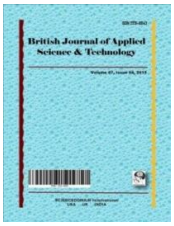

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Modeling Analysis of Stirred Tank Reactors

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Authors' contributions

This work was carried out in collaboration between all authors. Author CAI designed the study, performed the modeling and simulation both with MATLAB and Aspen Plus software, he also wrote the protocol and first draft of the manuscript. Authors OEL and MOA were involved in literature searches and data analysis respectively. Authors MOO and ARA supervised the study and interpreted the results. All authors read and approved the final manuscript

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ABSTRACT

Continuously Stirred Tank Reactor (CSTR) was modeled and the reactor performance analyzed with a view to coming up with an essential parametric quantity useful for assessing control at the steady-state design stage. The steady-state design of CSTR and its implementation, using Matrix Laboratory (MATLAB®) program for hypothetical reaction case and the commercial software Aspen Plus® for a real chemical case was performed. The approach adopted considered two separate first-order irreversible exothermic reaction processes, implemented in MATLAB® and Aspen Plus® software respectively and a target conversion and reactor stability ratio (RSR) determined. Results from this study revealed that at varied temperatures (320-360K) under steady-state design, a suitable target conversion of 95% and RSR values less than 0.50 present minimal control problems with irreversible exothermic reactions for both hypothetical and real chemical systems. Conversely, reactor design for low conversion and maximum temperatures can present control problems with exothermic reactions due to larger reactor size and low heat transfer area. The key to improved

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reactor performance with minimal control problems, is designing at a reasonable low RSR value and providing excess heat transfer area so that disturbances can be properly handled.

Keywords: CSTR; exothermic; MATLAB; aspen plus; parametric quantity.

NOMENCLATURE

T_r	*Reactor temperature (K)*
R	*8314* $(Jkmol^{-1}K^{-1})$
C_A	*Final concentration of reactant A* $(kmol/m^3)$
F	*Flowrate of product* (m^3/s)
A	*Jacket heat transfer area* (m^2)
D	*Reactor diameter (m)*
L	*Reactor length (m)*
T_j	*Jacket temperature (K)*
F_j	*Flowrate of coolant* (m^3/s)
Q	*Rate of heat removal from liquid in reactor (MW)*
V_j	*Jacket volume* (m^3)

1. INTRODUCTION

Process modeling and computer simulation have proved to be an extremely effective engineering tool for the design and optimization of physical, chemical and biological processes [1,2]. Chemical reactors and their reactions exist in numerous forms, and may or may not contain catalysts. The phases in the reactors can be liquid or vapor, adiabatic or non-adiabatic [3,4]. To obtain a mathematical model, two steps are required [5]. The first method involves formulating a model from first principles using the laws governing the system; this is generally referred to as mathematical modeling. The second approach requires the experimental data obtained by exciting the plant and measuring its response; this is called system identification [6].

However, obtaining a mathematical model for a complex system can be time consuming and tedious as it often requires some simplifying assumptions such as defining the operating point and carrying out linearization about that point and ignoring some system parameters, etc. This fact has led researchers to exploit the use of simulations to solve complex systems utilizing solely the input – output sets [5]. Commercial simulation tools like Aspen Plus® software and MATLAB® programming have been increasingly in use in many aspect of process engineering since their introduction as mathematical aids. While mathematical models developed from first principles can be implemented in MATLAB® by means of programming, Aspen Plus is more user friendly as it has built in models that allow for modeling of real chemical systems [3,7].

Once the mathematical relations have been established with a series of equations, the next step is determining which variable is to be solved for in each equation [1]. In other to obtain solutions to engineering problems via simulation, there are several levels of solution available to select from [8,9]. Software packages are also now available which have excellent graphical capabilities and ease the programming of specific problems; one popular package is MATLAB® [10,11]. At this point of the adaptive strategy, a valid representation of the actual process is needed [12,13] and it should be ensured that the result is within the context of engineering principles and decisions have to be made on whether or not the simulated process achieves the objectives stated in the definition of the problem. In this work, MATLAB® program and Aspen Plus® were applied for simulation and analysis of reactor performance.

2. METHODOLOGY

2.1 Mathematical Modeling of Continuously Stirred Tank Reactor (CSTR)

CSTRs are usually cylindrical agitated vessel containing reacting solutions and they operate at steady-state conditions (see Fig. 1). For a first-order exothermic irreversible reaction taking place in a CSTR with constant volume, used to convert reactant A to product B, is given as [14]:

$$A \rightarrow B \quad (1)$$

The rate of disappearance of A (r_A) and rate of formation of B (r_B) are given as:

$$-r_A = kC_A;\ r_B = kC_A \quad (2)$$

where $k = k_o \exp(-E/RT)$

Total material balance (kg/s) at constant density (ρ):

$$\rho_0 F_0 - \rho F \quad (3)$$

$$F_0 = F$$

Component A balance (kmol A /s) at constant reactor volume (V):

$$F_0 C_{A0} = FC_A + r_A V_r \quad (4)$$

or $F_0 C_{A0} = FC_A + V_r kC_A$

Reactor energy balance (J/s) where cooling of an exothermic chemical reaction, via a cooling coil (jacket) is included:

$$\rho_0 C_{P0} F_0 T_0 = \rho C_P F T_r + \lambda V_r kC_A + Q \quad (5)$$

where $Q = UA_j(T_r - T_j)$ and $A_j = \pi DL$ (6)

Steady state model of the cooling jacket is:

$$F_j C_j \rho_j T_{c,in} = F_j C_j \rho_j T_j + UA_j(T_r - T_j) \quad (7)$$

The conversion χ of reactant A is given by:

$$\chi = 1 - \frac{C_A}{C_{A0}} \quad (8)$$

2.2 Reactor Stability Ratio (RSR)

The reactor stability ratio (RSR) value is fundamental in order to determine the controllability of a CSTR [15]. Very large RSR (≥ 0.60) means there is little additional ΔT driving force to be able to increase heat removal rates in order to handle upsets. This limit can be determined by:

$$RSR = \frac{\Delta T_{design}}{\Delta T_{max}} \quad (9)$$

where ΔT_{design} is the differential temperature driving force between the reactor and the jacket (i.e. $\Delta T_{design} = T_R - T_j$). $\Delta T_{max} = T_R - T_{C,in}$ is the differential temperature driving force between the reactor and the supply coolant. The steady state equations of (3), to (9) further reduced to the following:

$$V_r = \frac{F(C_{A0} - C_A)}{kC_A} \quad (10)$$

$$Q = \rho C_P F(T_0 - T_r) - \lambda F(C_{A0} - C_A) \quad (11)$$

$$T_j = T_r - {Q}/{UA_j} \quad (12)$$

$$F_j = \frac{Q}{C_j(T_j - T_{C,in})} \quad (13)$$

$$D = 2\left(\frac{V_r}{\pi}\right)^{1/3};\ L = 2D \quad (14)$$

$$A_j = 2\pi D^2 \quad (15)$$

2.3 CSTR Model Development

Basically, the idea is to implement an irreversible hypothetical reaction by use of an explicitly coded numerical method in MATLAB and an irreversible real chemical reactions process simulation method in Aspen Plus. The kinetic and process parameters are presented in Tables 1 and 2 respectively. Reactors with different design values of conversion (i.e. 55 to 95%) and over a range of reactor temperatures (i.e. 320 to 360K) simulated.

2.3.1 MATLAB® implementation of hypothetical irreversible reaction case

For an irreversible exothermic reaction ($A \rightarrow B$), the forward reaction is first-order in concentration of A. The kinetics and process parameters are providedin Table 1.

$$r_A = -kC_A \quad (16)$$

The MATLAB program based on equations (10) – (16) was developed (see Appendix); the reactor temperature and conversion were varied to see the effect of these parameters on the size and heat transfer area of the reactor.

2.3.2 Aspen Plus® implementation of real chemical irreversible reaction case

The Aspen Plus® model of the rigorous continuous stirred tank reactor (RCSTR) with rate-controlled reactions based on known kinetics used in this work is as shown in Fig. 1. The reactor comprises a feed and product streams. The data used for the development of the RCSTR Aspen Plus model is provided in

Table 2 and a stepwise solution algorithm for the CSTR model development is presented in Table 3.

3. RESULTS AND DISCUSSION

For the purpose of this study, various simulation of CSTR has been performed with the use of MATLAB and Aspen Plus as presented in Figs. 2-5 for the effects of temperature and conversion on design parameters, different heat of reaction at 95% conversion, heat transfer coefficient at 95% conversion, temperature and volume on conversion and rate of heat transfer respectively. The MATLAB simulation gave more results that provide detailed information about the CSTR reactor performance. Aspen Plus simulation only gives result for the required heat transfer rates and conversions, however, the heat transfer area and differential temperature driving force can be computed if the jacket temperature is known. Higher reactor conversion (95%) at 320 K reactor temperature gives lower RSR value of 0.20, but increase slightly as reactor temperature is increased. Conversely, at varied temperatures, lower reactor conversions of 55 and 75% give high RSR values ranging from 0.52 to 1.0 as a result of lower heat transfers rate and differential temperatures driving force between the reactor and jacket. However, more heat transfer rate, reactor volume and heat transfer area are required for improved performance as indicated in Fig. 2. This means that with a target reactor conversion fixed at 95% a design where increase in the rate of heat removal and good reactor temperature control for RSR values less than 0.5 are possible. Figs. 3-4, ±20% changes were made to heat of reaction and heat transfer coefficient with a fixed target reactor conversion of 95% respectively. Both parametric changes were observed to have no effect on reactor volume and heat transfer area because these parameters are determined by flow rate, temperature and conversion, however, while heat transfer coefficient showed no further effect on the rate of heat removal, the heat of reaction indicates changes in the rate of heat removal. An increase in the heat of reaction increases the cooling water flow rate, RSR value and the rate of heat transfer, hence, higher heat of reaction requires higher heat transfer rate which lowers the jacket temperature and increase cooling water flow rate. The reverse is the case for increase in the heat transfer coefficient, hence for improved performance, the engineer should design at lower heat of reaction and high heat transfer coefficient. The effect of temperature and volume on conversion and rate of heat transfer has been illustrated with Aspen in Fig. 5, three reactors of different volumes were simulated and results showed that heat transfer rate increases with increase reactor volume, this agrees with results obtained with MATLAB. In terms of reactor conversion performance, the reactor with 900 m^3 capacity gave the optimal target conversion of 95% reached at a reactor temperature of 385 K and at this point the rate of heat removal stands at 1.60×10^7 W. This is high due to the feed conditions and reaction's activation energy.

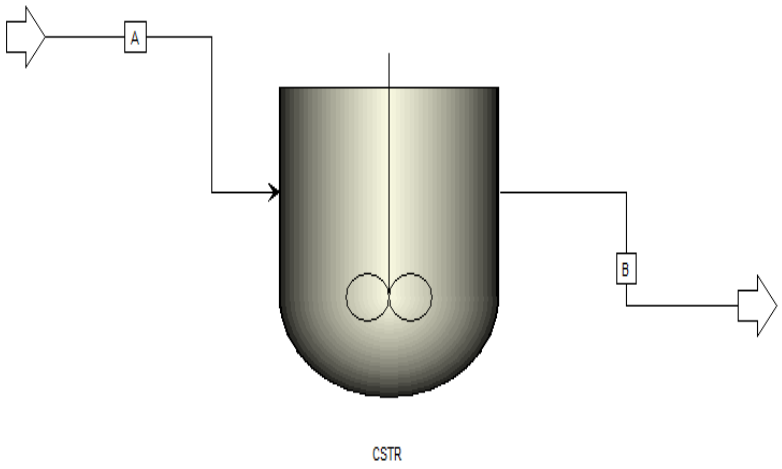

Fig. 1. Aspen Plus Rigorous CSTR model for exothermic irreversible reaction

Table 1. Simulation parameters for MATLAB CSTR modeling

Parameter	Value
Feed composition C_{A0}	8.01 kmol/m^3
Pre-exponential factor,k_0	$20.75 \times 10^6 s^{-1}$
Molecular weight, $M_{w(A)}$	100kg/kmol
Process densities,ρ_0 and ρ	801kg/m^3
Coolant density,ρ_j	1000kg/m^3
Heat of reaction,λ	-69.71$\times 10^6$J/kmol
Aspect ratio (L/D)	$8/4$
Heat capacities,c_{p0} and c_p	3137J/kg/K
Coolant heat capacity,c_j	4183 J/kg/K
Overall heat transfer coefficient, U	851W/m^2/K
Feed temperature,T_0	294K
Inlet coolant temperature,$T_{c,in}$	294 K
Feed flowrate,F_0	4.377$\times 10^{-3}$ kmol/s
Activation energy, E	69.71$\times 10^6$ J/kmol

Table 2. Simulation parameters for Aspen plus CSTR modelling

Parameter	Value
Feed Stream Condition:	
Temperature	298 K
Pressure	15 atm
Composition:	
Ethylene	0.4 kmol/s
Benzene	0.2 kmol/s
Property method	Chao Seadel
Reactor type	RCSTR
reactor temperature	430 K and varied
Reactor volume	100 and varied
Aspect ratio (L/D)	$8/4$
Valid-phase	Liquid only
Kinetic data:	
Reaction	$C_2H_4 + C_6H_6 \rightarrow C_8H_{10}$
Activation Energy, E	217.57$\times 10^6$J/kmol
Pre-exponential factor, k_0	1.56×10^6 s^{-1}
Reaction constant	$R = (C_{C_2H_4})(C_{C_6H_6})k_0 e^{(-E/RT_R)}$

Table 3. Solution algorithm for Aspen plus® implementation of CSTR

Step	Procedure
One	Start the Aspen Plus® software
Two	Select a reactor model type
Three	Add/specify other auxiliary equipment (streams and valves)
Four	Add chemical components
Five	Specify physical property package (thermodynamic model)
Six	Specify reaction (add reactions/kinetic parameters)
Seven	Reactor model setup (set T_r, P_r, V_r and valid phase)
Eight	Add reaction to reactor model
Nine	Run simulation

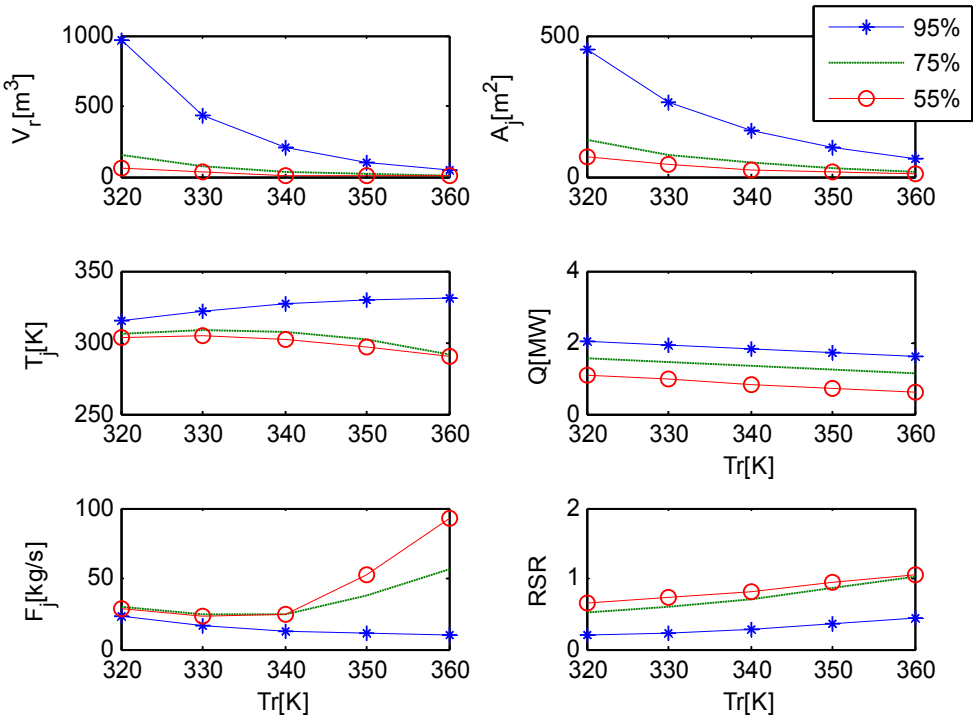

Fig. 2. Effect of temperature and conversion on design parameters

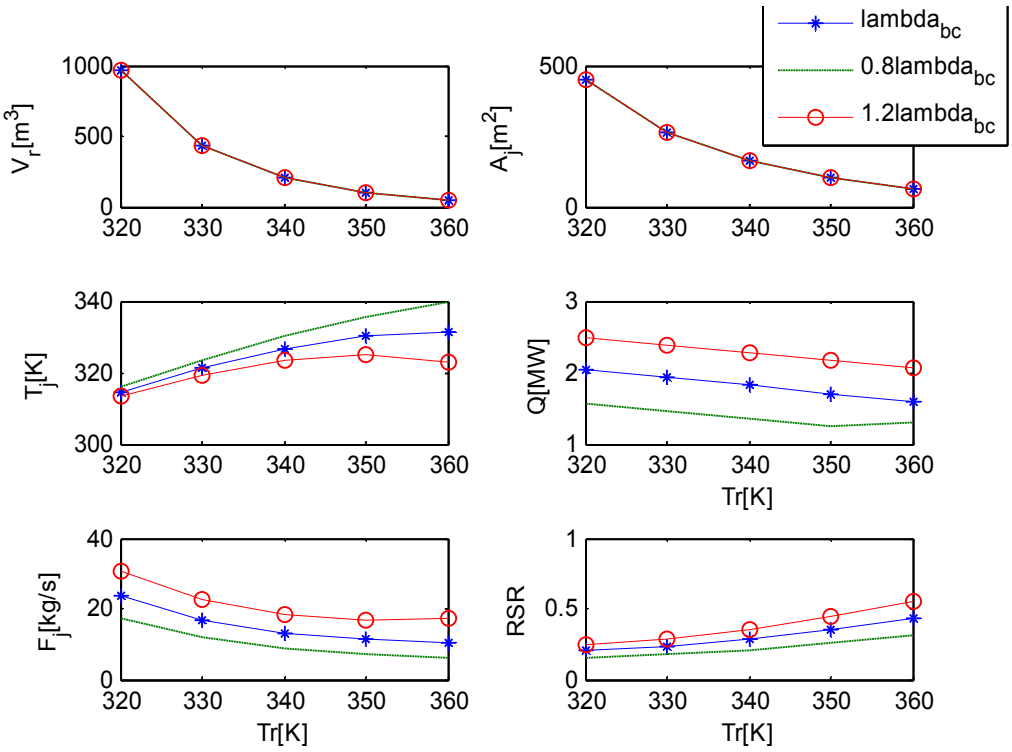

Fig. 3. Effect of different heat of reaction (λ_{BC},$0.8\lambda_{BC}$ and$1.2\lambda_{BC}$) at $\chi = 95\%$

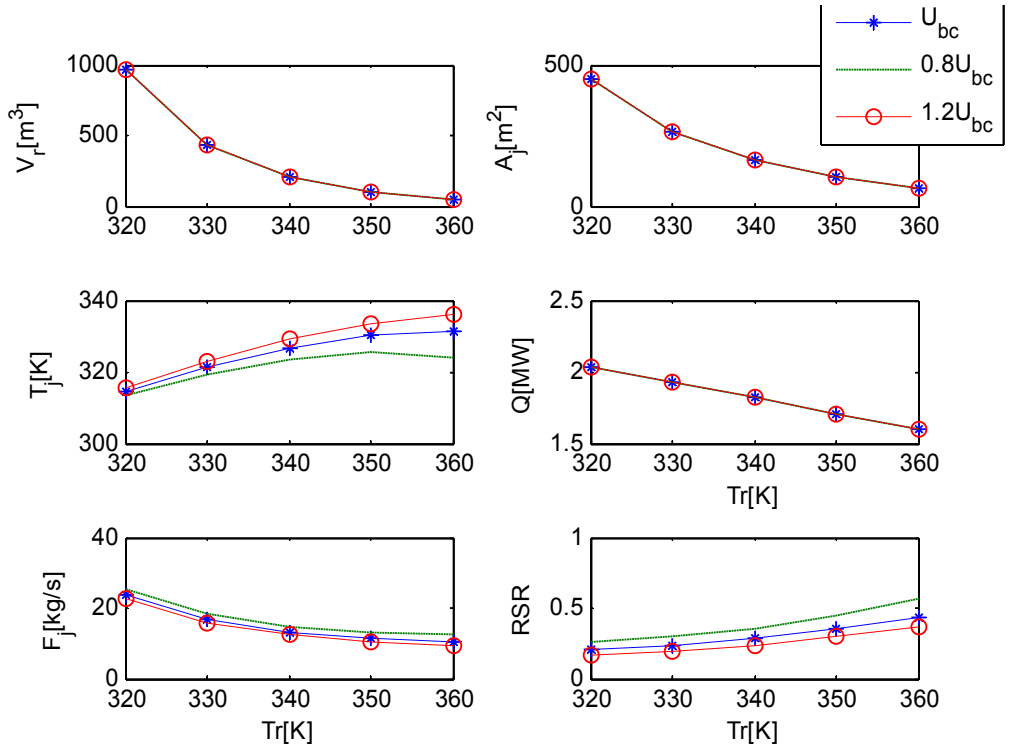

Fig. 4. Effect of heat transfer coefficient (U_{BC},$0.8U_{BC}$ and$1.2U_{BC}$) at $\chi = 95\%$

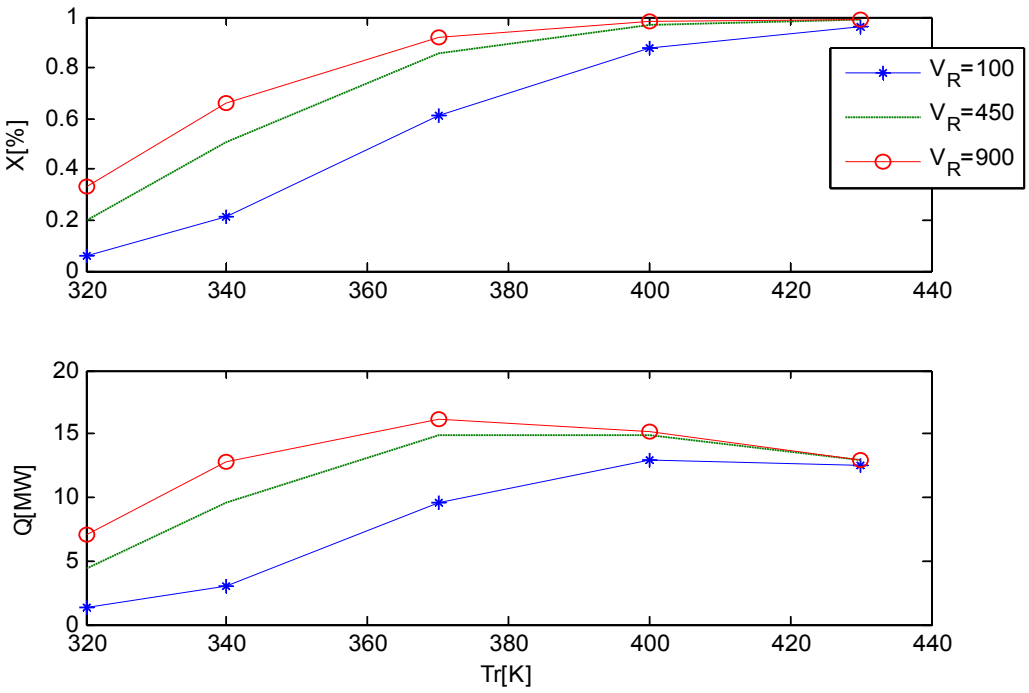

Fig. 5. Aspen plussimulation result for different reactor sizes

4. CONCLUSION

The study concluded that reactor performance analysis using MATLAB and Aspen Plus for irreversible reactions follows a similar path, however, MATLAB provides more detailed information about the CSTR. Higher conversion (target conversion of 95%) and temperatures (320-360 K) yield favorable RSR values, hence, present minimal control problems with irreversible exothermic reactions for both hypothetical and real chemical systems.

In general, the key to improved reactor performance with low control problems is designing at a reasonable low RSR value and providing excess heat transfer area so that disturbances can be properly handled.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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APPENDIX

```
%filename "modeling_Analysis_CSTR.m"
%
%parameter to vary
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Tr=320; conversion=0.95;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%data given in Table 1
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%
F=4.377e-3; E=69.71e6;T0=294;Tcin=294;U=851;CA0=8.01;k0=20.75e6;
Cp=3137;Cj=4183;roej=1000;lambda=-69.71e6;roe=801;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%
K=k0*exp(-E/Tr/8314);      %rate equation
CA=CA0*(1-conversion);     %final conc of reactant A
Vr=F*(CA0-CA)/K/CA;        %reactor volume
D= (2*Vr/pi) ^0.3333;      %reactor diameter
Aj=2*pi*D^2;               %jacket heat transfer area
Q=roe*Cp*F*(T0-Tr)-lambda*F*(CA0-CA);%rate of heat removal from reactor
Tj=Tr-Q/U/Aj;              %jacket temperature
Vj=0.3333*Aj;              %jacket volume
Fj=Q/(Cj*(Tj-Tcin));       %flowrate of coolant
deltatemp=Tr-Tj;  %differential temperature driving force between Tr and Tj
RSR=deltatemp/(Tr-294);
Tr, Vr, D, Aj, Q, Tj, Fj, RSR
```


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