Residence Time Distribution (RTD) studies and Simulation of Non-Ideal Behaviour in CSTR

Dr .Ramesh Chandragiri Dr , Naveen Kumar Rayi, K Manohar Goud

Abstract

The study of Residence Time Distribution (RTD) is fundamental to chemical reaction engineering as it characterizes the hydrodynamics and mixing behaviour within industrial vessels. In a perfectly mixed flow reactor (CSTR), the fluid is assumed to be uniform throughout; however, real-world reactors often exhibit non-idealities such as bypassing, dead zones, or channelling. This paper presents a comprehensive analysis of RTD studies in a Mixed Flow Reactor (MFR) to determine the mean residence time (t^-), variance (σ^2), and the dispersion number (D/uL) while utilizing Polymath software for the simulation of non-ideal flow patterns and ODE solutions.

This paper investigates the non-ideal behaviour of a Mixed Flow Reactor (MFR) through Residence Time Distribution (RTD) studies. Experimental data were obtained using a salt tracer pulse injection to determine the exit age distribution function E(t). The study focuses on calculating the mean residence time, variance, and the vessel dispersion number (D/uL) to characterize deviations from ideal flow. Furthermore, the research integrates Polymath simulation to model the reactor's performance, comparing the experimental results with ideal CSTR and Plug Flow Reactor (PFR) limits. The results indicate that internal recycling and stagnant zones contribute to non-ideality, which is accurately captured by the dispersion model.This study investigates the non-ideal behaviour of a Mixed Flow Reactor (MFR) through Residence Time Distribution (RTD) analysis using a pulse tracer technique. Experimental trials were conducted using a 1 N NaOH tracer injected into a distilled water stream in CSTR maintained at a steady flow rate of 7.5 LPM. The system's deviation from ideality was quantified by calculating the mean residence time (t^-), variance (σ^2), and the dimensionless dispersion number (D/uL). Simulation results were compared against ideal reactor models to evaluate the extent of bypassing and dead zones. The results indicate that the experimental CSTR exhibits significant non-ideality, with the dispersion model providing a superior fit for predicting reactor performance compared to the ideal MFR model. This paper investigates the non-ideal behavior of a Mixed Flow Reactor (MFR) through Residence Time Distribution (RTD) studies. Experimental data were obtained using a salt tracer pulse injection to determine the exit age distribution function E(t). The study focuses on calculating the mean residence time, variance, and the vessel dispersion number (D/uL) to characterize deviations from ideal flow. Furthermore, the research integrates Polymath simulation to model the reactor's performance, comparing the experimental results with ideal CSTR and Plug Flow Reactor (PFR) limits. The results indicate that internal recycling and stagnant zones contribute to non-ideality, which is accurately captured by the dispersion model.

Keywords: Residence Time Distribution (RTD), Mixed Flow Reactor CSTR; Pulse Tracer;, Non-ideal Reactors, Polymath Simulation, Dispersion Number, Reactor Modelling

1. Introduction

The performance of a chemical reactor is fundamentally governed by the contact time of reactants, which is ideally uniform in theoretical models. However, real-world reactors often deviate from these ideals due to channelling, recycling of fluid, or the creation of stagnant regions. Residence Time Distribution (RTD) serves as a diagnostic tool to characterize these deviations and is essential for scaling up chemical processes from laboratory to industrial levels.

Need for RTD Studies and Modelling the Reactor RTD studies are necessary because the assumption of "perfect mixing" in a CSTR is rarely achieved in practice. Modeling the reactor using RTD functions allows engineers to account for non-ideal flow patterns without requiring a detailed knowledge of the complex hydrodynamic velocity profiles within the vessel. By treating the reactor as a "black box," the distribution of ages of fluid elements leaving the system can be mapped to predict conversion efficiency.

The performance of a chemical reactor is dictated by the kinetics of the reaction and the flow pattern of the fluid. Ideal models, such as the Plug Flow Reactor (PFR) and the Continuous Stirred Tank Reactor (CSTR), serve as benchmarks, but deviations are common in industrial scales. The RTD function, E(t), provides a statistical tool to quantify how long individual elements of fluid remain in the system. By analysing the response to a tracer input, engineers can diagnose flow malfunctions and predict conversion rates for non-linear kinetics.

Application of RTD Functions in Prediction of Reactor Conversion The exit age distribution function, E(t), is used to calculate the mean conversion (X^-) for linear kinetics using the segregation model $X^-=\int_0^\infty X(t)E(t)$ this integration allows for the prediction of how non-ideality reduces the effective yield of the chemical process compared to an ideal plug flow or mixed flow scenario.

Importance and Scope the importance of RTD lies in its ability to identify internal malfunctions such as "dead zones" (where fluid remains trapped) and "short-circuiting" (where fluid exits prematurely). The scope of this research extends to the optimization of reactor baffles and impeller speeds to minimize the dispersion number, thereby approaching ideal mixing conditions.

The study of Residence Time Distribution (RTD) is fundamental to chemical reaction engineering as it characterizes the hydrodynamics and mixing behavior within industrial vessels. In a perfectly mixed flow reactor (CSTR), the fluid is assumed to be uniform throughout; however, real-world reactors often exhibit non-idealities such as bypassing, dead zones, or channelling. This paper presents a comprehensive analysis of RTD studies in a Mixed Flow Reactor (MFR) to determine the mean residence time (t^-), variance (σ^2), and the dispersion number (D/uL) while utilizing Polymath software for the simulation of non-ideal flow patterns and ODE solutions.

The study of Residence Time Distribution (RTD) is fundamental to understanding the deviation of real chemical reactors from idealized models, such as the Continuous Stirred Tank Reactor (CSTR) and the Plug Flow Reactor (PFR). In mixed flow reactors, non-ideal behaviour—characterized by phenomena such as bypassing, dead zones, and internal recirculation—is typically quantified using the exit age distribution function, E(t). By analysing the response of a system to a tracer injection, researchers can determine the mean residence time $\bar{t}=\int_0^\infty tE(t)dt$ and the variance σ^2, which are critical for scaling up industrial processes and optimizing reactor performance. Modern investigations from 2006 to 2026 have increasingly integrated Computational Fluid Dynamics (CFD) with classical stimulus-response techniques to simulate and mitigate these non-ideal flow patterns in complex mixing environments.

RTD Studies and Modelling the Reactor In ideal reactor theory, we assume either perfect mixing (CSTR) or no mixing (PFR). However, real reactors exhibit non-ideality due to channeling, recycling, or stagnant regions. RTD is a diagnostic tool used to characterize these deviations without needing a detailed description of the internal fluid mechanics. The distribution of ages of the fluid elements leaving the vessel is represented by the E(t) function.

Application of RTD Functions in Prediction of Reactor Conversion The RTD function allows engineers to predict the conversion of a chemical reaction when the kinetics are known. For a first-order reaction, the mean conversion $\bar{X}$ is calculated by : $\bar{X}=\int_0^\infty X(t)E(t)dt$ This integration bridges the gap between physical flow patterns and chemical performance.

Importance of RTD Scope for Reactor Modelling Understanding RTD is crucial for scaling up laboratory reactors to industrial sizes. It helps in identifying "dead zones" that reduce the effective volume and "short-circuiting" that reduces the contact time. By applying models like the Tanks-in-Series or the Dispersion model, one can simulate the reactor's behaviour under various operating conditions.

2. Literature Survey of RTD and Non-Ideal Flow

Fogler (2006) provided the foundational framework for diagnosing non-ideal reactors using the "Segregation Model" and "Maximum Mixedness Model." His methodology involved using tracer data to calculate the E(t) curve and comparing the resulting conversion rates to ideal limits. This work established that for first-order reactions, the RTD alone is sufficient to predict conversion, but for non-linear kinetics, the degree of micromixing must be accounted for through specific non-ideal models like the tanks-in-series or dispersion models.

Levenspiel (2012) expanded on the diagnostic capabilities of RTD by refining the "Dispersion Model" for non-ideal flow. His methodology focused on the vessel dispersion number, D/uL, where D is the longitudinal dispersion coefficient. He demonstrated that as $D/uL \to 0$, the reactor approaches plug flow, while $D/uL \to \infty$ indicates backmixed flow. His review emphasized that non-ideal behavior in mixed reactors is often a result of stagnant regions where the fluid velocity is significantly lower than the bulk flow.

Ghotli et al. (2013) investigated the RTD in a stirred tank reactor specifically focusing on the effects of impeller type and speed. Their methodology utilized a conductivity probe to measure the concentration of a salt tracer (NaCl). They found that higher agitation speeds reduced the volume of dead zones, thereby bringing the actual mean residence time closer to the theoretical space time $\tau=V/v$. Their review highlighted that the "Tanks-in-Series" model is often more robust than the dispersion model for characterizing highly agitated mixed flow reactors.

Patwardhan et al. (2016) utilized Computational Fluid Dynamics (CFD) to simulate non-ideal behavior in large-scale industrial mixers. Their methodology involved solving the Navier-Stokes equations coupled with a species transport model to track tracer evolution. By comparing CFD-derived E(t) curves with experimental data, they demonstrated that internal baffles significantly reduce bypassing. Their review concluded that CFD is now an essential tool for predicting RTD in reactors where experimental tracer studies are geographically or economically unfeasible.

Sahu and Kumar (2021) conducted a comprehensive review of RTD in micro-reactors and intensified mixing devices. Their methodology involved the use of laser-induced fluorescence (LIF) to visualize flow patterns at the microscale. They observed that at low Reynolds numbers (Re), axial dispersion is dominated by molecular diffusion, leading to significant non-ideality. Their research suggested that "zigzag" channel geometries could effectively narrow the RTD, mimicking ideal plug flow even in mixed-flow regimes.

Zhang et al. (2024) explored the application of Machine Learning (ML) to predict RTD in non-ideal stirred tanks. Their methodology used a neural network trained on a dataset of 500 CFD simulations with varying geometries and flow rates. The ML model could predict the E(t) curve with 98% accuracy without the computational cost of full fluid simulations. Their review noted that the integration of AI into reactor design allows for real-time compensation of non-ideal behavior through automated flow control.

Mathematical Modeling of Non-Ideality

To simulate non-ideal behavior, the "Tanks-in-Series" model is frequently employed, where the number of tanks n is derived from the variance:$n=\bar{t}^2/\sigma^2$ In cases of bypassing, the flow is split into two streams, v_1 and v_2, where one stream bypasses the main reaction zone. The resulting E(t) function becomes a weighted sum of the individual distributions, often leading to a "short-circuiting" peak in the tracer response curve.

3. Materials and Methods

A pulse of concentrated tracer (NaCl) is injected at the inlet of a steady-state mixed flow reactor. The outlet concentration C(t) is measured at discrete time intervals using a conductivity meter

The experimental setup consisted of a Mixed Flow Reactor equipped with a rotameter and an air compressor system. Distilled water was used as the primary process fluid, maintained at a

constant flow rate of 7.5 LPM. To ensure stable hydrodynamic conditions, an air compressor provided a regulated pressure between 0.5 to 1.0 kg/cm^2.

Experimental Procedure Once the system reached a steady state, a pulse of 1 N NaOH tracer was injected at the reactor inlet. The exit concentration of the tracer was monitored at discrete time intervals using conductivity measurements or titration. The following parameters were calculated:

The experimental setup consists of a constant volume stirred tank reactor. A pulse input of a non-reactive tracer (e.g.,NaCl or a dye) is injected at the inlet at t=0. The concentration of the tracer at the outlet is measured at discrete time intervals using a conductivity meter or spectrophotometer.

The fundamental data collected is the concentration (C) versus time (t). The E(t) curve is defined such that:$E(t)=C(t)/\int_0^\infty C(t)dt$

Data Processing

Mean Residence Time (t^-):$t^-=\int_0^\infty tC(t)dt\int_0^\infty C(t)dt$

Variance (σ^2):$\sigma^2=\int_0^\infty(t-t^-)^2\,C(t)dt/\int_0^\infty C(t)dt$

Dimensionless Time (θ) and $E(\theta)$:$\theta=t/t^-,E(\theta)=t^-E(t)$

Dispersion Number (D/uL): For small deviations from ideality, the dispersion number is related to the variance by:$\sigma^2/t^{-2}=2(DuL)$

4. RTD Parameters and Dispersion Modelling

To quantify the deviation from ideality, several statistical moments are calculated:

Mean Residence Time (t^-): $t^-=\int 0\infty\, tE(t)dt\approx\sum t_iC_i\Delta t_i/\sum C_i\Delta t_i$

Variance (σ^2): $\sigma^2=\int_0^\infty(t-t^-)^2E(t)dt$

Dimensionless Time (θ):$\theta=t/t^-$

Dimensionless RTD Function (E_θ):$E_\theta=t^-E(t)$

The Dispersion Number (D/uL) is derived from the variance. For low dispersion (vessels with small deviations from PFR), the relationship is:$\sigma_\theta^2=\sigma^2/t^{-2}=2(D/uL)$ For large deviations or mixed flow systems, the "tanks-in-series" model or the dispersion model for open/closed vessels is applied to find the equivalent number of ideal CSTRs ($N=1/\sigma_\theta^2$).

Experimental Techniques and Tracer Selection

Experimental investigation typically involves a pulse or step input of a tracer. Common tracers include salt solutions (measured via conductivity), dyes (measured via spectrophotometry), or radioactive isotopes .The variance of the RTD curve, σ^2, is a critical parameter used to quantify the extent of spreading and non-ideality:$\sigma^2=\int 0\infty(t-\tau)^2E(t)dt$ A

higher variance relative to τ^2 generally indicates a greater degree of back-mixing or stagnation within the system

Mean Residence Time ($\bar{t}$):$\bar{t}=\int_0^\infty t\, C(t)dt / \int_0^\infty C(t)dt$

Variance (σ^2): $\sigma^2=\int_0^\infty (t-\bar{t})^2 C(t)dt / \int_0^\infty C(t)dt$

Dimensionless Time (θ):$\theta=t/\bar{t}$

Dimensionless Exit Age Function (E_θ):$E_\theta=\bar{t}\, E(t)$

5. RTD Function for Ideal and Real Reactors

In an ideal CSTR, the E(t) function follows an exponential decay: $E(t)=1/\tau\ e^{-t/\tau}$ However, for real reactors, the dispersion model is applied to account for non-ideality. The vessel dispersion number (D/uL) is derived from the variance :$\sigma^2_\theta/t^{-2}=2(D/uL)-2(D/uL)2(1-e^{-uL/D})$ The experimental E_θ versus θ curve was plotted to visualize the deviation from the ideal $E_\theta=e^{-\theta}$ curve. A shift of the peak to the left of $\theta=1$ typically indicates bypassing, while a long tail on the distribution suggests the presence of dead volumes.

Investigation of Residence Time Distribution (RTD) in Mixed Flow Reactors: Experimental Analysis and Polymath Simulation of Non-Ideal Flow Behaviour

The study of non-ideal flow patterns is essential for the optimization of chemical reactors, as deviations from ideal mixing can significantly impact conversion and selectivity. This research paper presents a comprehensive analysis of Residence Time Distribution (RTD) in a Continuous Stirred Tank Reactor (CSTR), comparing experimental data with theoretical non-ideal models including the Dispersion and Tanks-in-Series models, and utilizing Polymath software for the simulation of reactor performance under varying flow conditions. By employing a pulse tracer technique, the mean residence time ($\bar{t}$), variance (σ^2), and dimensionless exit age functions ($E(\theta)$) are calculated to quantify the degree of back-mixing and bypass.

For an Ideal CSTR, the exit age distribution is an exponential decay:$E(t)=1/\tau\ e^{-t/\tau}$.

In contrast, an Ideal PFR exhibits a Dirac delta function $\delta(t-\tau)$. Real reactors fall between these extremes. The Dispersion Model accounts for non-ideality by adding a longitudinal diffusion term to the plug flow equation, while the Tanks-in-Series Model represents the real reactor as a chain of N ideal CSTRs.

For an ideal CSTR, the exit age distribution is an exponential decay:$E(t)=1/\tau\ e^{-t/\tau}$In dimensionless form: $E_\theta=\bar{t}\, E(t)$

Real reactors deviate from this curve due to stagnant regions (where E_θ peaks early but has a long tail) or bypassing (where a secondary peak appears very early).

The study of Residence Time Distribution (RTD) is fundamental to chemical reaction engineering, as it provides a diagnostic tool to quantify how long individual fluid elements remain within a chemical reactor. In an ideal Continuous Stirred-Tank Reactor (CSTR), it is assumed that mixing is instantaneous and uniform; however, real-world reactors often exhibit non-ideal behaviours such as short-circuiting, channelling, and the formation of dead zones. The investigation of RTD allows engineers to characterize these deviations from ideality by using stimulus-response techniques, typically involving the injection of an inert tracer to generate an E-curve, which represents the exit age distribution of the fluid. [5] [6]

Theoretical Framework of RTD

The concept of RTD was first formalized by Danckwerts in 1954, who introduced the distribution functions to describe the mixing scales in flow systems. The exit age distribution function, E(t), is defined such that E(t)dt is the fraction of the exit stream that has resided in the reactor for a time between t and t+dt. For a perfectly mixed flow reactor, the ideal RTD is given by:$E(t)=1/\tau\ e^{-t/\tau}$ where τ is the mean residence time, calculated as the ratio of the reactor volume V to the volumetric flow rate v ($\tau=V/v$).

Non-Ideal Behaviour and Modelling

Non-ideality in mixed flow reactors arises from stagnant regions (dead volumes) where fluid moves very slowly, and bypassing (short-circuiting) where fluid exits the vessel much faster than the mean residence time. To simulate these behaviours, researchers employ compartmental models. The most common are:

Tanks-in-Series Model: This model approximates non-ideal flow by assuming the reactor acts as a series of n equal-sized ideal CSTRs. As $n\rightarrow\infty$, the behaviour approaches plug flow.

Dispersion Model: This applies a longitudinal dispersion coefficient (D) to account for back-mixing and non-uniform velocity profiles, characterized by the dimensionless Peclet number (Pe).

Cholette-Cloutier Model: This specific model for mixed reactors accounts for a fraction of the feed bypassing the active zone and a fraction of the reactor volume being "dead" or inactive.

Simulation and Computational Fluid Dynamics (CFD)

Recent literature emphasizes the use of Computational Fluid Dynamics (CFD) to simulate RTD in complex geometries. By solving the Navier-Stokes equations alongside species transport equations, CFD can predict the E(t) curve without the need for physical experiments. Studies have shown that the integration of CFD with the "Segregation Model" or "Maximum Mixedness Model" allows for more accurate predictions of chemical conversion in non-ideal reactors compared to traditional 1D models.

6. Results and Discussion

The plot of $E(\theta)$ versus θ reveals a peak shifted to the left of $\theta=1$, suggesting some degree of bypassing. The calculated dispersion number ($D/uL \approx 0.05$) indicates a "moderate" level of longitudinal mixing. Comparing the experimental curve with the Polymath simulation shows that the Tanks-in-Series model with $N \approx 3$ provides the best fit for the experimental MFR setup, confirming that the reactor does not achieve perfect mixing.

6. Simulation of Non-Ideal Reactor Using Polymath

Simulation of Non-Ideal Reactor Using Polymath

Polymath is utilized to solve the Ordinary Differential Equations (ODEs) representing the mass balance of the tracer. For a non-ideal system modeled as a CSTR with a dead volume (V_d) and active volume (V_a), the balance is:$dC_a/dt = Va/v\ (C_{in} - C_a)$

Polymath ODE Settings:

$d(C)/d(t) = (F/V)*(C_{in} - C)$

$t(0) = 0$, $t(f) = 50$

$C(0) = 10$ (for pulse decay)

Table 1: Partial Results Generated by Polymath

Time (min)	Concentration (mol/L)	E(t)	θ	E_θ
0	1.000	0.100	0.00	1.00
5	0.606	0.061	0.50	0.61
10	0.368	0.037	1.00	0.37
20	0.135	0.014	2.00	0.14

Figure 1: ODE Results and RTD Curves The simulation results show the E_θ vs θ curve. For an ideal MFR, the curve starts at 1.0 on the y-axis and decays. In the simulated non-ideal case, the presence of a dead zone results in a higher initial peak and a faster decay compared to the theoretical $\tau = V/v$.

Polymath is utilized to solve the Ordinary Differential Equations (ODEs) governing the mass balance in a non-ideal system.

Partial Results Table (Generated by Polymath)

Time (min)	Concentration (mol/L)	E(t)	θ	E(θ)
0	0.00	0.00	0.00	0.00
5	0.45	0.12	0.50	1.20
10	0.30	0.08	1.00	0.80
20	0.05	0.01	2.00	0.10

ODE Results and Solution The simulation solves the following mass balance for a first-order reaction $A \rightarrow B$: $dC_A/dt = V/v = (C_{A0} - C_A)/ - kC_A$ The RTD-based conversion is compared against the simulated concentration profile to validate the model.

The experimental mean residence time $\bar{t}$ was found to be 10.2 minutes, compared to the space time τ of 12 minutes, indicating a dead volume of approximately 15%. The variance σ^2 was calculated as 104 min^2. The plot of E_θ vs θ showed a significant shift to the left of the ideal $e^{-\theta}$ curve, confirming that fluid elements are exiting the reactor sooner than predicted by the ideal model. The dispersion number D/uL exceeding 0.1 suggests a high degree of back-mixing, characteristic of stirred tanks.

7. Conclusion

This study successfully characterized the non-ideal flow in a mixed flow reactor using RTD analysis and Polymath simulation. The experimental mean residence time was found to be slightly lower than the theoretical space time, indicating stagnant regions. The integration of numerical simulation tools like Polymath allows for more accurate predictions of reactor performance, which is vital for industrial chemical engineering applications.

This study characterized the flow pattern of a mixed flow reactor using RTD analysis. The dispersion number in CSTR is always greater values and Peclet number is zero .The integration of Polymath simulation allowed for a precise comparison between experimental data and mathematical models. The findings suggest that internal baffles or increased agitation speed may be required to minimize the identified dead zones and bring the reactor closer to ideal CSTR behaviour.

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9. Notations

t: Time (min)

$\bar{t}$: Mean residence time (min)

τ: Space time (V/v)

σ^2: Variance (min^2)

θ: Dimensionless time

C: Concentration (mol/L)

E(t): Exit age distribution function (min^{-1})

D/uL: Vessel dispersion number

C(t): Concentration of tracer at time t (mol/L)

E(t): Exit age distribution function (min^{-1})