

Numerical Testing and Validation of a Model for Laminar Flow Tubular Reactor

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ABSTRACT: Non-ideality in the reactors is accounted traditionally using Residence Time Distribution (RTD) studies. However RTD studies are conducted on existing reactors. Therefore accounting for non-ideality at the design stage using RTD is not possible. There are several causes of non-ideality in the reactors. The non-ideality in Laminar Flow Tubular Reactor (LFTR) is due to variation in velocity in the radial direction, diffusion and convection effects of reacting and product species. One peculiar feature of LFTR is the non-ideality due to radial variation in velocity is mathematically deterministic. There is no work reported in the literature that makes use of this deterministic nature of non-ideality except some analytical methods for simple kinetics. The present paper deals with simple mathematical model that makes use of theoretical RTD of LFTR to predict the reactor performance for general kinetics by a numerical method. Testing and validation of the model is done for kinetics for which analytical solutions are not available. Algorithm for numerical testing is developed. The algorithm is used to develop computer code which is used to predict reactor performance and testing. The reactor performances predicted are compared with already well established methods. The results agree well.

KEYWORDS: Residence Time Distribution, Velocity Profile, Numerical method, Conversion, Laminar Flow Tubular Reactor.

I. INTRODUCTION

Reactor modelling that takes into account non-ideality at the design stage requires theoretical understanding of all the factors and phenomena that contribute to the reaction. The convection and diffusion effects of reacting and product species are computationally very intensive. Ideal reactor models make use of only macro mass conservation principles and some simplifying assumptions to arrive at equations called performance equations. Therefore though mixing contributes to the reaction, it does not play any role in the performance equations. The validity of assumptions to the real reactors plays an important role in the accuracy of performance prediction of the reactors using these equations. The simplest way of quantifying mixing adequate enough to incorporate kinetics in the evaluation of reactor is conventionally carried by using Residence Time Distribution (RTD) studies [1].

RTD studies are done on an existing reactor. It is a stimulus-response technique. There is no way RTD can be used at the design stage except the cases where RTD can be simulated using appropriate model. RTD information in the form of E-Curve is used to predict the reactor performance. Models used for this purpose are axial dispersion, recycle and tanks in series. These models are single parameter models [2] and are not adequate enough to be fitted to all reactors. In such cases multi-parameter models are used.

Reactor performance can also be predicted by numerically solving the Convection-Diffusion-Reaction (CDR) equations. This is computationally very intensive. Therefore low dimensional models are very popular and are used extensively despite their fallibility [3].

Another approach is to use Computational Fluid Dynamics (CFD) to obtain simulated RTD and then using this RTD reactor performance is predicted. Inappropriate RTD sampling and numerical diffusions can lead to significant deviations in the RTD predictions using CFD [4]. Advances in CFD and precision in measurements have improved the knowledge of the flow fields in the reactors. Velocity fields can easily be obtained from 3D CFD simulations. But an effective method for quantifying non-uniformity of mixing using such velocity fields is still not available in the literature. Measuring or computing flow pattern is helpful for some understanding of the non-uniform mixing but

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quantitative mixing measures cannot be obtained directly from velocity fields. RTD theory also cannot provide a definitive answer on the size, locations, and intensity of the non-uniformity [5].

Mixing in reacting flows is an important operation in the process industries. Laminar flow regime is very predominant in food processing and polymer processing and often involves viscous liquids. Modelling of the flow with reactions taking place during flow is a greater challenge and has been studied extensively in the last 50 years [6]. The RTD of a system modelled as a rigid pipe and laminar flow is a typical case in food processing industry [7]. Modelling of mixing processes in laminar flows though deterministic has not received much attention, and detailed analysis of such flows is still lacking, even though utility of these systems is significant [8]. The models that demand moderate computational time and still adequate enough to be practically useful are to be developed [9]. Despite the laminar flow is deterministic [10], not much work of its utility is available in the literature. In cases where diffusion is not a significant contributor to reaction, mathematically simpler models are to be developed. A model which makes use of velocity profile and predicts the performance of LFTR accurately has been recently reported [11]. The testing of this model is limited to analytical methods and therefore applicable to simple kinetics. The present work deals with testing of this model for generic kinetics using numerical methods.

II. VELOCITY PROFILE MODEL FOR LFTR

A model of LFTR which uses velocity profile has been presented by Kallur [11]. It is referred as VELOCITY PROFILE MODEL FOR LFTR (VPLFTR) in this paper. In this model, the tubular reactor is assumed to be split into several grid cells by slices, sectors and concentric circles as shown in Fig. 1. The velocity profile is assumed to be parabolic. The velocity at the geometric centre of face of the grid cell is known. Using this volumetric flow rate into the grid cell is determined. Using the geometry the volume of the grid cell is calculated. Thus space-time for each grid cell is determined. Assuming the grid cell to be ideal Continuous Stirred Tank Reactor (CSTR), conversion in each cell is determined. This calculation is done sequentially from the grid cells on the inlet face of the reactor proceeding towards the exit face of the reactor. Due to symmetry, processing is done for all the grid cells only in one sector (total of 40 in Fig. 1) and conversion at the exit cells are averaged to get the conversion in the reactor.

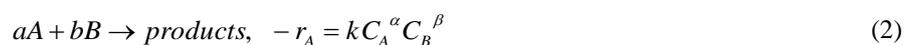


Fig. 1 Tubular Reactor with slices, sectors and concentric circles [11]

Important step in the algorithm of the model is the determination of conversion in the grid cell using the Equation (1).

$$X_{Ai} = \frac{\tau_i(-r_{Ai})}{C_{A0i}} \quad (1)$$

where i refers to a grid cell. For simple kinetics conversion can be determined analytically. For general kinetics given by



Solution of Equation (2) by analytical methods is not possible for all orders and all stoichiometric co-efficients. This paper deals with the development, testing of a numerical method to solve the performance equation for general kinetics.

Further the VPLFTR model was tested by comparing conversion in VPLFTR model with conversion in an independent method. The independent method used was segregated flow model limited to availability of analytical

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methods [11]. For general kinetics given above, numerical solution of segregated flow model is inevitable. There is no literature available for numerical solution of segregated flow model for general kinetics. This paper deals with an algorithm for numerical solution of segregated flow model and the same is used to test and validate VPLFTR.

III. NUMERICAL SOLUTION OF PERFORMANCE EQUATION

Using the kinetics given by Equation (2) in Equation (1), cell wise conversion is given by Equation (3).

$$k\tau_i C_{A0i}^{\alpha+\beta-1} (1-X_{Ai})^\alpha \left(M - \frac{b}{a} X_{Ai} \right)^\beta - X_{Ai} = 0 \tag{3}$$

Equation (3) is a polynomial of the order $(\alpha+\beta)$ in X_{Ai} .

An algorithm (Newton – Raphson) to solve Equation (3) was developed. Code was written and used to determine the conversion in the cells in a sequential manner to obtain the conversion in LFTR. For $a = b = 1$ and $\alpha = \beta = 1$, Equation (3) was solved analytically. The code which is in terms of a, b, α and β was run with all these values initialized to 1. Analytical solution and computer results were found to be in complete agreement. This confirms that the code solves Equation (3) for any values of a, b, α and β . After validating the code to solve Equation (3), the code was used to determine the conversion in each grid cell of VPLFTR in a sequential manner. Conversion in the VPLFTR model was thus determined for $a = b = 1$ and $\alpha = \beta = 1$.

Conversion thus obtained was tested against another independent method viz., segregated flow model for LFTR. Analytical Equation for conversion in LFTR is given by

$$X_A = k C_{A0} \bar{t} \left[1 - \frac{k C_{A0} \bar{t}}{2} \ln \left(1 + \frac{2}{k C_{A0} \bar{t}} \right) \right] \tag{4}$$

Conversion obtained in the VPLFTR model using Equation (3) and conversion obtained using Equation (4) for one case in which $C_{A0} = C_{B0} = 50$ is given in Fig 2. From Fig 2 it is clear that the conversions completely agree.

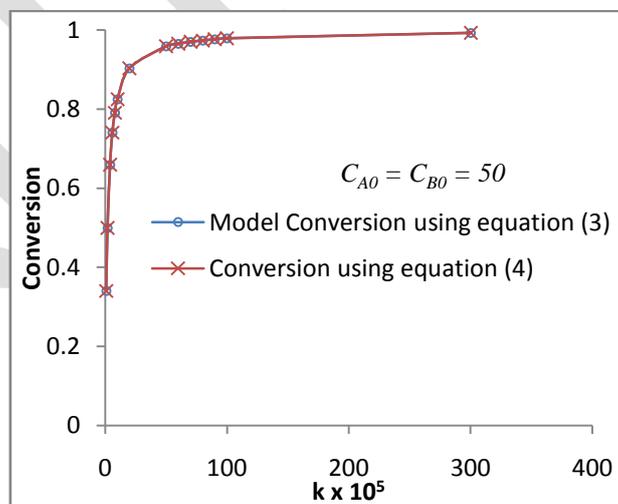


Fig. 2 Comparison of conversions in the VPLFTR model and LFTR

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The code to solve Equation (3) can take any values of stoichiometric co-efficients and orders.

IV. SEGREGATED FLOW MODEL AND NUMERICAL TESTING OF VPLFTR

Segregated flow model is one of the models available to determine conversion in a flow reactor for which RTD information is available. RTD information is obtained from a reactor by conducting stimulus-response experiment. During steady state operation of the reactor, a substance called tracer [1] is injected into the reacting mixture at the inlet and outlet tracer concentration as function of time is noted. From concentration vs. time, E-Curve which describes time distribution of different elements in the reactor is obtained. E-curve information is then used to model the flow reactor for which the experiment was conducted. Segregated Flow Model uses E-Curve information to predict the reactor performance. With known information on E-Curve either experimental or theoretical, the conversion in the reactor is given by Equation (5).

$$X_A = 1 - \frac{\bar{C}_A}{C_{A0}} = 1 - \int_0^\infty \left(\frac{C_A}{C_{A0}} \right)_{el} \cdot E dt \tag{5}$$

The segregated model assumes infinitesimally small batch reactors in transit, each reactor undergoing different extents of conversion. The term $(C_A/C_{A0})_{el}$ is the conversion taking place in such hypothetical batch reactor. This $(C_A/C_{A0})_{el}$ can be expressed as function of time in the Equation (5) and the performance of the reactor can be evaluated. Analytical solutions are available to solve the Equation (5) for simple kinetics. For higher order reactions and orders with fractional orders numerical methods are to be used. Numerical method for the reaction given in Equation (6) is presented here.



Applying batch reactor performance equation to the rate Equation in (6), we get

$$\left(\frac{\bar{C}_A}{C_{A0}} \right)_{el} = \int_0^\infty \left\{ 1 - \frac{M(1 - \exp[k C_{A0}(M-1)t])}{1 - M \cdot \exp[k C_{A0}(M-1)t]} \right\} \cdot E dt \tag{7}$$

Theoretical E-Curve of LFTR is given by Equation (8).

$$E(t) = \begin{cases} 0 & \text{for } t < \frac{\bar{t}}{2} \\ \frac{(\bar{t})^2}{2t^3} & \text{for } t \geq \frac{\bar{t}}{2} \end{cases} \tag{8}$$

Combining Equation (7) with Equation (8) results in Equation (9).

$$\left(\frac{\bar{C}_A}{C_{A0}} \right)_{el} = \int_{\bar{t}/2}^\infty \left\{ 1 - \frac{M(1 - \exp[k C_{A0}(M-1)t])}{1 - M \cdot \exp[k C_{A0}(M-1)t]} \right\} \cdot \frac{(\bar{t})^2}{2t^3} dt \tag{9}$$

Since integration in Equation (9) cannot be carried out till time equal to infinity, it was carried out till time equal to three times the space-time of the reactor. There was no change in the conversion for higher values of t. Comparison between model conversion and that obtained using Equation (9) for various values of M and k agree. This comparison for $C_{A0} = 50$ and $M = 1.2$ is given in Fig. 3.

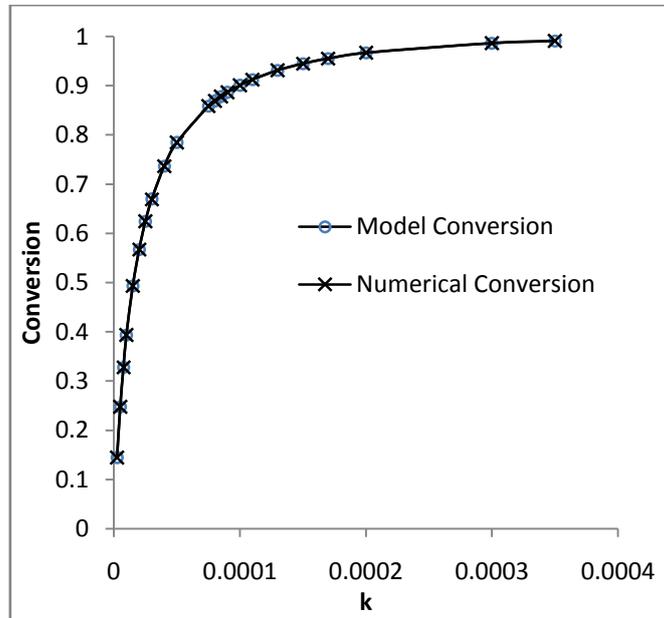


Fig. 3 Conversion in the VPLFTR model and numerical segregated flow model

For $M \neq 1$, the dimensionless number equivalent to N_{Da} is $kC_{A0}(M - 1)\tau$. The difference between model conversion and that in Ideal plug flow reactor were plotted against $kC_{A0}(M - 1)\tau$. This plot results in single curve for a given value of M . Fig. 4 gives these curves for two values of M .

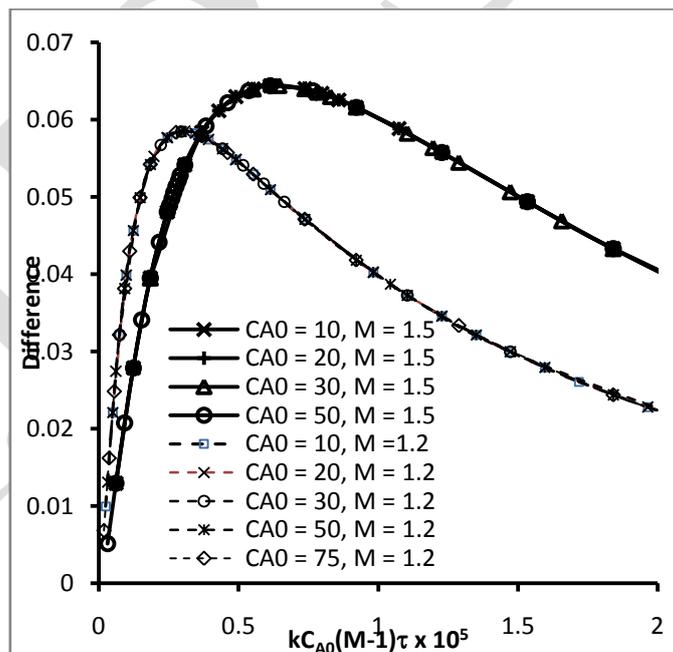


Fig. 4 Difference between VPLFTR model conversion and Ideal PFR conversion

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Testing of the VPLFTR for general kinetics given by Equation (2) gets more computationally intensive. Applying batch reactor performance equation to general rate equation given in Equation (2) we get,

$$t = \int_0^{X_{A,el}} \frac{dX_A}{kC_{A0}^{\alpha+\beta-1}(1-X_A)^\alpha \left(M - \frac{b}{a}X_A\right)^\beta} \tag{10}$$

$(C_A/C_{A0})_{el}$ is then given by Equation (11).

$$\left(\frac{C_A}{C_{A0}}\right)_{el} = 1 - X_{A,el} \tag{11}$$

For every value of t in Equation (5), $X_{A,el}$ is to be determined from Equation (10) and then $(C_A/C_{A0})_{el}$ is to be determined from Equation (11). Determination of $X_{A,el}$ in Equation (10) for given t is done by assuming a value to X_A and evaluating the integral numerically. For every value of X_A increasing from zero, the value of t was evaluated and compared. For every X_A so determined, $(C_A/C_{A0})_{el}$ was determined using Equation (11). This algorithm has two loops. One outer loop where t is changing in Equation (5) and for every t , $X_{A,el}$ is changing in an inner loop. The flowcharts for the algorithms for both inner and outer loop are shown in Fig. 5 and Fig. 6.

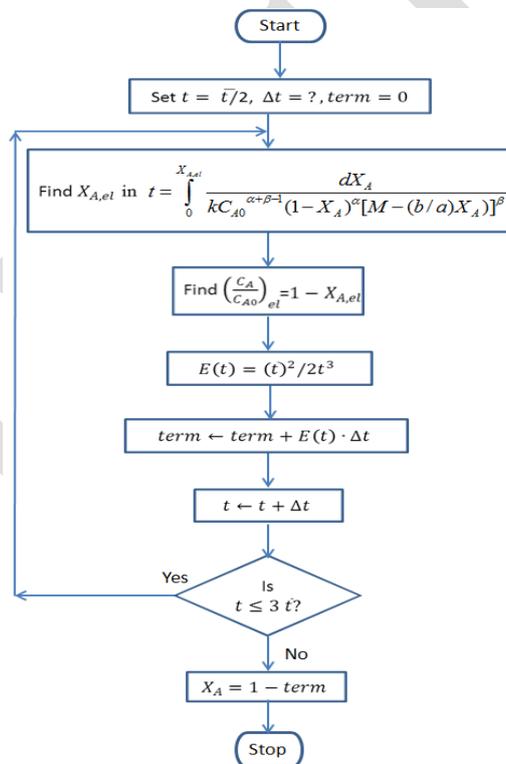


Fig. 5 Flow chart for outer loop

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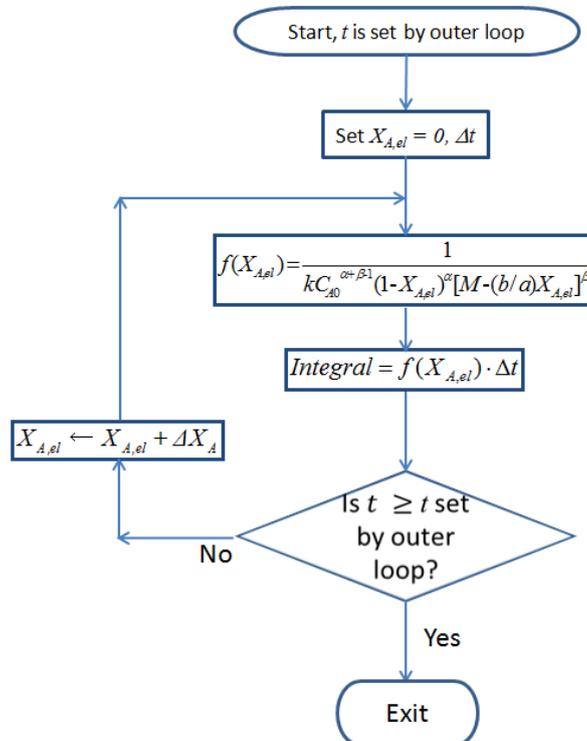


Fig. 6 Flow chart for inner loop

These flow charts are used to develop the algorithm and then a computer code was written. The VPLFTR model conversion and conversion for segregated flow model of LFTR (numerical) are compared in Fig. 6 and Fig. 7 for two cases.

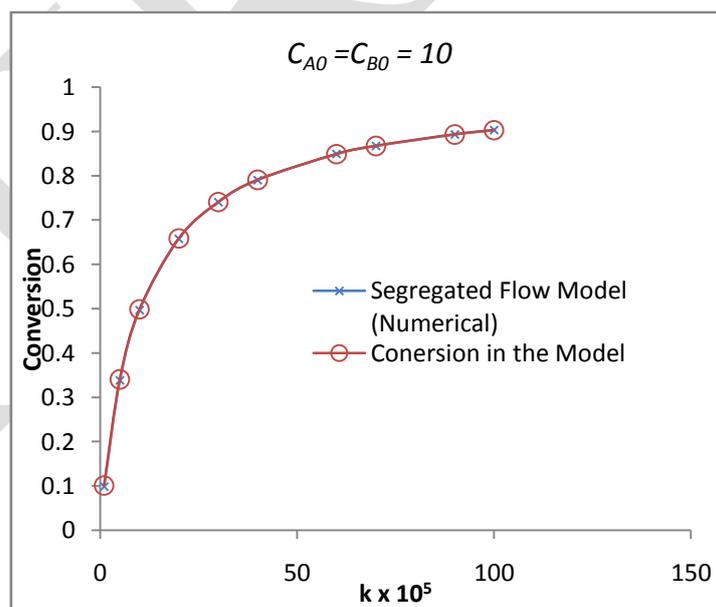


Fig. 6 Comparison of VPLFTR model conversion and Segregated Flow model conversion for $M = 1$.

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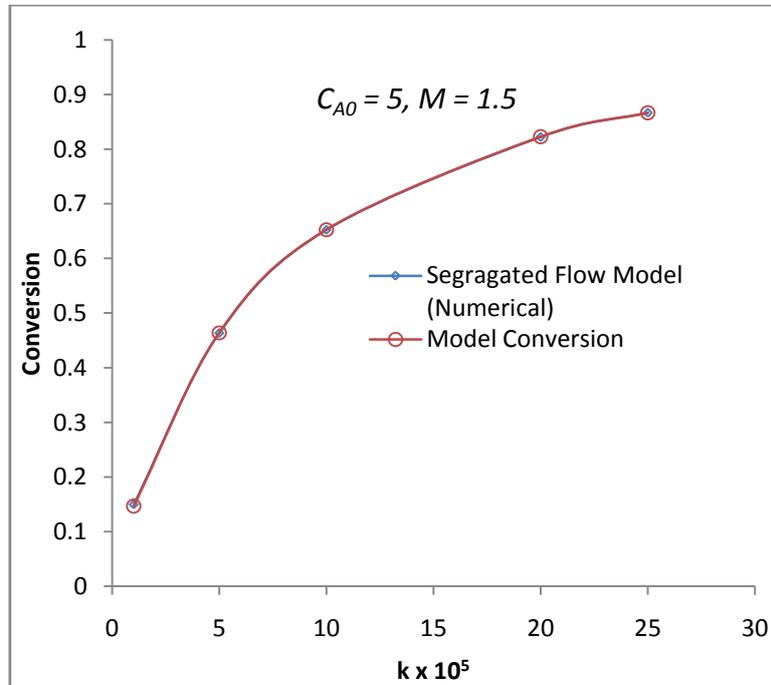


Fig. 7 Comparison of VPLFTR model conversion and Segregated Flow model conversion for $M = 1.5$

As shown in Fig. 6 and Fig. 7, conversions obtained in the VPLFTR model and conversions in LFTR using segregated model agree well.

V. CONCLUSION

VPLFTR model was validated and tested for more generic kinetics. It was identified that applying the VPLFTR model to general kinetics required numerical methods to determine conversion in the grid cells. Suitable algorithm and a computer code was developed in this paper and implemented. Validation of VPLFTR was done using segregated flow model for LFTR and an algorithm for the determination of conversion in LFTR using numerical method for general kinetics was developed, tested and implemented. In all the cases conversion in the VPLFTR model and conversion in LFTR model by segregated flow model completely agree.

This validates the VPLFTR model for more general cases. Thus non-ideality originating from parabolic velocity profile in LFTR can be accurately accounted at the design stage.

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