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Development of a Simulation and Analysis Tool for Chemical Reactors

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ABSTRACT
A reactor analysis and simulation tool (ASchem) for the design and performance analysis of batch, continuous stirred-tank and plug-flow reactors has been developed. The simulation tool is robust, allows for choice of reaction kinetics in liquid phase and has simplified graphical user interfaces. The tool also has unit converter, calculator, interpolator, graphical and tabular data output. The design and model equations of these reactors were encoded in a JAVA program. Results from the simulation tool were compared with those obtained from the simulation of the same model equations using MATLAB (2009b) with literature data. The deviations obtained were minimal with an average precision of 0.0258%, 0.0061% and 1.1923% for the batch, plug-flow and continuous stirred tank reactors respectively.

Keywords: reactor design, performance, analysis

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I. INTRODUCTION

In a chemical processes, the potential andyield with respect to the reactants used depend on the type and size of the reactors and its mode of operation[1]. The study of the behavior of chemical reactors is the key to the growth in chemical process as it helps in increasing the performance of chemical plants. Chemical reactors are simply the device that houses chemical reactions.AChemical reaction is a process that results in the conversion of chemical substances [2]. A mathematical model that can reliably predict the behaviour of the reactors becomes a valuable asset that can be used to study the behavioural performance of the reactors [3]. The model can be reconfigured and experimented with; which is usually impossible, too expensive or impractical to do in the system it represents. The operation of the model can be studied, and hence, properties concerning the behavior of the actual system or its subsystem inferred [4].This can be done by simulating and analysing the developed models.Models for the commonly used chemical reactors such as Batch Reactor (BR), Continuous Stirred Tank Reactor (CSTR) and Plug-Flow Reactor (PFR) were considered in this work.

Model simulation is a tool used to evaluate the performance of a system: existing or proposed, under different configurations of interest and over long periods of real time[5]. The development of analysis and simulation tool for chemical reactors' involves developing specialized computer software that can analyse and simulate reactors.Software modularity [6], user friendly interfaces and computing power have increasingly opened up new opportunities for the application of advanced mathematical models in process operations. This growing computational potential made possible the use of these models in process design, simulation and optimization; provides a means of analyzing and simulating different reactors by linking them with computers; thus ensuring a fast evaluation of many design alternatives [7]. Existing simulation tools developed over the years were restricted as most applications were for very specific existing systemsor component applications. This lack of flexibility made it rigorous to develop new products. Also, simulation tools that emerged for general systems werecomplicated, sophisticated in their approaches and lacked a user friendly interface which made it difficult for the user to easily learn;while in some, programming was a necessary part of the modeling process, thus consuming more time.

Mathematical model/design equationsthat represent the real life behaviour of the systems at different conditions were developed and programmed using a special computer language into the tool developed. This was developed for ideal, isothermal and adiabatic (no heat loss or gain) batch, continuous stirred tank and plug flow reactors

required in converting a given feed (reactants) to products, with the initial parameters and operating conditions. The reactors were considered at unsteady state conditions except for the plug flow reactor considered at steady state conditions.

II. TOOL DEVELOPMENT

A. DESIGN AND MODEL EQUATIONS

Application of the principle of conservation of mass for each reactor yielded the respective design and model equations as follows:

BATCH REACTOR (BR):

DESIGN EQUATIONS: Reaction time: $dt = C_{A_0} \frac{dX_A}{(-r_A)}$ (1)

Reactor Volume: $V = v_0 t$ (2)

MODEL EQUATION: $\frac{dX_A}{dt} = \frac{(-r_A)}{C_{A_O}}$ (3)

CONTINUOUS STIRRED TANK REACTOR (CSTR)

DESIGN EQUATION: Reactor volume: $V = \frac{F_{A0L}\, X_A}{(-r_A)}$ (4)

MODEL EQUATION: $\frac{dX_A}{dt} = -\frac{F_{A_O} X_A}{V} - (-r_A)$ (5)

PLUG FLOW REACTOR (PFR)

DESIGN EQUATION: Reactor volume: $dV = F_{A_{0L}} \frac{dX_A}{(-r_A)}$ (6)

MODEL EQUATION: $\frac{dX_A}{dL} = \frac{(-r_A)A_R}{F_{A_O}}$ (7)

B. REACTION KINETICS

The following reaction types were considered in this work:

Unimolecular-Type First Order Reaction:

$A \rightarrow Products$ (8)

Bimolecular-Type Second Order Reactions

Case 1: $A + B \rightarrow Products$ (9)

Case 2: $2A \rightarrow Products$ (10)

Tri-molecular-Type Third Order Reactions

Case 1: $A + B + C \rightarrow Products$ (11)

Case 2: $A + 2B \rightarrow Products$ (12)

Case 3: $3A \rightarrow Products$ (13)

These reactions were assumed to be elementary; hence the reaction rate expressions for these reaction types/schemes were written in terms of the stoichiometry [8] of the balanced equations and are generally of the form:

$(-r_i) = K[C_A]^{\propto}[C_B]^{\beta}$ …… (14)

$(-r_i) = K\left[C_{A_O}(1 - X_A)\right]^{\propto}\left[C_{B_O}(1 - X_A)\right]^{\beta}$ …… (15)

Where: i = reactants (A, B, ……); $\propto, \beta, \ldots\ldots$ are the coefficients of the reactants in the balanced equation, C_{A_O}, C_{B_O} …. are the initial concentrations of the reactants; C_A, C_B, …. are the concentrations of the reactants at any time t.

Thereaction kinetics based on the reaction types (equations 8 to 13) were developed following equations (14 and 15) and substituted into the various design/model equations of the respective reactors.

III. MATERIAL AND METHODS

The design equations for the batch and plug flow reactors wereordinary differential equationswhich were solved by numerical integration using the Simpson's rule algorithm while the design equation for the CSTR was an algebraic equation which was solved by algebraic manipulation. The model equations for the BR, CSTR and PFR were Ordinary Differential Equations (ODEs) which were solved numerically using the 4th order Runge-Kutta algorithm.The computer programs for the different modes of reactor(design or model) were developed following the mathematical algorithm of the methods stated for each.The computer programs were used to develop the simulation tool (ASchem) following the flow chart in Figure 1. The simulation tool was made interactive bydeveloping and incorporating a graphical user interface (GUI) using Java following the steps outlined in Figure 2.

The developed Software package (simulation and analysis tool named "ASchem" (Akpa-Somkene chemicals)is a continuously evolving window based software package with the following features: Choice of reaction kinetics, Choice of fluid phase: (constant density for liquid or ideal gas), Allows analysis of reactors of the same configuration in series, Unit converter incase units are not in the required/specified units, In-built calculator for numerical computations, Simulation Conditions:This enables the user to simulate using any valid conditions and not be constrained to a given step-size, Gives the user a view of the different reactors in 2D, Generates Tables & Graphs for the reactor analysis or performance.The software

also has the ability to run checks on the entered input values thus prevent errors from occurring during the input stage.

The accuracy of the developed simulation tool (ASchem) was ascertained by comparing its results with those obtained from the simulation of the same design/model equations using MATLAB software.

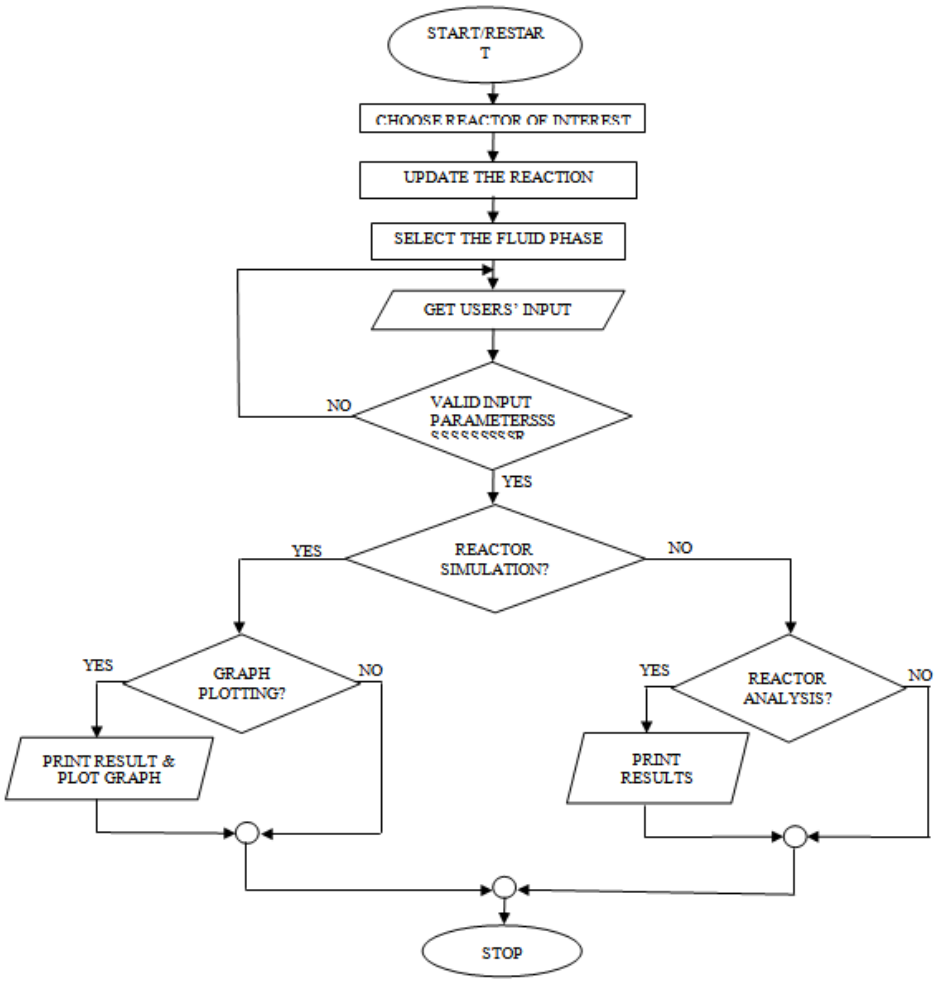


Figure 1: Flow Chart for Developing the Simulation Tool

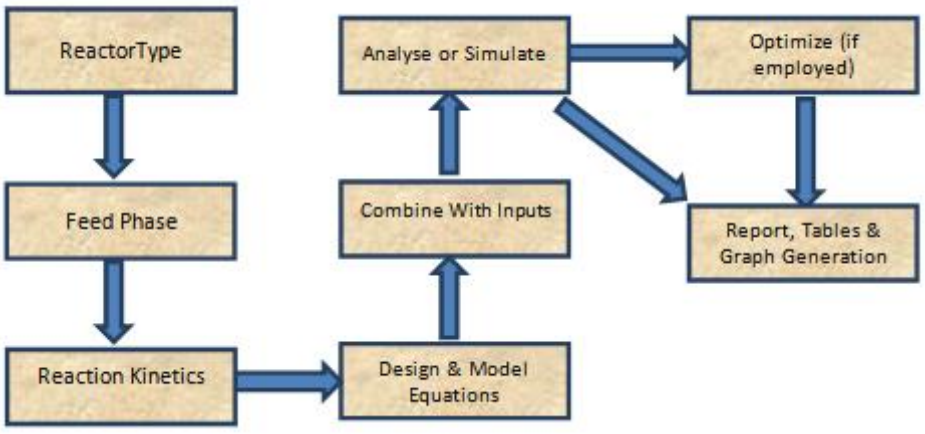


Figure 2: Flow Chart for the Design of the Graphical User Interphase

A brief description of the graphical user interface of ***ASchem*** to highlight its features and capabilities of entering data, analysing and simulating chemical reactors are presented.

I. Input Data Entering Form

The graphical User Interphase(GUI) has three different segments: the input parameters, model assumptions and reactor view segments. These can be visualized in Figure 3.

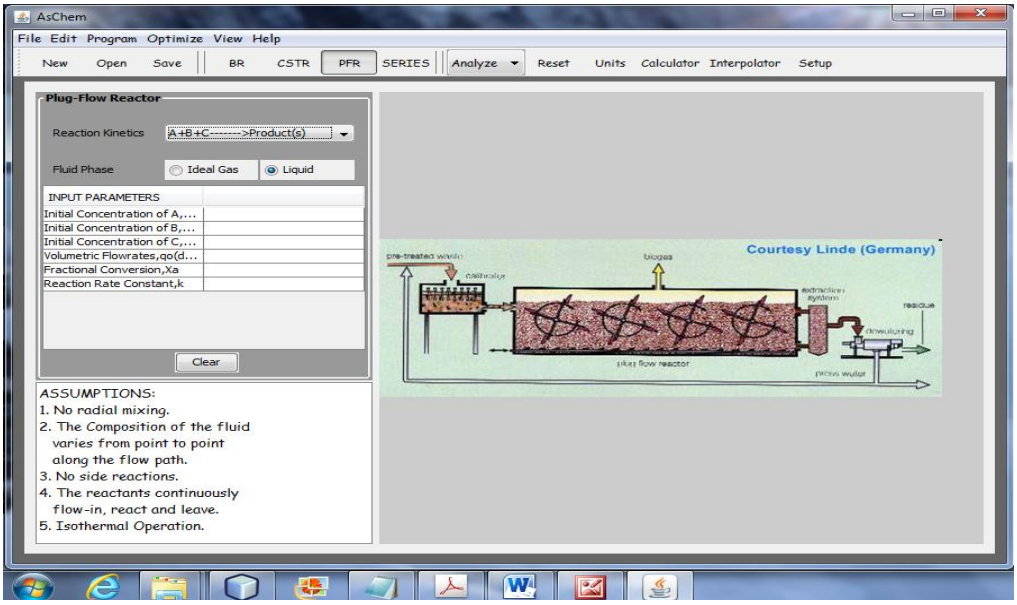


Figure 3: The Input Data Entering Form

Figure 3 shows the 'form' for the analysis and simulation of a plug flow reactor. Similar forms for other reactors can be generated by clicking their respective buttons on the tool bar.

II. Output Data Processing

After entering input parameters of any of the reactors, the program button on the menu bar executes the program depending on the task chosen, whether to analyse (design) or simulate (performance study). The results of the chosen task are displayed on the output data form; of either the reactor analysis shown in Figure 4; from which Tables, graphs and reports of the analysis are be generated as shown in Figures 5 and 6 respectively or the simulation results as shown in Figure 7.

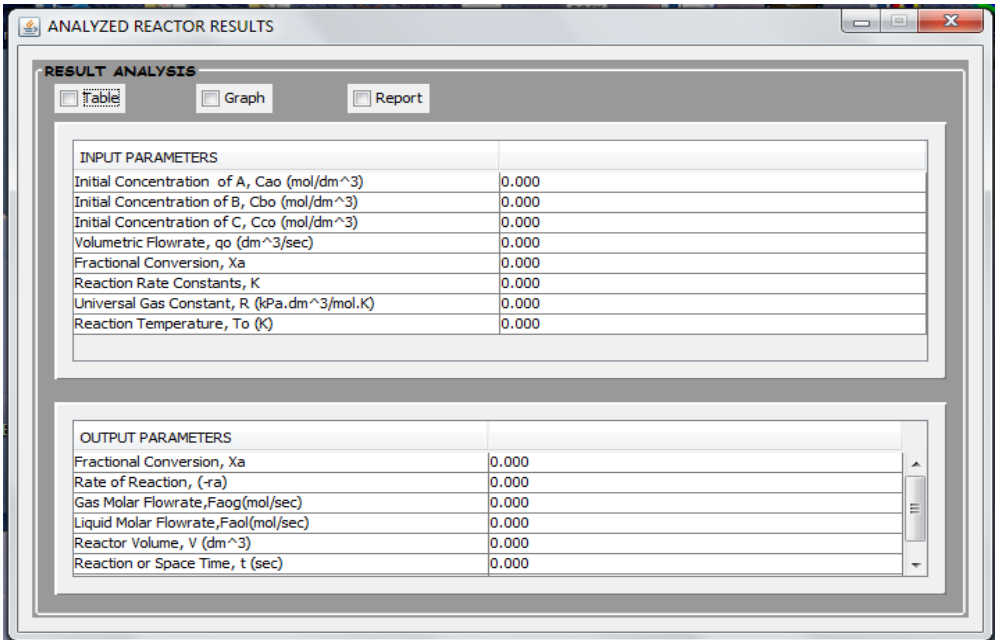
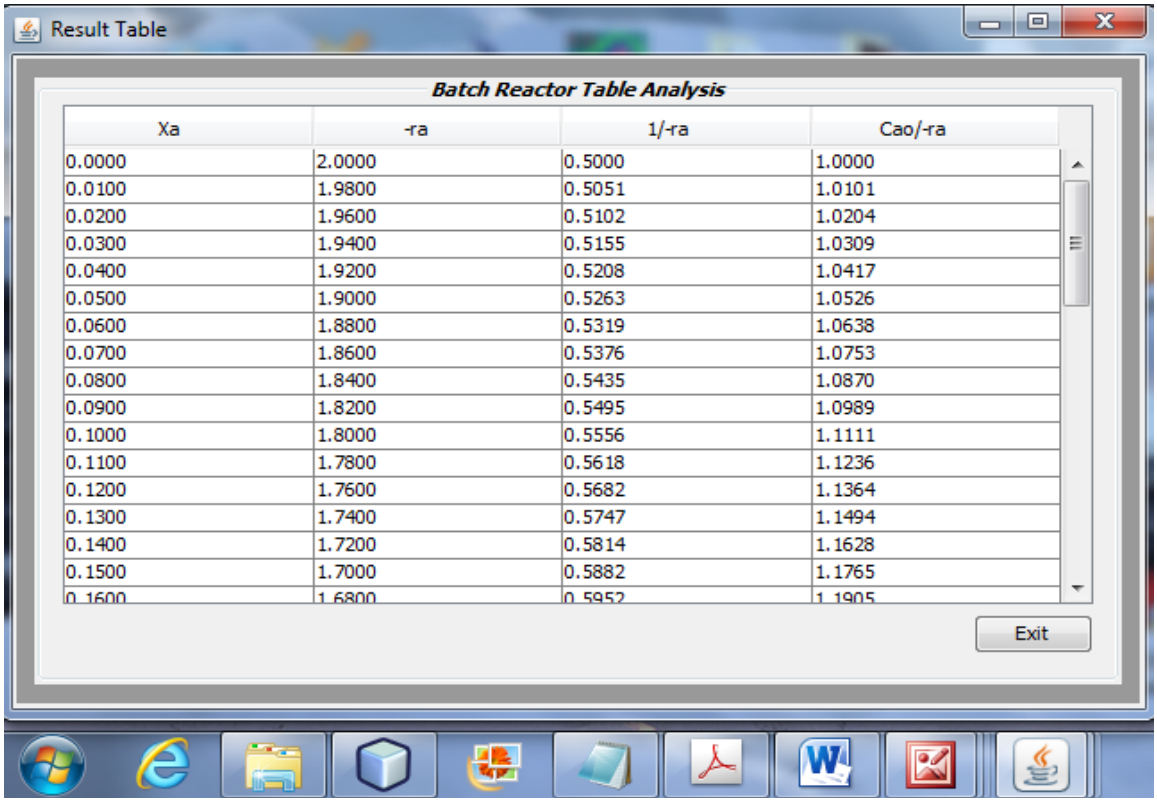


Figure 4: Reactor Analysis Form



Xa	-ra	1/-ra	Cao/-ra
0.0000	2.0000	0.5000	1.0000
0.0100	1.9800	0.5051	1.0101
0.0200	1.9600	0.5102	1.0204
0.0300	1.9400	0.5155	1.0309
0.0400	1.9200	0.5208	1.0417
0.0500	1.9000	0.5263	1.0526
0.0600	1.8800	0.5319	1.0638
0.0700	1.8600	0.5376	1.0753
0.0800	1.8400	0.5435	1.0870
0.0900	1.8200	0.5495	1.0989
0.1000	1.8000	0.5556	1.1111
0.1100	1.7800	0.5618	1.1236
0.1200	1.7600	0.5682	1.1364
0.1300	1.7400	0.5747	1.1494
0.1400	1.7200	0.5814	1.1628
0.1500	1.7000	0.5882	1.1765
0.1600	1.6800	0.5952	1.1905

Figure 5: Reactor Analysis Result Table

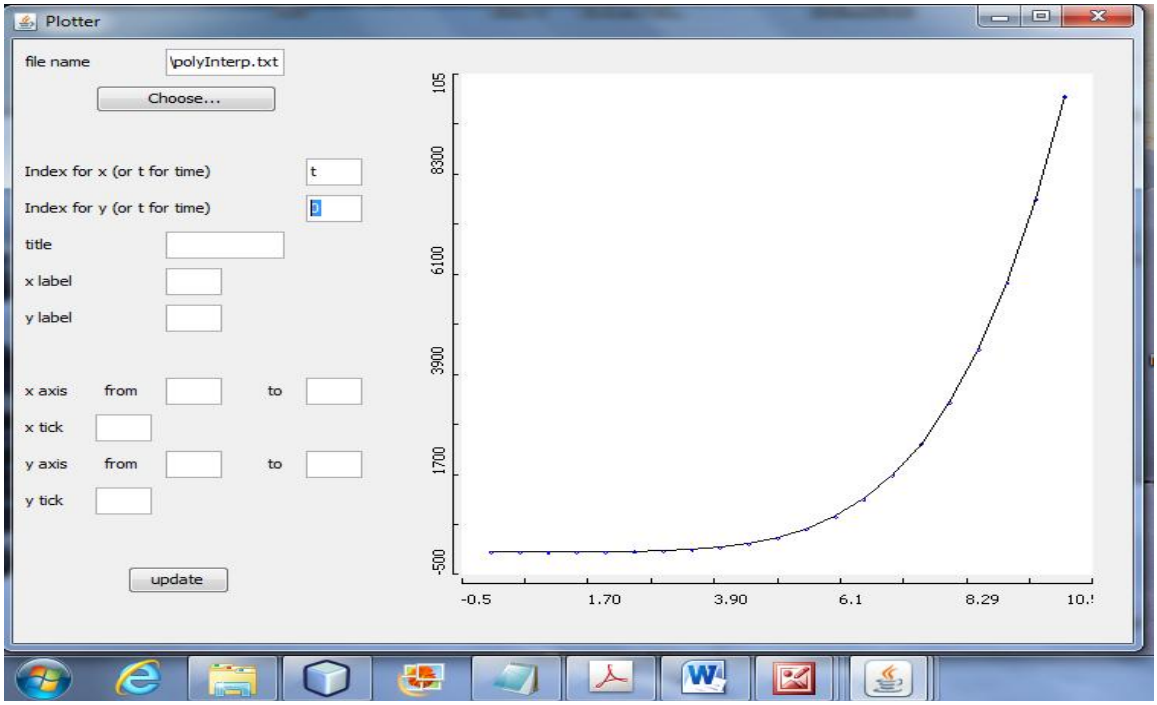


Figure 6: Reactor Analysis Result Graph

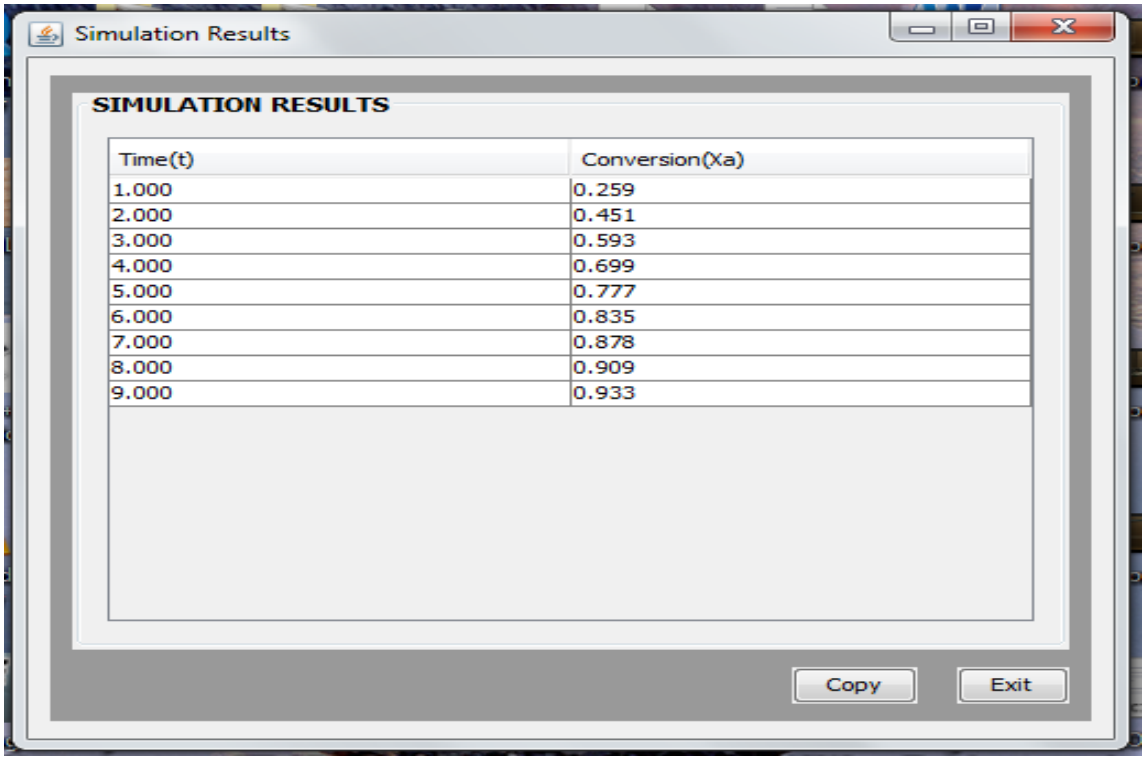


Figure 7: Reactor Simulation Result Form

IV. DISCUSSION OF RESULTS

The graphical profiles of the simulation results from the developed software ASchem and MATLABfor a Batch reactor (BR), Continuous Stirred Tank Reactor (CSTR) and Plug Flow Reactor (PFR) are presented in Figures 8, 9 and 10 respectively.

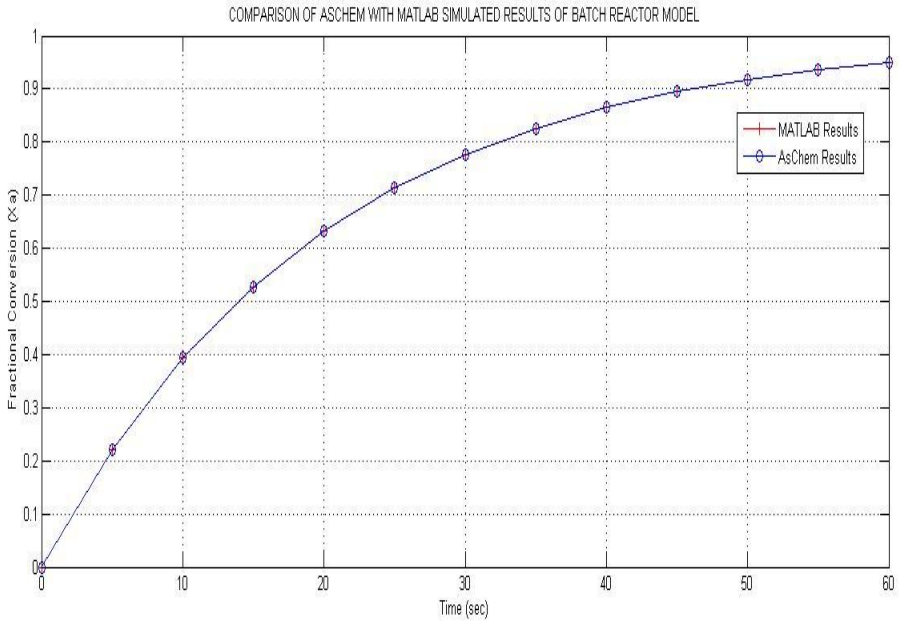


Figure 8: Comparison of ASchem with MATLAB Simulation Results of BR Model.

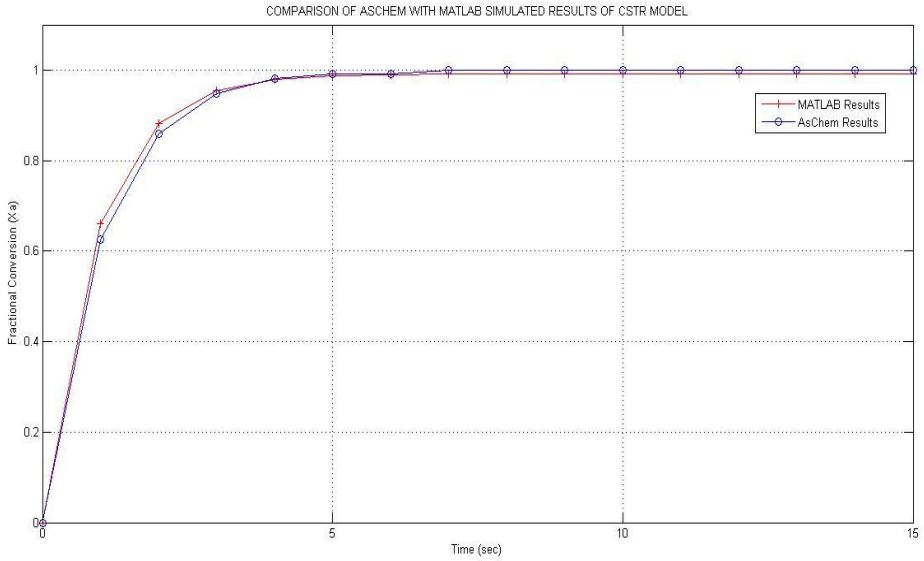


Figure 9: Comparison of ASchem with MATLAB Simulation Results of CSTR Model.

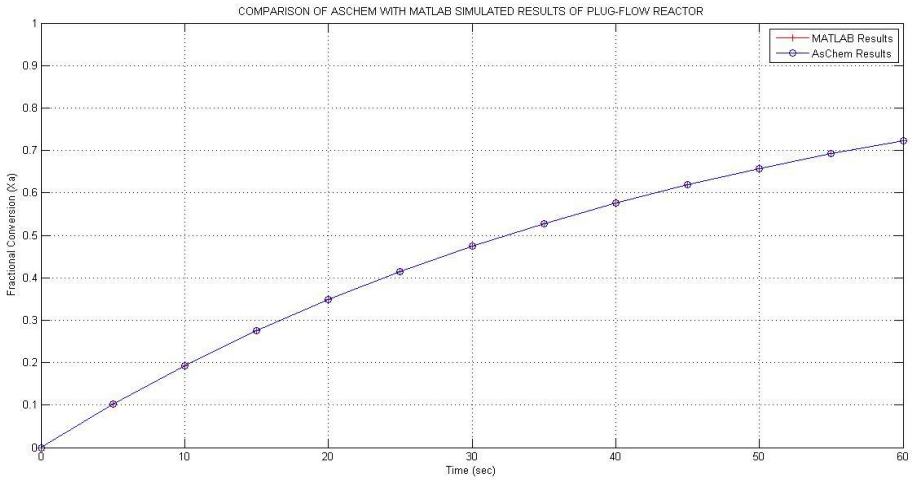


Figure 10: Comparison of ASchem with MATLAB Simulation Results of PFR Model.

The simulation results also showed average deviations of 0.0258%, 1.182% and 0.00608% between results obtained from the developed software ASchem compared with results obtained using MATLAB. Therefore the developed software is a valid tool for the simulation for the Batch, Continuous Stirred Tank and Plug Flow reactors.

V. CONCLUSION

A new software ASchem has been developed for the analysis and simulation of reactors (batch, continuous stirred tank and plug flow reactors). The design and model equations of these reactors were encoded in a JAVA program to develop the software.The software is robust, allows for choice of reaction kinetics in liquid phase (first, second and third order kinetics), provides a user-friendly interface, including a design environment, allows graphical interaction and expert system guidance on how to use the program. It will also stimulate creative thinking on the performance improvement for existing systems by providing a computer prototype of the real system.The software also has unit converter, calculator and interpolator. Results from the simulation tool were compared with those obtained from the simulation of the same model equations using MATLAB; the average deviation obtained was 0.0258%, 0.0061% and 1.1923% for the batch, plug-flow and continuous stirred tank reactors respectively.

REFERENCES

[1]. Maurizio, M., "Chemical reactors",*Process Engineering Aspects, Encyclopaedia of Hydrocarbons;*Volume V, 351-368, 2005.

[2]. Nanda, S., "Reactors and Fundamentals of Reactors Design for Chemical Reaction",*Dept. of Pharmaceutical Engineering, M.D. University Rohtak*-124001 Haryana,2008.

[3]. Aris, R., *Mathematical Modelling Techniques*. New York: Dover Publishers, 1994.

[4]. Shinnar, R., "Chemical Reactors Modelling-The desirable and the achievable". *In D. Luss & V. Weekman Jr. (Eds), Chemical Reaction Engineering Reviews, ACS symposium series:* 72, (p. 1), 1978.

[5]. Maria, A., "Introduction to Modelling and Simulation",*Proceedings of the 1997 Winter Simulation Conference*, 7-13,1997.

[6]. Hooper, J. R., Saleh, J. M. &Pike, R., "Design of multiphase and Catalytic Chemical reactors: a Simulation tool for pollution prevention", *Clean Prod.Processes*, 3, 92 – 103, 2001.

[7]. Rodrigues, A. E., & Minceva, M., "Modelling and Simulation in Chemical Engineering: Tools for process innovation",*Computers and Chemical Engineering*,29, 1167-1183,2005.

[8]. Fogler, S. H., *Elements of Chemical Reaction Engineering*, 3rd Edition.New Delhi: Prentice-Hall of India Private Limited,2004.

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