

## Educational Software for Rating and Sizing Chemical Reactors

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### Abstract

An educational software for Rating and Sizing Chemical Reactors is presented in this work. The user-friendly software designed using C# is presented in a step-by-step, simple-to-follow format. Design equations are analyzed for batch and flow reactors. Having been tested with sample problems from relevant literatures, it is believed that it can serve as an important tool in solving chemical Reaction Engineering problems. Results obtained show a high level of accuracy, although with slight differences from that obtained in the literature. This can be attributed to truncation errors when using manual calculation method.

### INTRODUCTION

Chemical Reaction Engineering is a branch of chemical Engineering concerned with the rational design and/or analysis of performance of chemical reactors. Reactor design is at the heart of producing almost all industrial chemicals. The knowledge of chemical kinetics and reactor design, the ability to handle chemical reactions, as well as the process of converting one or more chemicals into other chemicals that are more valuable is the major distinguishing factor between a Chemical Engineer and other Engineers. Thus, chemical engineers need to understand chemical reactions and be able to model equipment in which the chemical.

The selection of a reaction system that operates in the safest and most efficient manner can be the key to the economic success or failure of a chemical plant (Fogler, 1999). For example, if a reaction system produced a large amount of undesirable product, subsequent purification and separation of the desired product could make the entire process economically unfeasible. However, to find what a reactor is able to do we need to know the kinetics, the contacting pattern and the performance equation (Levenspiel, 1999).

The computer has come to find wide application in our everyday life, ranging from household to industrial chores. Jobs that would have taken a long time to be completed are now done in split seconds. Difficult and tasking jobs are now being done with ease. The growing trend in the use of computers has also had a great impact in the Chemical Engineering field. Design and Optimization of batch and semi-batch reactors was carried out by Zhang and Smith (2004), where they carried out a systematic study of ideal and non-ideal mixing in batch and semi-batch reactors. Also, Anyanwu et al (2012) designed a 50L per batch, stirred tank reactor, and based on that design, developed a simple algorithm using Microsoft visual C# language to enable scaleup of the reactor. Meanwhile, Jason (2015) did a detailed study of a homogeneous reaction of dye and bleach for an experimental module in Chemical Engineering Reactor Design, thereby developing design equations to compare models to experimental results using the kinetic behavior of the system. This paper presents a user-friendly software for computing design parameters for batch and continuous stirred tank reactors.

### Design Equations

The general material balance equation is given as:

Input = output + disappearance by reaction + accumulation

### Performance Equation for a Batch Reactor

For a batch reactor, the performance indicator is time. The performance equation for a constant volume batch reactor is given as

$$t = C_{A0} \int \frac{dX_A}{-r_A} \quad 1$$

For a first order batch system, the rate law is given as

$$(-r_A) = k_A C_A \quad 2$$

For a second order batch system, the rate law is given as

$$-r_A = -\frac{dC_A}{dt} = -\frac{dC_B}{dt} \quad 3$$

Or

$$(-r_A) = k_A C_A C_B$$

Steps in solving for time in a Batch Reactor is summarized in the table below

Mole balance		$\frac{dx}{dt} = \frac{-r_A}{N_{A0}} V$	
Rate law	First order $-r_A = kC_A$		Second order $-r_A = kC_{A^2}$
Stoichiometry		$C_A = \frac{N_A}{V_0} = C_{A0}(1 - X_A)$	
Combine	$\frac{dx}{dt} = k(1 - X)$		$\frac{dx}{dt} = kC_{A0}(1 - X)^2$
Integrate	$t = -\frac{1}{k} \ln(1 - X)$		$t = \frac{X}{kC_{A0}(1 - X)}$

Table 1: Summary of batch reactor time computation steps

### Continuous stirred tank reactor

For a CSTR, the performance equation is volume

$$V = \frac{F_{A0}\Delta X_A}{-r_A} \quad 4$$

If  $FA_0 = V_0C_{A0}$  is the molar feed rate of component A to the reactor, then considering the reactor as a whole we have

$$\text{Input of A, moles/time} = F_A/(1 - X_{A0}) = F_{A0} \quad 5$$

$$\text{Output of A, moles/time} = F_A = F_{A0}(1 - XA) \quad 6$$

### Software Description

The software consists of fifteen (15) windows. On running the software, the homepage which allows the user specify reactor type is displayed. The user is then taken to another page depending on the type of reactor selected. Each of the two forms (describing the two types of reactors) has six (6) radio buttons for each of the six parameters to be computed, namely: volume, time, fractional conversion, initial concentration, final conversion and number of moles. Again, the user is taken to a new form depending on the parameter to be computed. Here, the window displayed enables the user input available parameters. However, before the textboxes which are used to input the given data are activated, the user has to specify the given parameters by checking the boxes on the right side of the form. The output i.e. required parameter is displayed in a label below the compute result button.

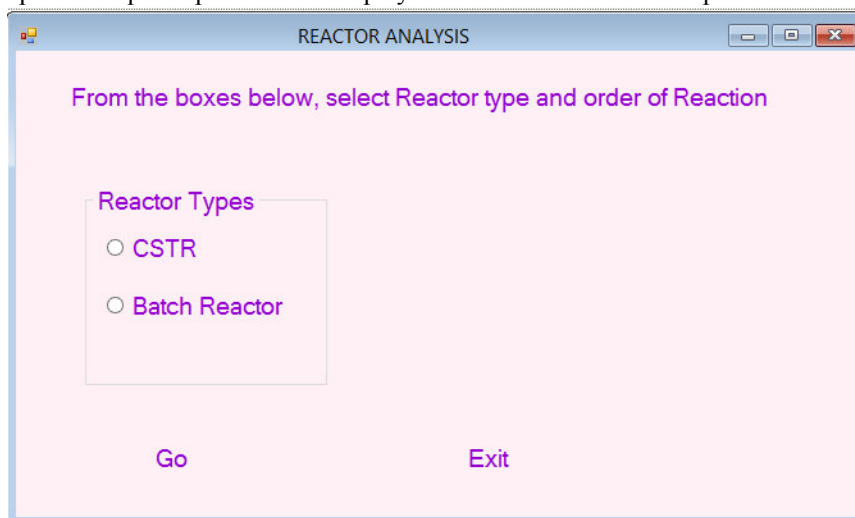


Fig. 1: homepage window

After selecting one of the buttons and clicking the “go” button, the user is taken to the either the CSTR page or the Batch reactor page depending on the reactor type selected. One of such pages is shown below.

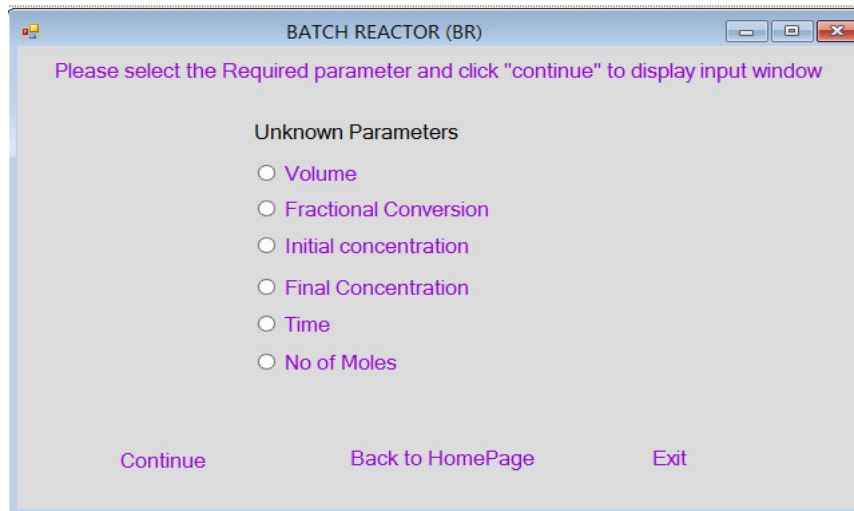


Fig. 2: Batch Reactor Window

On selecting one of the buttons, the page for the parameter is displayed. Example of one of such pages is shown below

The click event of the buttons automatically navigates the user to a different page. In figure 2, the continue button is to go to the next window where the input parameters are to be entered. Clicking the 'back to homepage' button takes the user back to the first window where the reactor type is selected. The exit button stops the program and closes the form.



Fig. 3: Batch Reactor Time window

In figure 3 above, the enable property of the textboxes is tied to the checked-changed event of the checkboxes. They can only be active when the user checks the corresponding checkbox. Also, trying to enter text in the first textbox i.e. the rate constant textbox, without selecting any of the checkboxes gives an error message prompting the user to select one of the checkboxes to proceed.

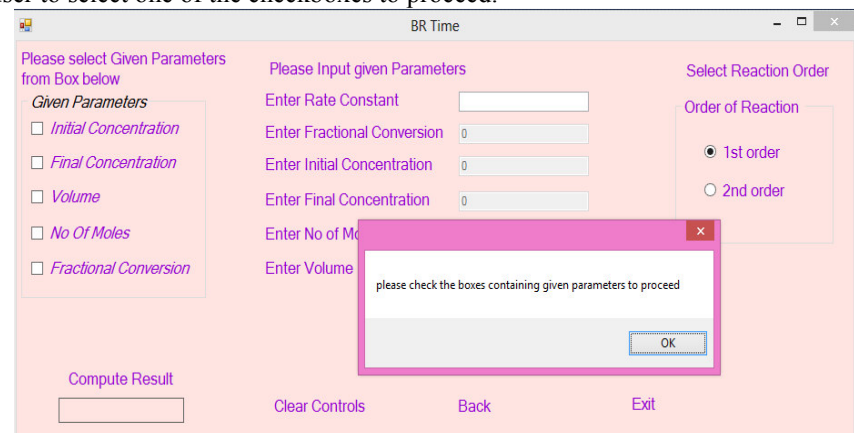


Fig. 4: an instance of an input window showing error message for wrong input during run time.

## SAMPLE QUESTIONS

The software is tested with the following sample problems

### Sample problem 1

Determine the time required for 80% conversion of 7.5 moles of A in a 15L constant volume batch reactor operating at 300K, the reaction is 1<sup>st</sup> order with respect to A with specific rate constant of 0.05min<sup>-1</sup> at 300K (Missen et al, 1998).

Inputs:

Fractional conversion,  $X_A = 0.8$

Number of moles of A,  $N_A = 7.5$  [moles]

Volume of reactor,  $V_R = 15$  [Litres]

Rate constant,  $K = 0.05$  [min<sup>-1</sup>]

### Sample problem 2

A liquid phase reaction  $A + B \longrightarrow C$  is conducted in an isothermal batch reactor the reaction is first order with respect to each reactant with  $K_A = 9.92 \times 10^{-2}$  L/molS at 25°C. Determine the reactor volume required to produce 175mols/hr of C if  $X_A = 0.9$ ;  $N_{A0} = N_{B0} = 0.15$  mol/L and the downtime between batches is 30mins (Missen et al, 1998).

Inputs:

$K_A = 9.92 \times 10^{-2}$  Lmol<sup>-1</sup>S<sup>-1</sup>

$C_{A0} = 0.15$  molL<sup>-1</sup>

$C_{B0} = 0.15$  molL<sup>-1</sup>

$X_A = 0.9$

$t_d = 30$ mins

$F_C = 175$  molhr<sup>-1</sup>

### Comparison of Design Results with literature Results

Sample problem	Design Parameter	Results		Relative Deviation (%)
		Literature	Software	
1. Missen et al (1998) p. 300. Example 12.1	Time (s)	1932.0(32.2mins)	1932.098	0.005
2. Missen et al (1998) p.301. Example 12.2	Time (s)	6050(1.6mins)	6048.389	0.026
	Volume (m <sup>3</sup> )	2.83	2.825	0.177

### Limitations of the software

Presently, the software has a limited scope of application. First, it cannot account for changes in volume therefore cannot be used to compute for parameters in gas phase equations. Secondly, the software cannot be used for non-isothermal, adiabatic problems. Thirdly, it does not take into consideration the number of species and stoichiometric amount involved in the chemical reaction. Finally, the user is restricted to the MKS system of units. Consequently, improvements upon the software will be constantly made in order to make the software as versatile as is humanly possible.

### Conclusion

From the sample problems presented, it is evident that the software has a higher degree of precision when compared with manual computations. Results obtained show slight differences between the one obtained from the software and that obtained in the literature with the highest deviation being 0.177%. Presented in an easy-to-understand format, the software, which is designed and implemented using Microsoft visual C# 4.0 platform, would serve as an important tool for computing chemical reaction parameters such as volume, time, concentration etc.

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