Chemical Reaction Simulation using Open Source Software XCOS

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***Abstract*— Modelling and simulation of chemical processes have high importance in chemical industrial development. Use of various simulation of chemical processes and reactions is gaining lot of significance in academics and research. Most of the time the work is cramped by unavailability of open source software. The current work represents effortless way to overcome this obstacle using XCOS, open source software for simulating chemical reactions. The well-known reactions are modelled mathematically and simulated using XCOS. The simulation results are discussed at the end to demonstrate the successful application of open source software XCOS for chemical reactions simulation.**

Keywords: XCOS, open source software, chemical reaction, simulation.

I. INTRODUCTION

Since last three decades, process simulation has changed the face of science and technology. It has reached new heights with different newly developed software both licensed and open ware. Chemical reactions have moved from in person laboratory to the computer in a virtual chemistry laboratory. Chemical reactions discussions have been switched from classrooms to process simulators as a new method for viewing simulations provide additional ways of learning chemistry. Importance of simulating chemical reactions in various ways has been underlined several times by different groups and is an established fact in current situations.

Representation of real-world reactions in terms of a set of mathematical equations [modeling]and solving the mathematical model to reach different reaction results [simulation] is combined considered in process simulation exercise.

Different simulation tools are available from various workers for simulating chemical reactions. These mainly include AACT simulators by the American Association of Chemistry Teachers, PhET interactive simulations by University of Colorado at Boulder, goREACT, ChemReaX are the popular open software for chemical reactions simulation.

In this work presented here, an attempt is made for simulating chemical reactions of different types using XCOS, a well-known toolbox from Scilab, an open ware from Engineering field. The first section of the paper introduces the XCOS toolbox. The second section throws a light of some of the well-known reactions from chemistry literature followed by third section describing the XCOS models for the chemical reactions discussed in section two. The fourth last section talk over the results and conclusion.

XCOS is Scilab toolbox dedicated to the modeling and simulation of hybrid dynamic systems including both continuous and discrete models. It helps in seamless integration of continuous and discrete process models. XCOS is a very robust system modeling and simulation open source tool, with comparable capabilities that to Simulink, which is the most sought-after commercial block-based modeling and simulation tool. The main aim of this work is to introduce XCOS a modelling and simulation tool for Chemical reactions for beginners and students and professional with non-simulation background.

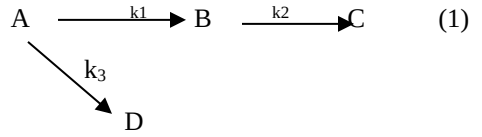
II. MODELLING AND SIMULATION OF CHEMICAL REACTIONS WITH XCOS

Complex reaction schemes of two different kinds were studied: the classical reactions of Van de Vusse and Trambouze1. The process model objective functions are distinct, but were based on the priority for the

desired product formation in all cases. For both these reaction schemes a standard Plug Flow Reactor [PFR] model was considered with the standard assumptions.

A. Van de Vusse reaction:

The first chemical reaction case studied is the most popular reaction of Van de Vusse [1]. In the Van de Vusse reaction, cyclopentenol (B) is produced from cyclopentadiene, with the formation of cyclopentanadiol (C) and dicyclopentadiene (D) as byproducts, according to the following reactions van de Vusse, J. G., 1964. {other examples like Ibuprofen, biofuel etc.} Considering the constant density throughout the reactor and the ideal level control, for simplicity, the chemical dynamics of the system is described by the differential equations, resulting from the mass balance of the reactor. It is composed of a combination of a parallel reaction with two series reactions, involving four species, A, B, C and D and B as the desired product component is represented as



(1)

For this reaction scheme a standard Plug Flow Reactor [PFR] model was considered with usual assumptions. The basic data assumed for simulating the model is as below:

Feed flow rate: F_0 = 200 mol/s, Initial concentration of pure component A: C_{A0} = 50 mol/lit, Volume of the reactor: V= 380 m^3, Reaction kinetics rates with their rate constants are k_1 = 10 s^{-1} (first-order); k_2 = 1.0 s^{-1} (first-order); k_3 = 1.0 L $(mols)^{-1}$ (second-order).

The standard process model for the Van de Vusse reaction are for PFR can be represented with following set of mathematical equations 2-5:

$$\frac{dC_A}{dt} = \frac{-F}{V}(C_{A0} - C_A) - k_1 C_A - k_3 C_A \quad (2)$$

$$\frac{dC_B}{dt} = \frac{-F}{V}(C_B) + k_1 C_A - k_2 C_B \quad (3)$$

$$\frac{dC_C}{dt} = \frac{-F}{V}(C_C) + k_2 C_B \quad (4)$$

$$\frac{dC_D}{dt} = \frac{-F}{V}(C_D) + \frac{1}{2} k_3 C_A^2 \quad (5)$$

This mathematical model was developed block wise in XCOS toolbox of Scilab. The simulated model is figured in figure 1 below. The results for concentration variations for all four components A, B, C and D were obtained in a single plot using 'mux block'. The same is discussed in the next section along with the results of other two reactions under consideration.

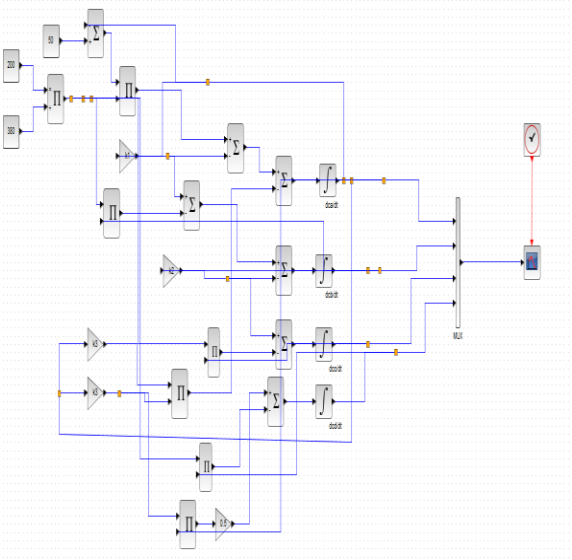
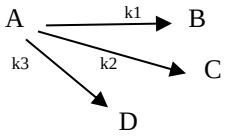


Figure 1: XCOS model for Van de Vusse reaction in Plug Flow Reactor under given conditions.

B. Trambouze reaction:

The second chemical reaction case studied is the reaction of Trambouze [2]. It is composed of three parallel reactions with no series reactions, involving four species, A, B, C and D and B as the desired product component is represented as



(6)

The basic data assumed for simulating the model is as below [2]: Feed flow rate: F_0 = 200 mol/s, Initial concentration of pure component A: C_{A0} = 10 mol/lit, Volume of the reactor: V= 200 m^3, Reaction kinetics rates with their rate constants are k_1 = 0.025 s^{-1} (first-order); k_2 = 0.2 s^{-1} (first-order); k_3 = 0.4 s^{-1} (first-order).

The standard process model for the Trambouze reaction are for PFR can be represented with following set of mathematical equations 7- 10:

$$\frac{dC_A}{dt} = \frac{-F}{V}(C_{A0} - C_A) - k_1 C_A - k_2 C_A - k_3 C_A \quad (7)$$

$$\frac{dC_B}{dt} = \frac{-F}{V}(C_B) + k_1 C_A \quad (8)$$

$$\frac{dC_C}{dt} = \frac{-F}{V}(C_C) + k_2 C_A \quad (9)$$

$$\frac{dC_D}{dt} = \frac{-F}{V}(C_D) + k_3 C_A \quad (10)$$

This mathematical model was developed block wise in XCOS toolbox of Scilab. The simulated model is figured in figure 2 below. Similar to the Van de Vusse reaction case, the results for concentration variations for all four components A, B, C and D were obtained in a single plot using 'mux block'.

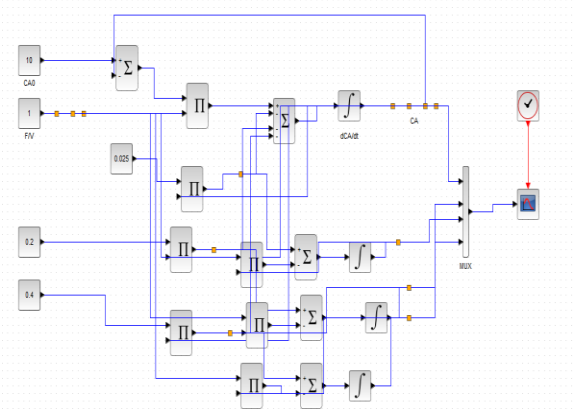


Figure 2: XCOS model for Trambouze reaction in Plug Flow Reactor under given conditions.

III. RESULTS AND DISCUSSION

Figure 3 shows the concentration profiles for the components A, B, C and D respectively with respect to time for Van de Vusse reaction carried out in a plug flow reactor. As compared with the standard component concentration profiles from literature.

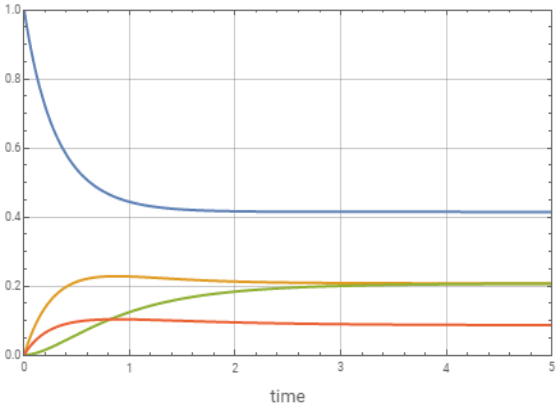


Figure 3: Concentration profiles for the components A, B, C and D for Van de Vusse reaction [component A: , component B: , component C: , component D:]

Figure 4 illustrates the concentration profiles for the components A, B, C and D respectively with respect to time for Trambouze reaction carried out in a plug flow reactor. The profiles for components B, C and D matches with the one observed and demonstrated in literature through experiment works. The concentration profile for component A i.e. reactant is differing with respect to literature reviewed due to the variation in kinetics related to order of reaction considered during modelling and simulation.

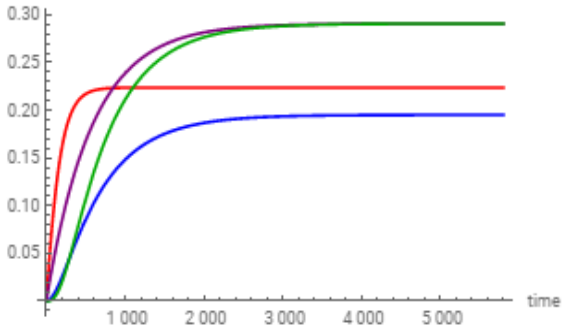


Figure 4: Concentration profiles for the components A, B, C and D respectively for Trambouze reaction. reaction [component A: , component B: , component C: , component D:]

IV. CONCLUSION

The concentration profile variations were satisfactory for all the three reactions types considered in the work. The work presented in this paper demonstrates the use of XCOS in chemical reaction modeling and simulation. The results obtained for component concentration profiles were encouraging. The main objective of this work to introduce XCOS a modelling and simulation tool for chemical reactions for beginners and students and professional with non-simulation background is satisfied by the simulation work. Nevertheless, use for XCOS for such different chemistries and with various types of reactors can be considered for future work ensuring large scale use of the open ware toolbox XCOS.

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