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RTD Modeling of a Non-Ideal Coiled-Tube Reactor through Experimental Investigation for Pulse Input Using Methylene Blue Dye

Avdesh Singh Pundir[1]*, Kailash Singh[2*], Varshika Singhal[1], Mayank Pandey[1], Garvit Gupta[1], Moh. Rohaan[1], Sunil Rajoriya[1*] and Girish Tyagi[1]

[1]Department of Chemical Engineering, MIET, Meerut, U.P-250005
[2] Department of Chemical Engineering, MNIT, Jaipur, Rajasthan-302017

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Abstract

This paper focuses on the grasp of a deep understanding of flow behavior in a coiled tube reactor through Residence Time Distribution (RTD) studies. The reactors, in general, are classified ideally: mixed and plug-flow patterns. Unfortunately, in the real world, it has been observed that they show very different behavior from that expected. Thus, the characterization of the nonideal coiled tube reactor is needed to carry out. The calculations were carried out in the Matlab for distribution of residence time of the coiled tube reactor that is used in the Chemical Reaction Engineering Laboratory at MIET College. Pulse input tests were used significantly to analyzed the flow behavior using methylene blue (MB) tracer. A significant disparity in RTD curves in the presence of the secondary flow was examined and data were recorded. Finally, a suitable mathematical model was selected from the Tank in Series (TIS) and Axial Dispersion Models (ADMs) based on residual error and was used to validate these outcomes. The deconvoluted of the signal was used to get C_{in} for the verification of the pulse input behavior. The results were compared with the experimental data that concluded the modeling of the reactor is in good agreement.

Keywords: Pulse input, Methylene blue, RTD, Coiled tube reactor, Non-ideal

1 Introduction

For an ideal reactor, the flow and mixing conditions are needed to be exactly known, which allows us to develop the theoretically mathematical model equation (1). However, in reality, for built reactors, these complex characteristics much deviate to some extent from ideal behavior due to various possible reasons such as a consequence of a short-circuiting, absence of turbulence, macroscopic internal currents, and stagnant zones (2). In an actual system, the velocity distribution profile leads to a residence time distribution (RTD). Experimental determination of RTD is carried out via measuring the outlet response of an inert tracer which injected into the flow stream to be study and so-called stimulus-response technique. In general, tracers are normally a soluble dye, acid, or color compound that can be effortlessly detected the concentration at the exit of a reactor with the assistance of an online or manually measuring device. The applied techniques are all primarily based on the measurement of some properties at the output flow of a reactor based on regarded modifications to the input flow which may additionally consist of the following strategies for making use of the tracer to a system (a) a step enter method, in which the regarded input concentration is modified from one regular stage to some other regular level;(b) a pulse enter method, in which a pretty small recognized quantity of tracer is injected into the feed circulate in the negligible feasible time; and (c) a sinusoidal enter method, in which the frequency of the sinusoidal variant is modified with time, therefore, producing a frequency-response layout for the system. Each approach can be modified into the other two as per our convenience. However, practically, it is a good deal to handle a less complicated approach to monitoring a tracer response that approximates a step-change or a pulse enter due to measurement complexity related to sinusoidal variations, besides, to consume much greater time and want for a unique measuring device (3).

The applications of continuous processing in the chemical industry have been increasing day by day. There are many causes why a chemical product manufacturer may choose to run chemical reactions in continuous mode instead of batch. The main causes for choosing continuous instead of batch reaction system are rapid kinetics, exothermic reaction, hazardous chemicals, high temperatures, and pressures. In general, a reactor used in chemical industries has non-ideal behavior. Therefore, it's important to know the real behavior of the reactor through modeling and simulation in practice. To simulate a real reactor, it's necessary to estimate RTD. RTD describes how much time a particle spends inside the reactor (4). For a better understanding of flow reactors, two different ideal reactor models i.e. Continuous Stirred Tank Reactor (CSTR) and Plug Flow Reactor (PFR) are used at the industry level. An Ideal CSTR assumes perfect mixing, while an ideal PFR assumes no mixing. No real reactor has consisted accurately the characteristics of either of the two ideal reactors, in general. Many researchers have shown that a real reactor can

***Corresponding author:** (a and b) Avdesh Singh Pundir and Sunil Rajoriya**,** Department of Chemical Engineering, MIET, Meerut, U.P-250005. Emails: avdesh.pundir@miet.ac.in and sunil.rajoriya@miet.ac.in (c) Kailash Singh, Department of Chemical Engineering, MNIT, Jaipur, Rajasthan-302017. E-mail: ksingh.mnit@gmail.com

be modeled as reactor data tank-in-series (TIS) and axial dispersion model (ADM) which are widely used (5). In many practical situations, the fluid in the reactor is neither well mixed nor plug flow. Therefore, there is a need for time to model a real reactor and it can be possible in several ways. The RTD describes us how long the various reacting fluid elements have been retained inside the reactor, however, it does not convey any information regarding the exchange of matter among the fluid elements. The mixing of different reacting species is one of the main factors responsible for controlling the behavior of chemical reactors. For the different order reactions system, more especially for the first-order system, the knowledge of the time with which each molecule remains in the reactor is required to predict the conversion of a reactant. Therefore, once the RTD is determined, it is quite easy to predict the reaction conversion that will be achieved in a real reactor with the known value of the specific reaction rate for the first-order reaction. For reactions other than the first-order only knowledge of RTD is not adequate to predict conversion. In such cases, in addition to RTD, the degree of mixing of molecules must be known (6). In this study, no reaction mixture has been considered while an investigation of flow behavior has been carried out using a methylene blue dye as a tracer for pulse input.

The main aim of this study is to develop a reliable model for a continuous reactor, especially for a coiled-tube reactor which is mostly used in many chemical and allied industries. A model is to develop for the flow of Newtonian fluid (because mostly organic solvents may have similar properties to water) in a coiled-tube reactor. This model is used to define the design rules for the reactor. The model describes the RTD as a function of the rheological behavior of the system and operational parameters for fixed tube dimensions. The first emphasis lies on determining the suitable model for a coiled tube reactor from experimental data and validation of the assumption by determining the dispersion coefficient, D_{Axial}. During experimentation, it is normally assumed that the input tracer concentration has perfect pulse shape, and then a suitable analytical expression is normally used without verifying the pulse input shape. That is why a different way for the calculation is presented, not only taking the moments but the whole distribution into account. The geometry configuration of the coiled tube reactor introduces a secondary motion which ultimately affects the dispersion. To accomplish this, the solutions of the three models are fitted to the measured RTD data. At first, a one-parametric tank in a series model is used due to its simple nature without taking into account complex phenomena such as bypass or channeling. Second dispersion models have been applied to solve the dispersion convection equations and fitted to the measured RTD data by using the least-squares method. At last, by using the deconvolution technique, a validation of the pulse input shape has been carried out along with an optimization scheme for an overdetermined system. All calculations were carried out in Matlab. This study has been carried out and presented in such a manner so that it can be more accessible to many postgraduate and research students who are working presently in this field. The prime objective of the present study is to determine a suitable model that predicts the output in a known manner from data gathered in an undergraduate laboratory through a lot of experiments. This study adds “off the shelves” method to the chemical engineering discipline.

2 Experimental setup

The experimental setup consists of two feed tanks and one tank is used through which water is fed to the reactor. The flow rate of water can be adjusted by operating the provided needle valve and measured with the help of a rotameter. The compressed air is used for the circulation of water. The reactor is a helical coil tube type made up of stainless-steel pipe. The methylene blue dye solution enters at the lower end coming out of the top of the coil from where samples are collected for analysis of outcomes. To investigate the flow behavior by using the RTD characteristics, a simple arrangement is made available to inject MB as a tracer into the lower end of the reactor, using a syringe, manually. Pressure regulator & pressure gauge are fitted in the compressed airline for ease of varying the water flow rate. The coiled tubular flow reactor consists of 60.96 cm length of the tube and 12.33 mm inner diameter provided with one inlet/outlet at one end opposite to each other and inclined at 90˚ with the axis of the tube. The diameter of the pipe before the inlet point of the reactor is 10 mm and through which a pulse input is given. The volume of the reactor is 2.911×10^{-4} m^3. The coiled tube reactor is kept in an isothermal rectangular tank fitted with a temperature sensor. The temperature of the stirred water bath tank is kept constant with the help of a PID controller and uniform by stirring action.

3 Effect of shape of the coiled tube reactor

The coiled1tube reactor consists of two main flows: a primary flow occurring along the axial direction of the fluid motion and a secondary flow acting perpendicularly to this due to centrifugal force. By the secondary flows, drag effects in the proximity of wall surfaces come in the picture (7). The secondary flow in helical pipes was firstly investigated by Dean (8). He used the dimensionless group to characterize the flow behavior inside the coiled-tube reactor, normally called Dean number, *De*:

$$De = \frac{Re}{\sqrt{\lambda}} = \frac{\rho u d_t}{\mu}\sqrt{\frac{d_t}{D_c}} \quad (1)$$

where λ is the ratio of coil-to-tube diameter. ρ and μ are the density and dynamic viscosity of the fluid and u is the mean axial velocity, respectively. For a better understanding of the physical meaning of Dean number, De, it can be re-written in terms of the forces which come in the picture are inertia, centrifugal acceleration, and viscous forces.

$$De\ \alpha \quad f\left(\frac{\sqrt{(centrifugal\ force)\times(inertia\ force)}}{(viscous\ force)}\right) \quad (2)$$

Under the condition of low values of Dean numbers ($De \ll 1$), viscous forces are dominant and the secondary flow is approximately absent (9). Conversely, with the increment in De, centrifugal and inertial forces overcome against drag which ultimately leading to the formation of secondary flow. Therefore, the Dean number is more informative than Reynold's number to describe the flow behavior in a curved/helically coiled-tube reactor. There are many analytical solutions available for the equation which describes the flow for incompressible laminar flow and lower values of curvatures radius (high λ). However, the nondimensional solution provided by analytical depends heavily on De. The action of centrifugal force due to the curvature of the reactor tube develops two opposite-rotating vortices, which supports secondary mixing. The centrifugal force pushes hard on the fluid elements which are moving in and around the center of the tube, and from the fluid mechanics' theory, it is clear that the axial velocity is maximum at the center point of the tube. The central region's fast-moving fluid is forced to move outward and it is constantly replaced by the fluid near the wall, so there is some sort of inter-transfer movement of inner and

outer fluid elements. Due to that reason, the position of maximum axial velocity is off-centered and moves toward the outer wall.

4 Results and discussion

There are many approaches available to model a real non-ideal reactor but two models have been significantly in use. These two models have one unknown parameter. One parameter model is also known as the Tank-In-Series (TIS) model and Axial Dispersion Model (ADM). There are two most common injection methods available: the first one is being called pulse input (mathematically, called "Dirac delta function" in case of ideal input) and the second one is called step input. In this study, the pulse input injection method has been used. Figure1 shows the actual experimental setup used in this study.

4.1 Measurement of the RTD

The main aim of this study is to introduce the reader to the analysis of the coiled tube chemical reactor. In it, reactions with complex kinetics can be carried out. It is normally work in unusual condition, such as unsteady-state operation. The mathematical analysis is a necessary tool for the characterization of flow and kinetic models. A software tool is also necessary to solve a complex problem in the design of a coiled tube reactor (10). In the last four decades, many researchers have published literature but out of them, the detailed review has been published by Nauman (11) along with the introduction of the development of the RTD theory. He adopted both the experimental as well as the modeling techniques and many applied applications. The RTD is defined as the product of function $E(t)$ and t such that as $E(t)dt$. E(t) represents the fraction of fluid elements whose residence time in the reactor lies in the time range dt. It is called the residence time density function. Alternatively, the fraction of fluid elements residing in the vessel between time limits t_1 and t_2 is given by $\int_{t1}^{t2} E(t)\,dt$. From the other point of view, the fraction of fluid element with age lessor than t can be represented by $\int_0^t E(t)\,dt$. As the nature of being a probability distribution function, $E(t)$ function can be presented as the normalization function: $\int_0^\infty E(t)dt = 1$. Under the normalization condition, the shaded area under the residence time density function is unity. It means that the fraction of fluid elements remains into the reactor for time limits between 0 and ∞ is 1. There are two important type reactors which normally encounter in chemical industries which are the plug flow and the mixed flow (continuously stirred tank reactor, CSTR) reactors. In the case of an ideal plug flow reactor, the RTD is a delta function that is centered at the point of reactor space-time τ and under ideal condition, it is assumed that there is no distribution of residence times, every fluid element lives for the same amount of time τ inside the reactor.

$$E_{PFR}(t) = \delta(t - \tau) \tag{3}$$

The spent period called macroscopic residence time normally depends on the reactor geometry and the operating conditions. For a tubular reactor with constant cross-section:

$$\tau = \frac{V}{\vartheta} \tag{4}$$

where V and L are the volume and length of the reactor, respectively, v is the volumetric flow rate and u is the averaged fluid velocity. To calculate the space-time for any kind of reactor, the knowledge of the reactor volume and the fluid flow rate is a must.

The major flow pattern in RTD theory other than a plug flow reactor is a CSTR. Each element of fluid at the inlet is instantaneously and perfectly mixed with the solution already present in the reactor. It can be easily shown that the RTD for a CSTR is the exponential function (12):

$$E_{CSTR}(t) = \frac{1}{\tau} E^{\frac{-t}{\tau}} \tag{5}$$

The RTD of a real reactor can be approached to the behavior of these ideal reactors and the extent of the deviation must be investigated by using well established RTD studies. There are many experiments possible which permit the RTD of a real reactor to be derived.

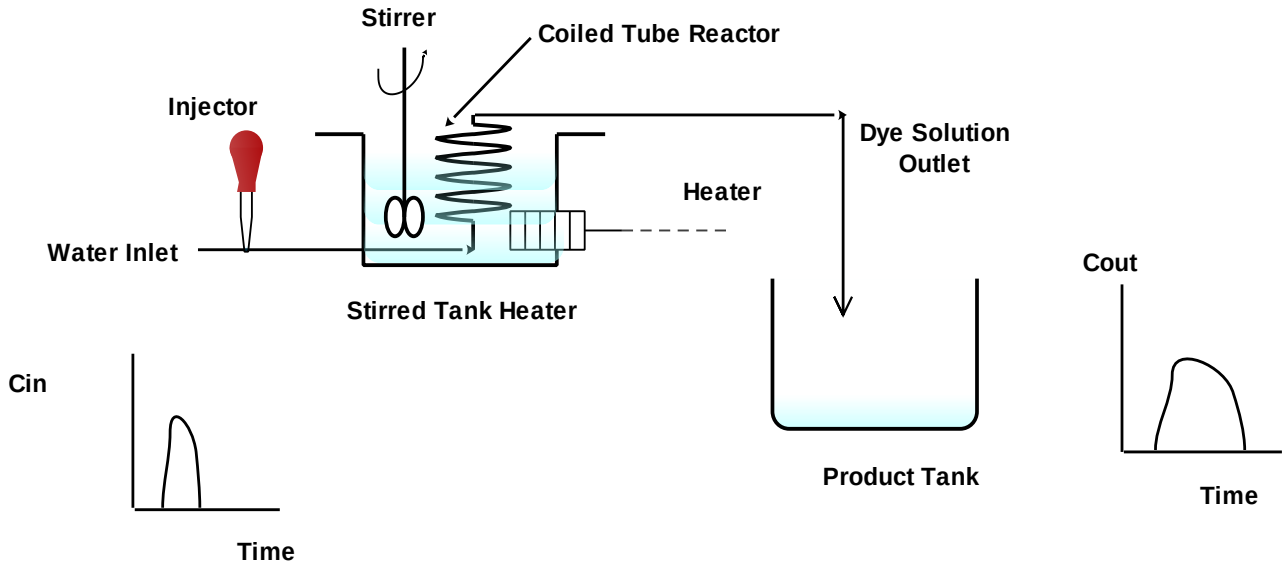


Figure 1: Schematic representation of the RTD experimental setup with a pulse input

In this study, only the simplest ones are introduced which doesn't demand any special skill or much chemical and sophisticated equipment for injection. The experimental measurement of the RTD is carried out by injecting a tracer, which is methylene blue (MB) in this study, into the coiled-tube reactor at a fixed time. This MB is an inert chemical. The MB concentration at the outlets of the reactor is measured by the colorimeter with the progress of time. The necessary condition for the selection of a trace is that it must be inert, soluble in the reacting mixture, and easily detectable. Besides, it should not have any interaction with the walls of the reactor so that it can be used to reflect, as best as possible, the real behavior of the reacting materials which are flowing through the reactor. Table 1 represents the values of the process parameters used and evaluated in this study.

Table 1: Various parameters used in this study

Parameter	Value (unit)	Parameter	Value (unit)
D_m	6.47E-10 (m^2/sec)	τ	21.83 (sec)
ρ	950 (kg/m^3)	N_{Re}	430.26
L	0.6096 (m)	De	117.62
L/d_t	49.44	λ	13.38
Pe_L	10.01	D_{Axial}	0.0017 (m^2/sec)
V	600 (ml)	u	0.0279 (m/sec)
$\bar{t}$	22.08(sec)	σ	87.42
Bo	0.2025	d_t	0.01233 (m)

4.2 C, E and F curves

The RTD is determined experimentally by injecting a small amount of MB dye, called a tracer, into the coiled tube reactor at a predefined time and then measuring the tracer concentration, C, (= C_{out}) in the effluent stream with the progress of time. In a pulse experiment, however, the uniform distribution of the MB dye is not practically possible which emphasizes the investigation of deconvolution study. The measured concentration of the MB at the outlet plotted against the time which is called C-curve and from this C-curve, E-curve was produced. The E-curve gives the "fraction" of the volume element exiting the system at a particular time. The E-curve can also be produced as a normalized distribution which means that the total area under the curve is unity. From the above-discussed theory, the E-curve can be determined:

$$E(t) = \frac{C(t)}{\int_0^\infty C dt} \quad (6)$$

Once the values of $E(t)$ are known, the mean residence time can be calculated as $\bar{t} = \int_0^\infty E(t)dt$ This is called the first moment of the distribution. The mean residence time $\bar{t}$ is equal to the space-time only under the ideal flow behavior condition. It is also useful to calculate the variance of the distribution, which is the second moment about the mean:

$$\sigma_t{}^2 = \int_0^\infty (t-\bar{t})^2 E(t)dt. \quad (7)$$

The calibration experiments were carried out on the UV-VIS detection system and presented in figure 2. The fitted calibration equation was used to estimate the concentration of the MB dye at the reactor outlet. Figure 3 depicts the outlet concentration measured with the progress of time. The evaluated cross ponding E and F curves from figure 3 have been shown by figures 4 and 5 along with its dimensionless forms. These figures show the smooth curve as expected.

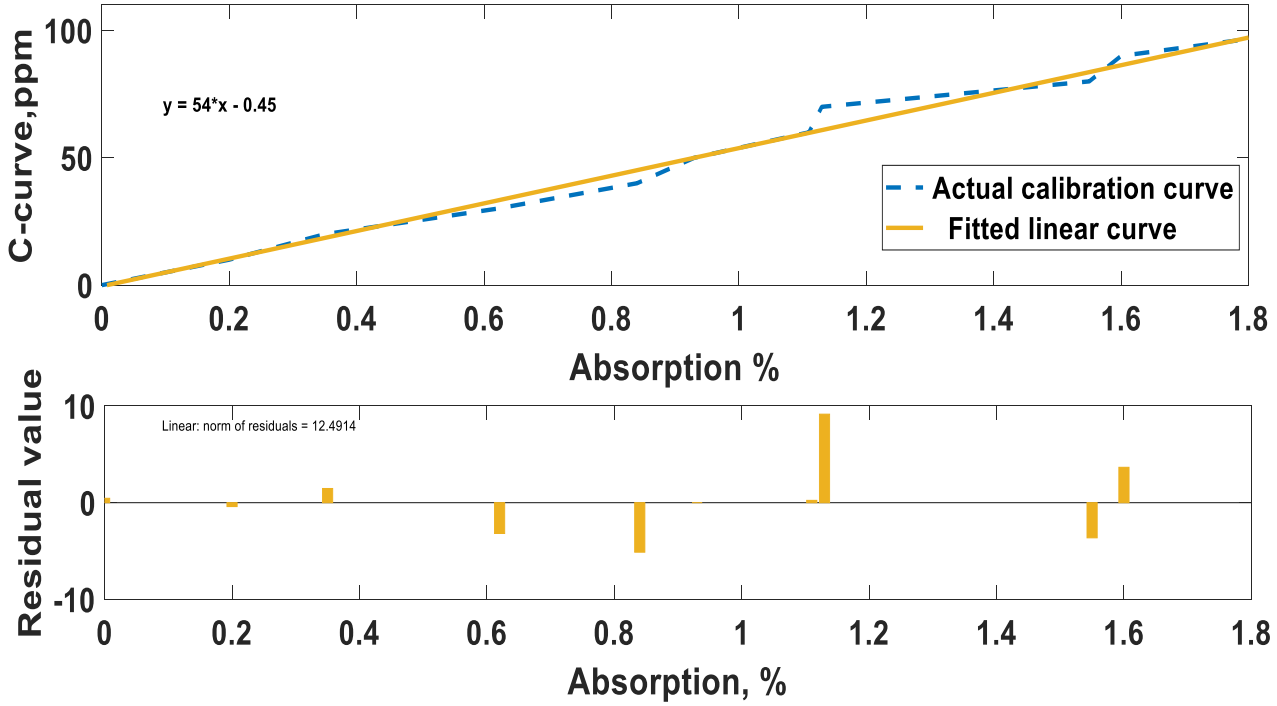


Figure 2 Calibration and residual error curves for concentration measurement

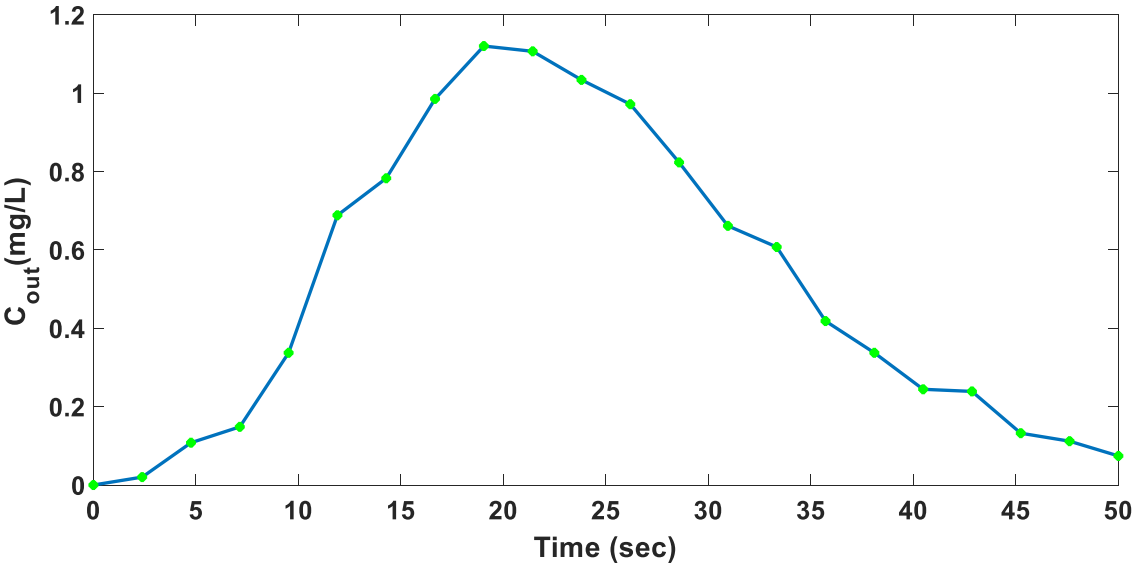
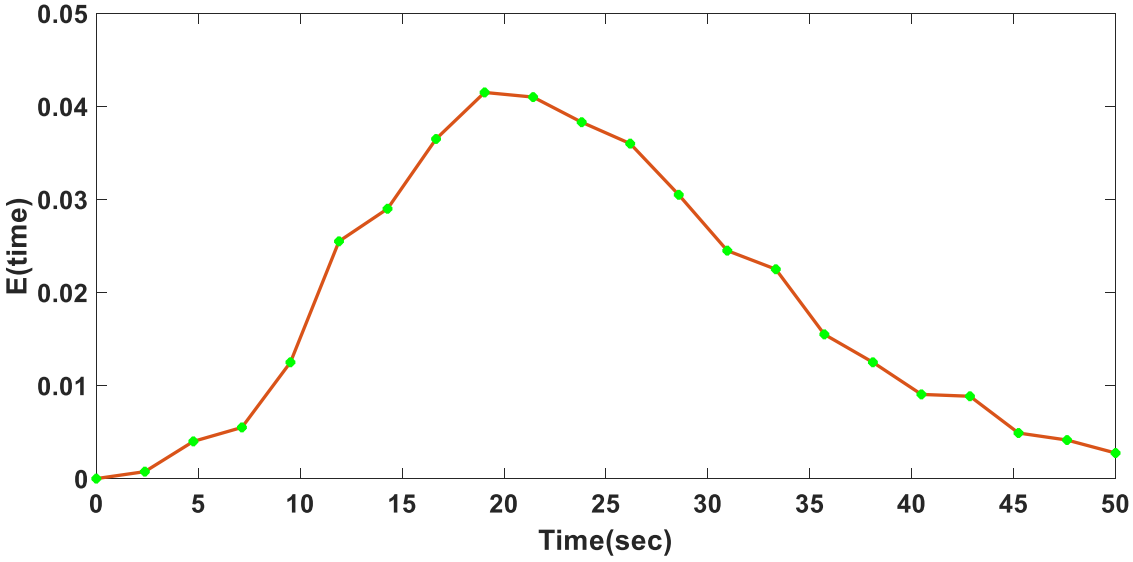
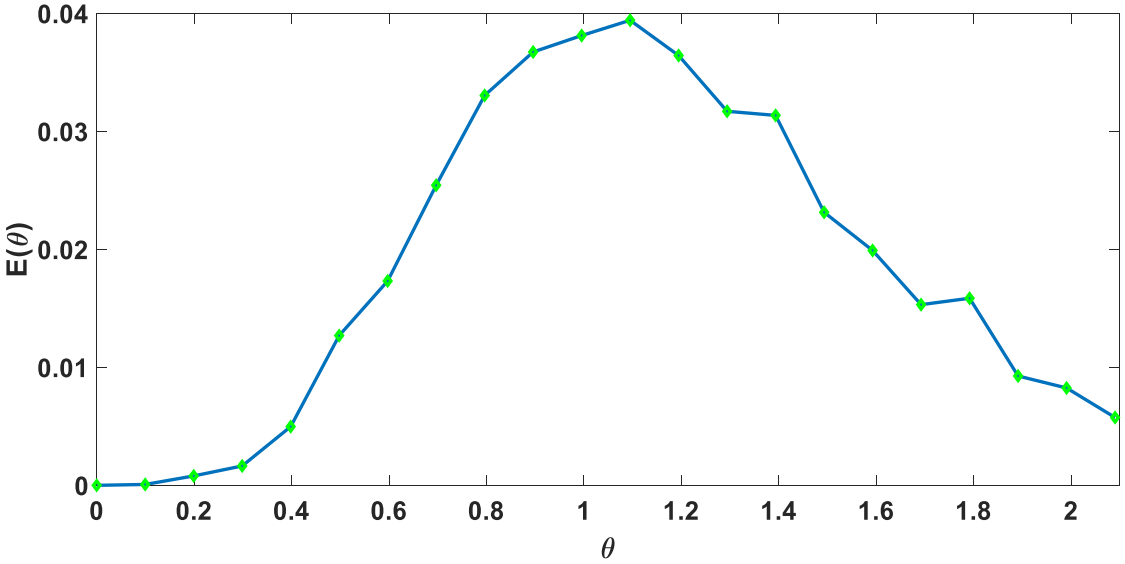


Figure 3: Concentration at the outlet of the coiled tube reactor

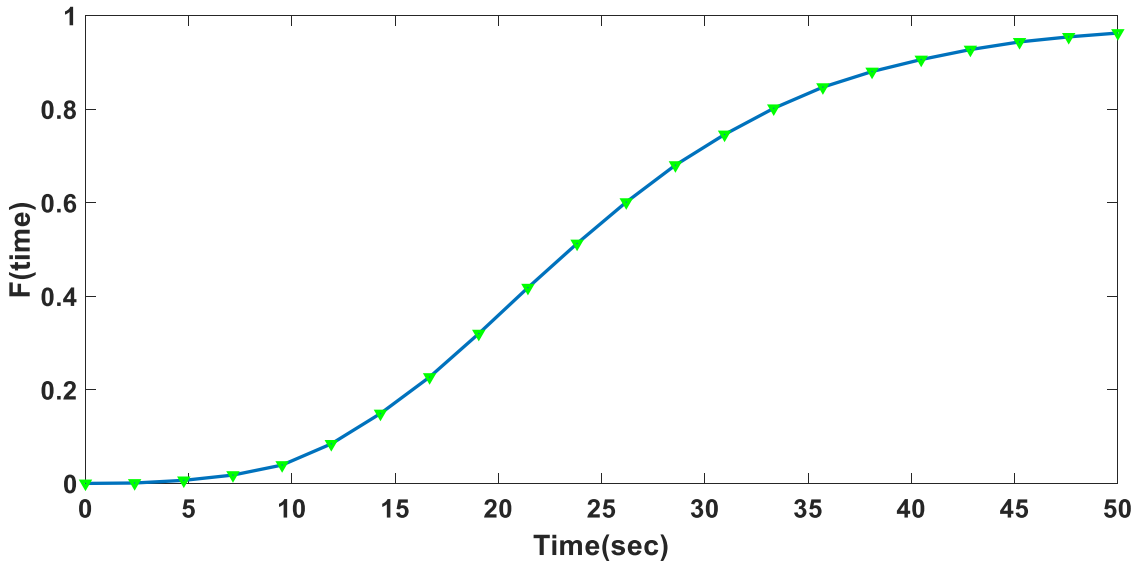


(a)

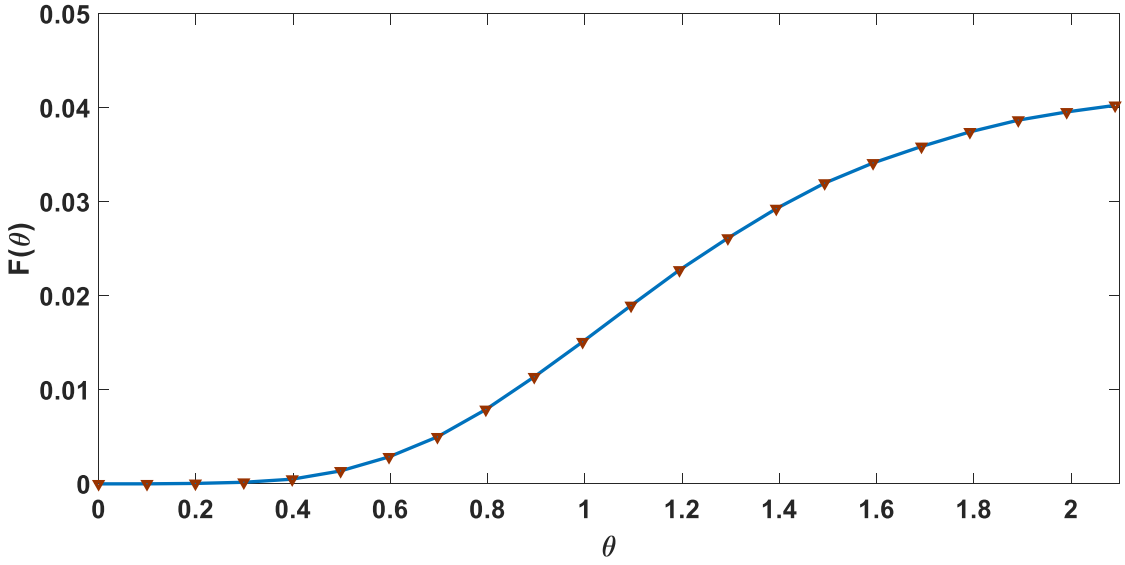


(b)

Figure 4: E curves of the coiled tube reactor with time (a) and without time dimension (b)



(a)



(b)

Figure 5: F curves of the coiled tube reactor with time (a) and without time dimension (b)

4.3 Tank in series model (TIS)

In this approach, we study the RTD of a coiled tube reactor to determine the number of CSTRs in series that will represent approximately the same RTD behavior as of the coiled tube reactor. We started the investigation with two CSTRs in series expression for the expression of the RTD, and then generalize it for "n" reactors connected in series. In this way, it is obtained an equation that allows us to calculate the number of tanks that best correlates the RTD data of the coiled tube reactor(13).

$$E_{CSTRs} = \frac{t^{n-1}}{n-1!t_i^{-n}}\exp(-\frac{t}{t_i}) \quad (8)$$

Here t_i = t/n, where t in the numerator represents the total volume of all reactors divided by the volumetric flow rate. Figure 6 shows the actual approach of the TIS model. Figure 7 shows the RTD mapping for different CSTR numbers in series. As n increases, the behavior is closer to plug flow behavior. The number of reactors in series can be calculated from the dimensionless variance (14):

$$\sigma^2 = \int_0^\infty (t-\bar{t})E(t)dt = \frac{\bar{t}^2}{n} \quad (9)$$

It is clear from figure 7 and 8, as we increase the number of tanks, the error gets reduce but after n = 6, the value of error gets an increase. Therefore, the best-fitted value for the TIS model is n = 6. But from figure 7, it is also clear that this value has a large error which is not acceptable for the real system.

4.4 Axial dispersion model (ADM)

In this study, the simplest model was to describe flow inside the coiled reactor which consists of both the convection and the diffusion terms which are most important of the axial dispersion model as reported by many researchers (15–17). The model is represented by the following equation:

$$\frac{\partial C}{\partial t} = D_{Axial}\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} \quad (10)$$

where C, the concentration of a tracer, is a function of time and the axial coordinate of the system x, D_{Axial} is the axial dispersion coefficient and u is a constant mean axial velocity, which does not vary with x. The model described a one-

dimensional dispersion process of a plug-flow reactor. Here, it is assumed that the axial dispersion coefficient is independent of the axial position as well as the tracer concentration. It describes the rate of axial dispersion inside the reactor. To make the model more approachable from the numerical solution point of view, we have converted the model in a non-dimensional form (18).

$$\frac{\partial C}{\partial \theta} = \frac{1}{Pe_L}\frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} \tag{11}$$

with $\theta = \frac{t}{\tau} = \frac{uL}{L}$ and z = x/L, where L shows the length of the reactor. It is clear that this model is a single parameter-based model which is generally known as the Peclet number, $PeL = uL/D_{Axial}$. However, the literature shows different definitions of this parameter under different conditions which differ in the way of representing the characteristic length and the diffusion coefficient (molecular or axial diffusion coefficient). The analytical solutions available are different when subject to different boundary conditions (19–21). The changing dispersion parameter due to the reactor geometry and operating conditions can be estimated by comparing the RTD experimental data with the analytical solution available.

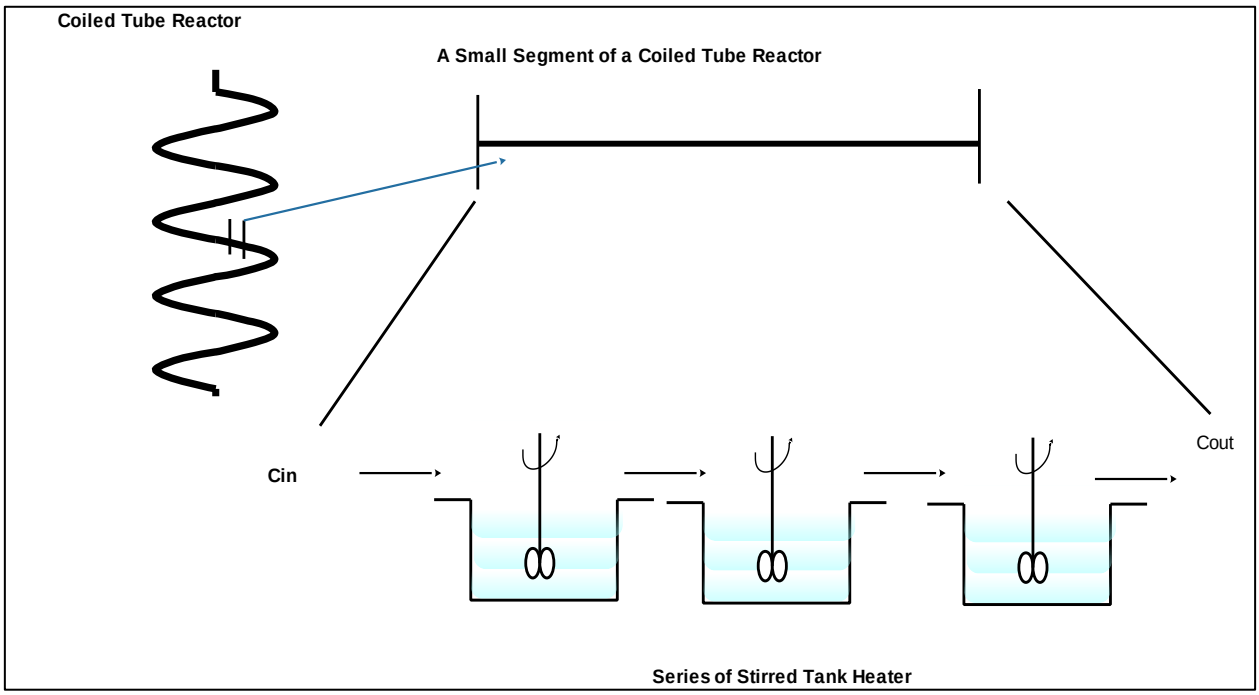


Figure 6: Schematic diagram for the tank in series model (TIS)

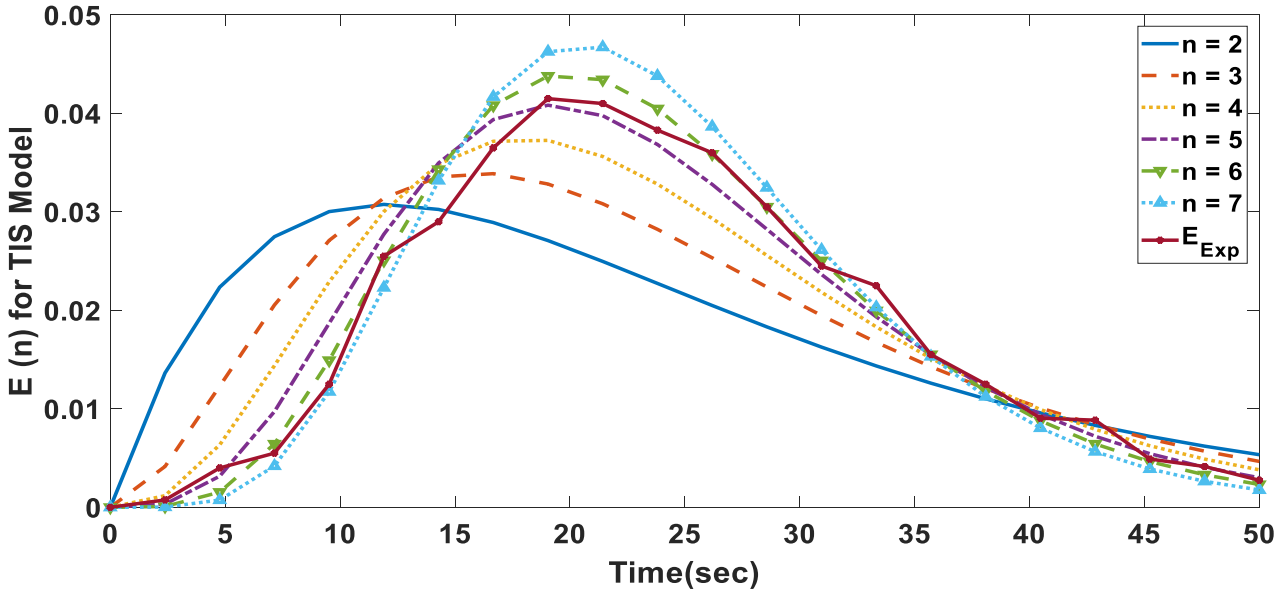


Figure 7: RTD mapping of the tank in series (TIS) model with the experimental data

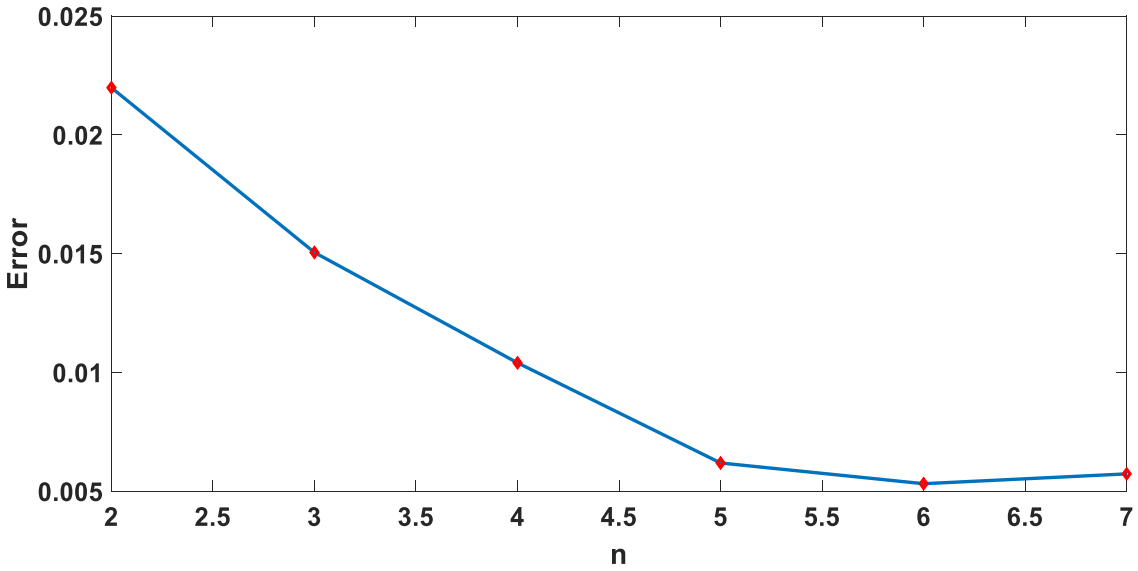


Figure 8: RTD mapping error of the tank in series model with the experimental data

Once we knew that unknown parameter then one can define the extent of hydrodynamic dispersion inside the reactor using that parameter value. To do so it is more convenient to work with dimensionless groups. The inverse of Pe_L is the vessel dispersion number, N_L. This is a measure of the spread of tracer in the whole reactor and is so defined:

$$N_L = \frac{1}{Pe_L} = \frac{D_{Axial}}{uL} = \frac{L/u}{L^2/D_{Axial}} \approx \frac{t_{Convection}}{t_{diffusion}} \quad (12)$$

The experimental RTD values were compared with the obtained analytical solution of the axial dispersion model (22), which holds in this study (Bo = 0.20, L/d_t = 49.44) . Levenspiel (17) suggested the analytical solution for small deviations from plug-flow (N_L > 0.01) under open-open ends boundary conditions as (21)

$$E\ Model\ 1 = \frac{1}{\sqrt{4\pi D_{Axial} t}} \exp\left(-\frac{(L-u_t)^2}{4D_{Axial}t}\right)$$ for large dispersion number, N_L > 0.01 (13)

$$E\ Model\ 2 = \sqrt{\frac{u^3}{4\pi D_{Axial} L}} \exp\left(-\frac{(L-u_t)^2}{4D_{Axial}L/u}\right)$$ for small dispersion number, N_L < 0.01 (14)

Bodenstein number is, $Bo = \frac{ud_t}{D_m}$ (15)

where L is the length of the reactor, u the cross-section average velocity and D_{Axial} the axial dispersion coefficient, which need be calculated from the Taylor expression for dispersion (5):

$$D_{Axial} = D_m + \frac{u^2 {d_t}^2}{192\ D_m} \quad (16)$$

if Bo < 10, diffusion dominates over convection, the second term on the right-hand side of the above equation can be omitted. But for Bo > 100, the first term can be neglected. This criterion seems not to fit well in our study. It seems from the experimental evidence that this study comes in an intermediate stage which consists both of diffusion as well as convective mechanism. For the coiled tube reactor, there is no straight forward relation available for the applicability of the model. The residual error of the fitting may be used for validation purposes. It is reported that for Dean number, De < 0.5, applicability validation relation for straight tube can be used (23). But in this study, Dean number, De, has a value of 117.61. However, for crosschecking purposes, we have applied that relation too. The analytical solutions provide by equations (13 & 14) depend on the vessel dispersion number N_L which is not known before fitting of the experimental data. Therefore, both solutions need to be applied to find a suitable model. To check the applicability of the axial dispersion model, the following relation has been used.

$$\tau_{ADM} = \frac{\bar{t}}{{d_t}^2/D_m} > \frac{6}{N_{Re}} \quad (17)$$

valid condition: $0 < \lambda < 280\ and\ N_{Re} < 1000$ and the mean residence time of the vessel, $\bar{t} = u/L$.Our study parameters come under this valid range. The geometry of the coiled tube reactor is responsible for the development of two major mechanisms: the first one is secondary flow and the second one is interchanging velocity between adjacent fluid layers. The development of these mechanisms can be verified by Dean number, De. Dean's number expresses the magnitude of the developed secondary flow. If De < 1.5, it can be assumed that the secondary flow is absent while 1.5 < De < 3, fully developed secondary flow can be assumed. Therefore, the secondary flow comes in the picture in this study. For methylene blue dye in water, molecular diffusivity goes around 6.74±1.32×10-6 cm^2/sec. In general, the liquid diffusivity has exponent in the range of -6. In equations 13 and 14, the only unknown parameter is the axial diffusion. The length of the coiled tube reactor was measured and the mean internal velocity was calculated as $u = \dot{v}/A$ with $\dot{v}$ the volumetric flow rate and A the cross-section area of the coiled tube reactor. The unknown axial dispersion coefficient was estimated using the least-squares minimization technique.

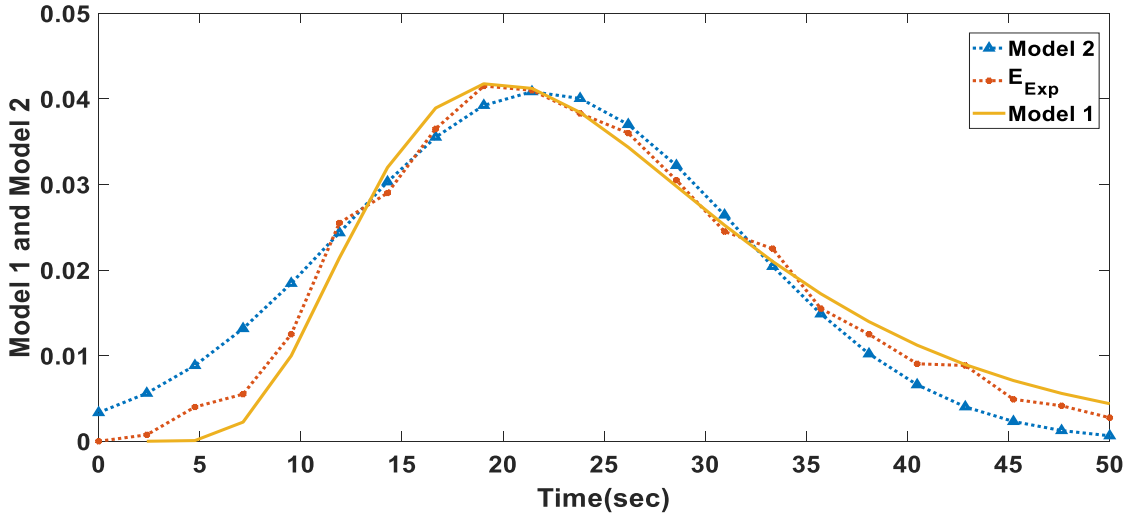


Figure 9: Fitting of Model 1 and Model 2 to the experimental data.

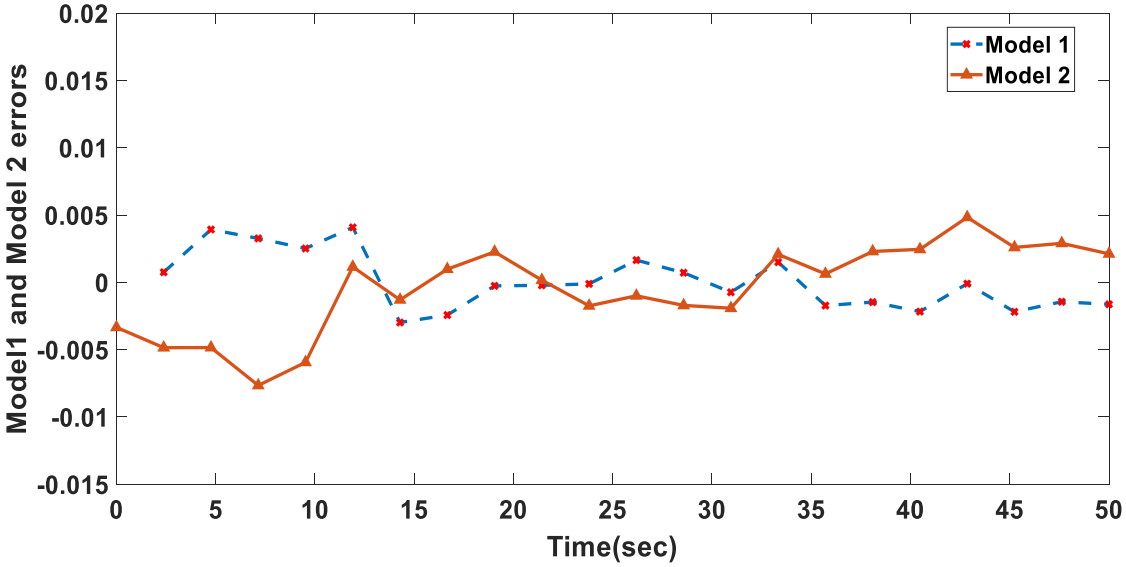


Figure 10: Models 'error with respect to the experimental data

Figure 9 depicts the output of the Model1 and Model 2 with time. It is clear that Model 1 is more reliable and seems good to fit in comparison to Model 2. The same conclusion can also be drawn from figure 10.

4.5 Convolution and deconvolution

The convolution integral is an important property to investigate RTD data. From our previous experience about carrying out the RTD experiments, the major challenge is generally related to the injection of the tracer. In addition, the injection point of MB dye may be located at a fixed distance from the inlet boundary of the vessel, the shape of the MB dye stimulus produced by the dye injector change as it moves towards the vessel entrance. As a result, the RTD curve cannot always be derived directly from the experimental measurement of the transient concentration in the effluent stream, C_{out}. However, if one knows C_{in}, by detecting it as a function of time at the inlet, the convolution integral method allows the extracting of the RTD of the coiled tube reactor. This methodology is called deconvolution, E being one of the factors of the convolution product. The convolution operation is used to get the output response of a linear and time-invariant system. If the input and impulse responses of a system are $C_{in}[o]$ and $E[n]$, respectively, then the output $C_{out}[o]$ of the system is given by convolution operation (24).

$$C_{out}[1 \times o] = C_{in}[1 \times m] * E[m \times o] = \sum_{-\infty}^{\infty} C_{in}[1 \times m]E[m \times o] \quad (18)$$

The convolution implemented between the discrete-time signals is usually called a convolution sum. If $C_{in}[m]$ is m points sequence and $E[n]$ is an n points sequence then $C_{out}[o]$ will be (m+n-1) points sequence. Deconvolution operation is performed by the reversed operation of the convolution (25). It is used to separate the mixed signals. This is an important part of this study. To the best of authors 'knowledge, no such study over the coiled tube reactor has been reported so far. For illustration purposes, a simple representation has been shown in figure 11. In this study, C_{out} is the only measurable. Different samples were taken at the outlet point of the coiled tube reactor and the corresponding concentrations, C_{out}, were measured using a colorimeter. Using C_{out}, E_{Exp} was calculated both in the time domain and in the dimensionless form.

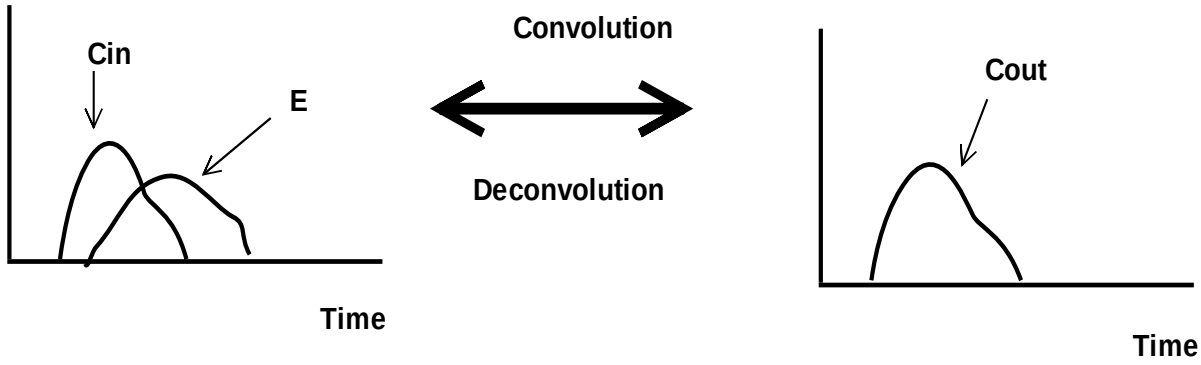


Figure 11: Convolution and deconvolution of the concentration signals

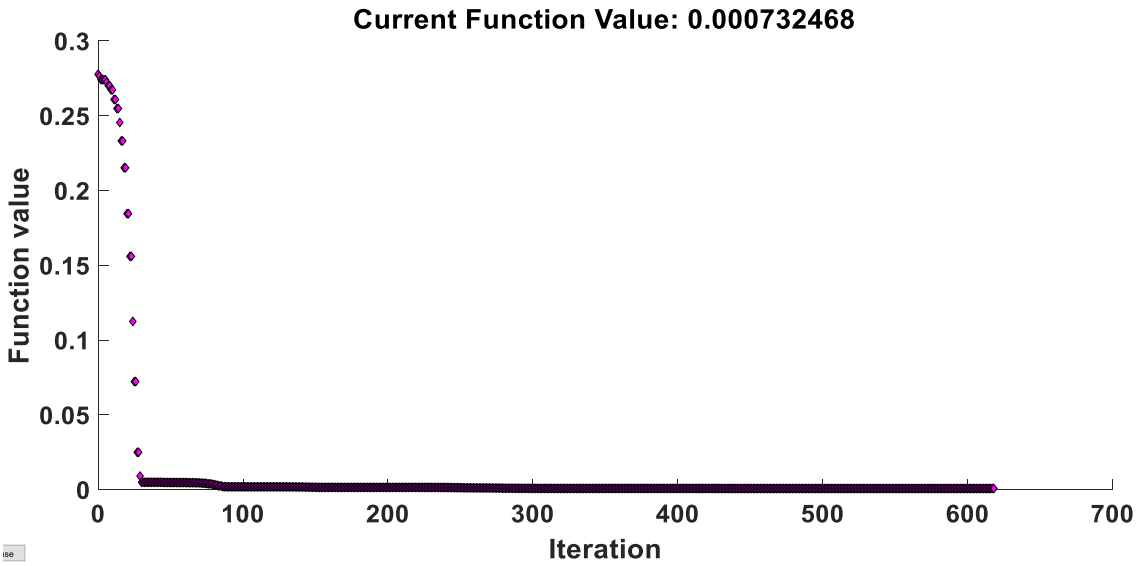


Figure 12: Optimization function values with respect to the number of iterations

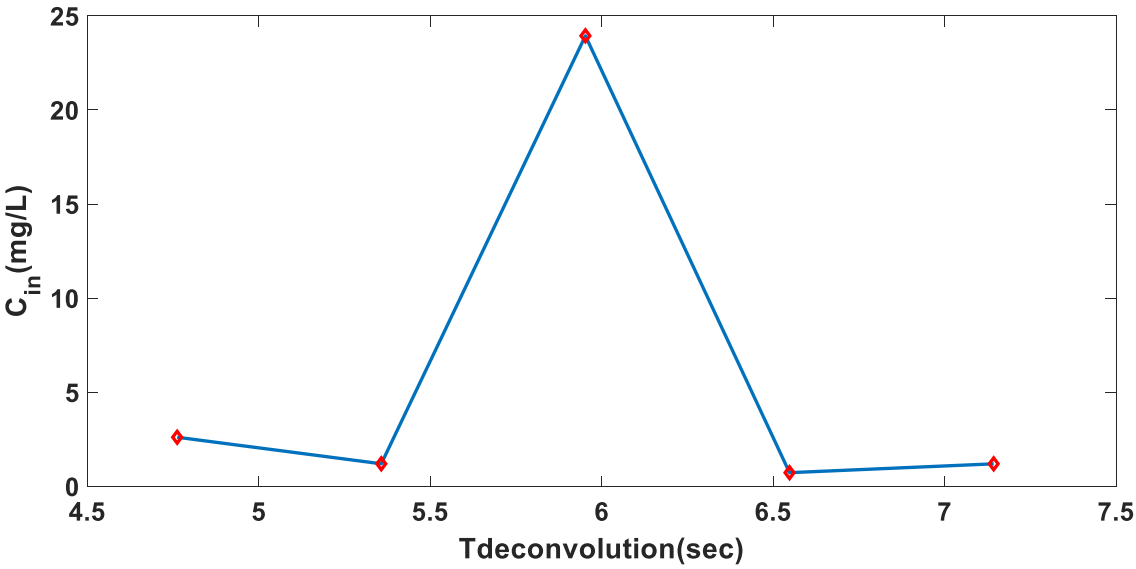


Figure 13: Deconvolution signal C_{in} from E and C_{out} signals

The concentration of tracer is in mg/l at the outlet of a continuous system. The deconvolution theorem has been applied to a de-combination of the RTD and C_{out} of the coiled tube reactor. In general, to calculate the signal exit of a reactor is known along with calculated RTD when the input signal is unknown. The major changeling in such a study is associated with the sampling of the output signals and the corresponding calculated RTD signals. In this study as shown in figure 11, the reactor distribution is E_{Exp} and the signal output is C_{out}, and we need to deconvolute both signals to get C_{in} (26):

$$C_{out} = \sum_0^\infty E_{EXP} \otimes C_{in} \quad (19)$$

It is noted that the deconvolution of the two signals is not possible if each signal has a different sampling increment interval. For deconvolution purpose, E_{Exp} = [E_1, E_2, E_3 ,..... E_{17}] has n = 17 values and C_{out} = [C_{out1}, C_{out2}, C_{out3} ,..... C_{out22}] has o = 22 values.

$$\begin{pmatrix} C_{out1} \\ C_{out2} \\ . \\ . \\ C_{outo} \end{pmatrix}_{o\times 1} = \begin{bmatrix} E_1\ 0 \dots\ 0 \\ E_2 E_1 \dots 0 \\ \vdots \\ 0\ 0 \dots E_{17} \end{bmatrix}_{o\times m} \cdot \begin{pmatrix} C_{in1} \\ C_{in2} \\ . \\ . \\ C_{in5} \end{pmatrix}_{m\times 1} \quad (20)$$

For simplification point of view, it can be written in the following matrix form

$$C_{out_{o\times 1}} = E_{EXP_{o\times m}} \otimes C_{in_{m\times 1}} \quad (21)$$

where E_{Exp} being the "matrix convolution," with values of *E* in the form of columns. The computation was done using a simple Matlab script. In Matlab, the sizing of the sample plays an important role. Here, 'o' represents the number of rows of the C_{out} vector,.i.e. o = m+n-1, where 'n' and 'm' represent the number of columns of E_{Exp} and C_{in} vectors, respectively. The calculations of the time vector associated with C_{in} were evaluated using cross ponding time vector of C_{out} and $E_{Exp.}$ As we can see, we have m = 5 unknowns and o = 22 equations, so the system is overdetermined and it has multiple solutions. For calculating the C_{in} curve, it is necessary to do the optimization by minimizing an objective function (O.F.) in the form of the sum of squared residuals between the C_{out} curve which is known and the product [E_{Exp}·C_{in}]:

$$OF = \sum(\ C_{out_{o\times 1}} - E_{Exp_{o\times m}} \otimes C_{in_{m\times 1}})^2 \quad (22)$$

Figure 12 represents the objective function values with respect to the number of iterations. The function value falls sharply after 20 iterations and continuously decreases with the number of iterations. The system calculation gets converged after 620 iterations and function obtains a minimum value of 0.000732. Figure 13 shows the evaluated deconvolution signals from E and C_{out} signals.

5 Conclusions

The study of the distribution of the residence time in a reactor helps to characterize the mixing phenomena and internal transport in the reactor. The comparison between the theoretically computed and experimentally determined RTD was guided us to develop a realistic mathematical model of the reactor understudy. Different mathematical models were tested to determine the performance of the coiled tube reactor. TIS model was tested first and n = 6 tanks found to be reasonable but it had shown the large deviation from the experimental data. Therefore, axial dispersion models were fitted. Two models were tested which are valid only for open-open boundary conditions. Model1 was more realistic to the experimental data and had fewer errors. In all the methods of testing and validation used, the results agree well. To validate the perfect pulse assumption, deconvolution of outlet concentration and exit age distribution signals was carried out. The evaluated inlet concentration seems to fit well with assumed assumptions.

Ethical issue

Authors are aware of and comply with, best practices in publication ethics specifically with regard to authorship (avoidance of guest authorship), dual submission, manipulation of figures, competing interests, and compliance with policies on research ethics. Authors adhere to publication requirements that submitted work is original and has not been published elsewhere in any language.

Symbols used

C_{out} (= C), C_{in}	[mg L^{-1}]	tracer outlet, inlet concentrations
d_t	[m]	diameter of the reactor
D_{Axial}	[m s^{-2}]	axial dispersion coefficient
E	[–]	residence time distribution (RTD)
E_θ	[–]	dimensionless RTD
E_{Exp}	[s]	experimental RTD
F		cumulative distribution function (CDF)
F_θ	[–]	dimensionless CDF
L	[m]	length of the reactor
N_{Re}	[–]	Reynolds number
t	[–]	time of measurement
u	[m s^{-1}]	average tracer speed
Bo	[–]	Bodenstein number
De	[–]	Dean number
Pe_L	[–]	Peclet number
o	[–]	length of C_{out} column vector
m	[–]	length of C_{in} column vector
n	[–]	length of E_{Exp} column vector
N_L	[–]	vessel dispersion number
D_m	[m s^{-2}]	molecular diffusivity
$\bar{t}$	[s^{-1}]	mean residence time

Greek letters

θ	[–]	dimensionless time vector
ρ	[kg m^{-3}]	density
λ	[–]	length to coil diameter ratio
τ	[s]	residence time of coiled tube reactor

Competing interests

The authors declare that no conflict of interest would prejudice the impartiality of this scientific work.

Authors' contribution

All authors of this study have a complete contribution to data collection, data analyses, and manuscript writing.

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