¹

$$\sigma^2 = \int_0^{\infty} (t - tm)^2 E(t)dt \quad (21)$$

Expressing this variance as dimensionless variance, σ^2_{θ} gives;

$$\sigma^2_{\theta} = \frac{\sigma^2}{\tau^2} = \int_0^{\infty} (\theta - 1)^2 E(\theta)d\theta \quad (22)$$

Expanding equation (22) gives;

$$\sigma^2_{\theta} = \int_0^{\infty} \theta^2 E(\theta)d\theta - 2 \int_0^{\infty} \theta E(\theta) d\theta + \int_0^{\infty} E(\theta) d\theta \quad (23)$$

$$\int_0^{\infty} E(\theta)d\theta = 1 \quad (24)$$

Since the fraction of all the materials that has resided for a period of time, t, in the reactor between $t = 0$ and $t = \omega$ is 1. Therefore

$$\sigma^2_{\theta} = \int_0^{\infty} \theta^2 E(\theta)d\theta - 1 \quad (25)$$

Substituting equation (20) into (25) gives;

$$\sigma^2_{\theta} = \int_0^{\infty} \theta^2 \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta} d\theta - 1 \quad (26)$$

$$\sigma^2_{\theta} = \frac{n^n}{(n-1)!} \int_0^{\infty} \theta^{n+1} e^{-n\theta} d\theta - 1 \quad (27)$$

Integrating will give,

$$\sigma^2_\theta = \frac{n^n}{(n-1)!} \left[\frac{(n+1)!}{n^{n+2}} \right] - 1 \quad (28)$$

$$\sigma^2_\theta = \frac{1}{n} \quad (29)$$

Taking the dimensionless variance back to time gives;

$$\frac{\sigma^2}{\tau^2} = \frac{1}{n} \quad (30)$$

$$n = \frac{\tau^2}{\sigma^2} = \frac{1}{\sigma^2_\theta} \quad (31)$$

The number of tanks in series is given by n, where τ is the space-time in the combined tanks in series, but it is equivalent to the mean residence time, t_m , in the non-ideal plug flow reactor. The number of tanks increases as the variance decreases, and the curve width or variance changes from $\sigma^2_\theta = 1$ for $n = 1$ to $\sigma^2_\theta = 0$ as $n \rightarrow \infty$. This indicates that the behavior of stirred tanks in series ranges from perfect mixing to plug flow.

RTD functions for ideal reactors: Non ideal reactor design for segregated flow involves the solution of

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

Where $E(t)$ is the residence time distribution function (RTD) and $C_A(t)$ is the concentration from a batch reactor at time t. C_A is the calculated outlet concentration.

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

$$\frac{d\bar{C}_A}{dt} = E(t)C_A(t)$$

I. $C = 0$ at $t = 0$

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 $E(t) = \frac{\tau}{2t^3}$ when $t \leq \frac{\tau}{2}$ else it is zero.

Here τ 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.

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

EofPLUG =

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 $\tau = 1$.

EofCSTR=exp (-t/tau)/tau

EofNCSTR= (t^ (N-1)/tau^N/(N-1)!*exp(-t*N/tau)

Where N is number of CSTR's in series

Simulation of Non Ideal Reactor Using Polymath: The

polymath entry for all the discussed RTD functions is shown in figure 2 for the case where $k=0.2$, $\tau=0.5$, and $n=10$ to a time of 30.0. The partial results table from the polymath solution shown in figure-2 gives general information on various problem variables before the user is prompted for various plots or tubular output.

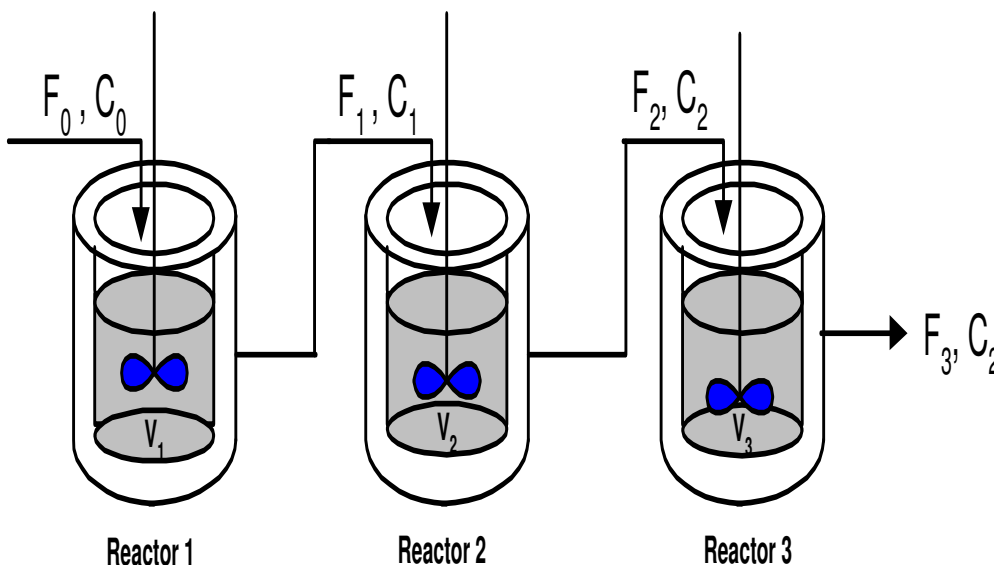


Figure-1
Continuous Stirred Tank Reactor (CSTR) in Series

Table-1
Partial Result Table Generated By Polymath

Sr. No.	Variable	Initial value	Minimal value	Maximal value	Final value
1	t	0	0	30.0	30.0
2	CAplug	0	0	0.4802366	0.4802366
3	CAbatch	1.0	0.1428571	1.0	0.1428571
4	CAlaminar	0	0	0.5486197	0.5486197
5	CAcstr	0	0	0.5960335	0.5960335
6	CAnostr	0	0	0.512182	0.512182
7	tau	5.0	5.0	5.0	5.0
8	Eoftplug	0	0	0	0
9	Eoftlaminar	0	0	0.6227395	0.000463
10	n	10.0	10.0	10.0	10.0
11	k	0.2	0.2	0.2	0.2
12	Eoftcstr	0.2	0.0004958	0.2	0.0004958
13	Eoftncstr	0	0	0.2627993	4.864E-16

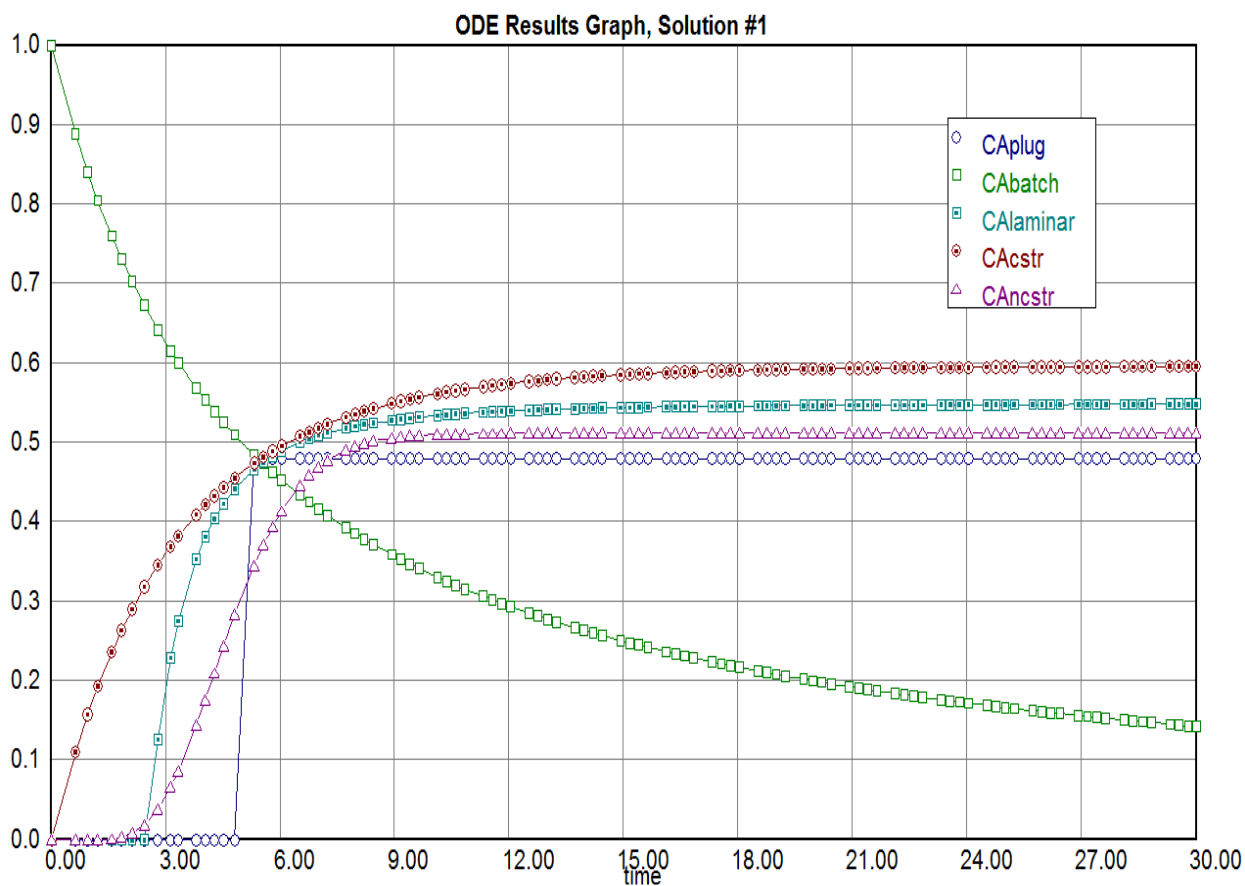


Figure-2
RTD Solution for Average Concentrations Exiting Various Ideal Reactors

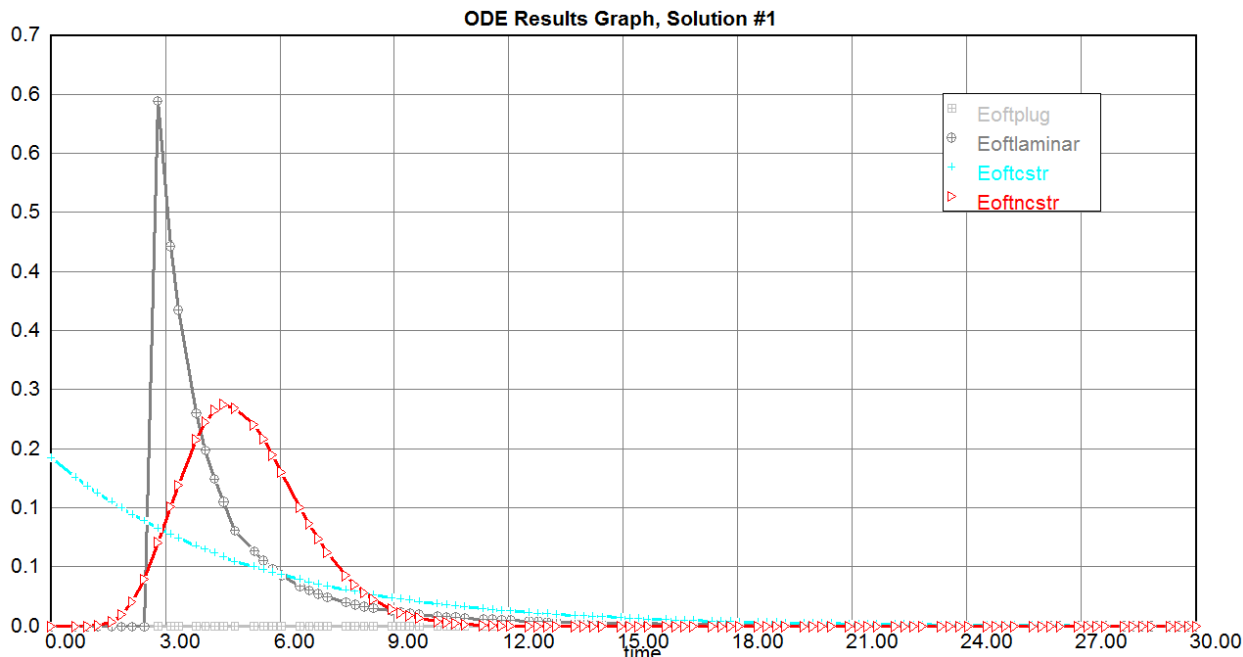


Figure-3
RTD Functions for Various Ideal Reactors

Results and Discussion

From the RTD data we require the $18.86 \approx 19$ tanks in series. Dispersion no. $\frac{D}{UL} = 0.027$, which indicate as intermediate amount of dispersion. From the data the number of tank increases as the variance decreases. There is approximately 22.86 % deviation between experimental and distribution mean residence time.

Table-2

Run. No.	$\tau_{exp.}$	$\tau_{theo.}$	σ^2	σ_{θ}^2	D/UL	N
Run No.1	10.89	8.4	6.378	0.053	0.027	18.86
Run No.2	10.60	7.63	5.433	0.048	0.024	20.83
Run No.3	8.6	5.6	5.0	0.067	0.034	14.92
Run No.4	7.67	4.94	4.354	0.074	0.038	13.51
Run No.5	5.19	4.2	2.804	0.104	0.055	9.61

The graphical results of all four reactors are presented in graph 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.

As expected, the calculated concentrations decrease according to the reactor types CSTR, Laminar Flow, n-CSTR, and Plug Flow. The conversion increases 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

Table-3

Sr. No.	Flow system	Concentration
1.	C_A cstr	0.5960335
2.	C_A laminar	0.5486197
3.	C_A ncstr	0.512182
4.	Plug Flow	0.4802366

Conclusion

From the experimental data, it's find out that 19 identically sized ideal stirred tank operating in series would have an equivalent performance with the non ideal plug flow reactor. There is approximately 22.86% deviation between the experimental and the distribution mean residence time. However, the main purpose was to use the information from the RTD curve to improve the reactor operation. The result of RTD provided vital information concerning the effect of operating conditions. As expected, from the experimental result the number of tanks increases as the variance decreases.

Notations: V=Volume of the Tank (Lit), v=Volumetric Flow Rate (Lit/min), C=Tracer Concentration (ml/Lit), E(t)=Residence Time Distribution Function, t=Time, Measured From Moment of Tracer Injection (min), t_m = Mean Residence Time (min), k =Rate Constant (min)⁻¹, τ = Space Time (min), Θ =Dimensionless Time, σ^2 = Variance, (Dimensionless), n =number of tanks (nos.),

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