ABSTRACT FOR ISOTHERMAL BATCH REACTOR

Description:

This abstract is for the code written for Isothermal batch reactor. Function of this program is to solve set of reaction design equations (Using complete segregateness model i.e. batch reactor model) with the option to solve them either simultaneously or sequentially. The time entered for simultaneous condition is the total time for reaction, whereas for sequential, it is the time taken by each reaction, making the total time to be entered time*no. of reactions.

Assumption:
1) Constant Volume Batch Reactor
2) The reactions are irreversible, comprising of only forward reactions (The code can be extended easily to reversible reaction with few changes)
3) Temperature of reactor is maintained at nearly the constant temperature by use of external cooling/heating medium

Mole/Mass Balance of a particular specie in batch reactor is written as:

$$\frac{dc_1}{dt} = k\gamma c_1^a c_2^b$$

Where, c_1 is the concentration of specie 1 in a **constant volume** batch reactor
c_2 is the concentration of specie 1 in a **constant volume** batch reactor
t denotes time
k is the forward reaction constant
a/b is the order of reaction with respect to 1/2
γ is the stoichiometry of specie 1
For a specie undergoing multiple reactions, involving multiple species, the equation can be rewritten as:

$$\frac{dc_1}{dt} = \sum k\gamma_i c_1^a c_j^b$$

Subscript i denotes the number of reactions and j represents other base-components
This system of equations need to be solved simultaneously to get solution of multiple reactions being performed at same time. In this code, the equations are accurately solved using function "OdeExplicitRungeKutta45".

Reference: Fogler 4th edition "Elements of chemical reaction engineering"

Examples:

Q1) Component system: CH_3CHO, CO, CH_4, O_2, CO_2
Thermodynamic Package: Peng Robinson/Lee Kesler
Reaction: $CH_3CHO \rightarrow CO + CH_4$ $k_{f1} = 0.5\ s^{-1}$

$\frac{1}{2}O_2 + CO \rightarrow CO_2$ $k_{f2} = 0.5\ (kmol/m^3)^{0.5}s^{-1}$

The initial feed composition is 0.5 moles O_2 and 0.5 moles CH_3CHO. Order is assumed to be the stoichiometries of corresponding reactants and assume irreversible reactions. Initial time = 0 and Final time = 1 s. Time step of 0.001s is considered. Volume = 1

Components	Results (in moles) (Simultaneous)	
	ASPEN	Custom Code
CH_3CHO	0.3033	0.3033
CO	0.1904	0.164
CH_4	0.1967	0.1967
O_2	0.4968	0.4834
CO_2	0.00637	0.0332

The result generated through DWSIM satisfies custom model atomic mass balance. The discrepancy in results of CO, CO_2 and O_2 might be because of solving coupled equations using different discretization methods. The similarity in results of CH_3CHO and CH_4 further strengthens ur argument, which were a solution of single differential equation. It may also be possible due to rounding errors in either of codes.