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Process Simulation of Reactor Using Open Source - A Review

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Abstract: *Process simulation is a successful tool for design, optimization and control of chemical processes. Chemical industry process simulations support the entire life cycle of a chemical process from development, design and construction to optimization of operation. Reactors are usually the heart of the chemical processes in which relatively cheap raw materials are converted to more economically favourable products. Reactions play essential safety and environmental protection roles. Proper design and operation of the reactor is required to provide the desired outcome. We study the various types of reactors use in the simulation and also various simulations software use for reactor simulations. DWSIM is the open media simulators use to simulate various unit operations and processes like reactors, distillation, heat exchangers, adsorption column etc. There various types of reactors give the outlet property of reactions by simulating them in to simulators. Like DWSIM lot of chemical simulators are available some paid version and some of open media like DWSIM. Conversion reactor are used for calculating conversion of reaction. Similarly, Gibbs and equilibrium reactors are used to calculate equilibrium constant.*

Keywords: Reactor, Process Simulation, Modelling and Simulation, Open Media., etc.

I. INTRODUCTION

Process simulation is a successful tool for design, optimization and control of chemical processes. Chemical industry process simulations support the entire life cycle of a chemical process from development, design and construction to optimization of operation. Simulation represents the application of modeling techniques to real systems which enabling information on plant characteristics to be gained without either constructing or operating the full-scale plant or the system under consideration. Modeling is the process of producing a model which is a representation of the construction and working of some system of interest. A model is similar to system but simpler than the system it represents. One purpose of a model is to enable the analyst to predict the effect of changes to the system. A model should be a close approximation to the real system and incorporate most of its salient features. Reactors are usually the heart of the chemical processes in which relatively cheap raw materials are converted to more economically favorable products. Reactions play essential safety and environmental protection roles. Proper design and operation of the reactor is required to provide the desired outcome.

Introduction to Simulation Software DWSIM

DWSIM is a open source simulator in which all calculations are made in a per-module basis according to connections between the objects. An object has all of its properties defined and if yes passes the data for the downstream object and calculates it. Process in a loop until it reaches an object that doesn't have any of its downstream connections attached to any object. Flowsheet can be calculated as many times as necessary without having to tell DWSIM which object must be calculated. This is done indirectly if the user defines all the properties and make all connections between objects correctly.

II. LITERATURE SURVEY

Ammonia and methanol synthesis which may be described through a relatively simple reaction pathway and the relative available kinetic scheme. To define the conversion of bioethanol into syngas/hydrogen or into building blocks

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such as ethylene. For thermodynamic study Gibb's reactor model adopted to calculates chemical and phase equilibrium by minimizing the Gibbs-free energy without specifying any reactions. [2]

To assess the economic optimization of a methanol synthesis plant presented by Luyben. Methanol yield and availability of reliable kinetic data fundamental in order to correctly size the plant. Methanol synthesis involves the reaction of both carbon dioxide and carbon monoxide with hydrogen. Peng–Robinson (PR) equation of state selected as the thermodynamic model which guarantees accurate calculation results in modelling light gases, alcohols and hydrocarbons. PR equation provides results similar to Soave–Redlich–Kwong (SRK) equation and better to predict densities of many components in liquid phase are non-polar. [2]

The ammonia synthesis mechanism carried out on promoted Ru/C catalysts under conditions (T = 370–460 ^{O}C, P = 50–100 bar). Biomass is converted by steam into syngas (H_2 + CO) and a combustion reactor fed with sand and char to supply thermal energy to the former. Process simulators (Aspen Plus, Pro II, Hysys, DWSIM) predefined models to simulate biomass gasification.[2]

Syngas (H_2 and CO) is then converted into methane by conversion step is methanation which is catalytic exothermal process at temperatures of 473-673 K and high pressure from 20 to 70 bar. Syngas enters methanation reactor with H_2/CO molar ratio of 3. The reactions considered in the proposed model are CO methanation and Water Gas Shift conversion (WGS). Process simulation of methanation reactor developed considering an isothermal fixed bed reactor with steam recovery and CO methanation kinetic on Ni catalyst. [5]

By comparing calculated gas concentration profiles (CH_4, CO, CO_2 and H_2) with experimental data obtain on bench-scale and with industrial data. Percentage error 12 %. Simulation value mixture leaving methanation reactor contained 47.3 % of CH_4, 1.2 % of H_2, 6.6 % of CO_2, 0.1 % of CO and 44.7 % of H_2O. Industrial Process values mixture leaving methanation reactor contained 46.9 % of CH_4, 1.4 % of H_2, 7.4 % of CO_2, 0.3 % of CO and 43.9 % of H_2O. In simulation values increase fraction of methane and water produce and decrease value of unwanted gases. [5].

At higher temperatures rate of disappearance of CO an H_2 and the rate of formation of H_2O and CH_4 increase. At 593 K CO is completely converted at end of the reactor. Concentrations of CH_4 and H_2O at the outlet reach almost equilibrium concentration of 12.5 mol% for CH_4 and H_2O. [5]

Configuration of reactor a maximum of 83.5% of conversion of Sulphur present in oil crude stream and residence time inside the reactor was 4.3 min. The catalyst quantity deposited in the system such as the void fraction of the catalyst. The catalyst produces a drop pressure of 2.5 MPa. Hydrotreatment process with recycle for designed a cooler with a flash separator. Hydrogen stream with a 99.8% of purity compressed to be mixed with the inlet stream. Methane enters at temperature of 298 K while the combustion gases from the outlet stream had a temperature of 680 K. [8]

Effect of reactor temperature always going to be crucial in this exothermic reaction mechanism. Optimum reactor volume predicted to be 430 K and the optimum reactor volume found to be 100 m3. Optimum feed flow rates were 0.4 kmol/sec w.r.t benzene and 0.2 kmol/sec w.r.t ethylene. Maximum yield of ethyl benzene predicted to 49.75% w.r.t benzene and 99.9% w.r.t ethylene. [11]

Simulation of saponification of ethyl acetate in presence of Sodium hydroxide in a plug flow reactor and continues stirred tank reactor using Aspen Plus simulation Software. CSTR use key unit operation variables when using a continuous agitated-tank reactor to reach a specified output. PFR used due to the non-mixing property. Plug flow reactors when there is a need for continuous large-scale reaction or fast reaction. PFR have high volumetric unit conversion as the occurrence for side reactions is minimum. [12]

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A simulation of a double tubular catalytic membrane reactor for the water–gas shift (WGS) reaction under steady-state operation which consists of dense Pd layer deposited on a porous glass cylinder support. The membrane at a temperature of 673 K, pressure of 2 atm, argon flow rate of 400 cm^3/min and steam-to-carbon (S/C) ratio of 1. CO conversion efficiency of up to 93.7% whereas a maximum value of only 77.5% attained without using a membrane. Optimum operating conditions in which complete CO conversion achieved at S/C ratio = 4, total retentate pressure =12 atm and membrane thickness =5 μm. [14]

Software's Use for Chemical Process Simulation

1. Aspen One
2. Pro II
3. Pro Sim Plus
4. DESIGN II
5. CHEMCAD
6. ProMax®
7. Super Pro Designer®
8. COCO
9. Op Sim/DW Sim
10. EMSO/EML

Equilibrium Reactor

The equilibrium reactor is a vessel which models equilibrium reactions. The outlet streams of the reactor are in a state of the chemical and physical equilibrium. The reaction set can contain an unlimited number of equilibrium reactions, which are simultaneously or sequentially solved. For this type of reaction, the quantity of each component at the equilibrium is related to equilibrium constant.

The value of equilibrium constant can be obtained by,

1. Considering it as a constant.
2. Considering it as a function of temperature.
3. Calculating it automatically from the Gibbs free energy at temperature of the reaction.

Example– $CO + H_2O = H_2 + CO_2$

Conversion Reactor

The reactor in which conversion reactions are performed called as conversion reactor. You can only attach reaction sets that contain conversion reactions. It should be specified the stoichiometry of all reactions and the conversion of the limiting reactant. This reactor calculates the composition of the outlet streams. Conversion reaction assumed that the user has information regarding the conversion of one of the reactants as a function of temperature. By knowing the conversion and the stoichiometric coefficients, the quantities of the components in the reaction can be calculated.

Example– $CO + 2H_2 = CH_3OH$

Gibbs Reactors

Gibbs reactors can work with equilibrium reactions or without any reaction information The element mass balance and try to find a state where the Gibbs free energy will be at a minimum. In the simulation Gibbs reactor can install without creating the reaction as Equilibrium reactor cannot be installed before creating reaction in software of simulation. Gibbs reactor will take non ideal effect from thermodynamic package. Gibbs reactor are most widely used to calculate Gibbs energy of reaction. Example Reaction – $CaO + CO_2 = CaCO_3$

CSTR

The CSTR (Continuous-Stirred Tank Reactor) is a vessel in which Kinetic and Heterogeneous catalytic reactions can be performed. The conversion in the reactor depends on the rate expression of the reactions associated with the reaction

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type. The inlet stream is assumed to be perfectly (and instantaneously) mixed with the material already in the reactor, so that the outlet stream composition is identical to that of the reactor contents. To simulate the CSTR we need to know the volume of the reactor. Example -$CH_4 + 2O_2 = CO_2 + 2H_2$

PFR

The PFR (Plug Flow Reactor or Tubular Reactor) generally consists of a bank of cylindrical pipes or tubes. Flow field is modeled as plug flow, implying that the stream is radially isotropic. Axial mixing is negligible. To simulate PFR we need to know volume and length of reactor.

Procedure for Equilibrium Reactor Simulation

1. Start a new DWSIM Simulation
2. Add components required for simulation
3. Ensure that all the components are added from same property package.
4. Select and add property package and click Next.
5. Drag and drop the Material stream from the object and rename as Feed. This serves as input.
6. On clicking “Feed” stream general information about block will displayed on left of screen.
7. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams. Choose “Temperature and Pressure” as the flash specification method for the inlet material stream.
8. Add two more Material streams and rename them as “Vapor” and “Liquid”. Serves as output streams.
9. Add an energy stream from the object palette
10. Locate the Equilibrium reactor block. Drag and drop into the flow sheet.
11. Select the checkboxes adjacent to the component names which has to be included in reaction. Give the stoichiometry of the reaction and choose appropriate base component. By default, basis activity and liquid phase. Change it to partial pressure and specify phase as vapor and click “OK”
12. Click on “EQ-React” block. click the dropdown button and select the necessary connections. If all the connections are given correctly all the blocks will turn blue.
13. Run the simulation by pressing “Solve flow sheet” button on top corner of the screen.
14. To analyze/display the results, select on “Master property table” icon on the tool bar. The property table will be opened showing all the results as shown in the figure below.

Procedure for Conversion Reactor Simulation

1. Start a new DWSIM Simulation
2. Ensure that all components are added from same property package. Click “Next” button.
3. Specify thermodynamic package as Raoult’s law.
4. Customize system of units in which simulation has to be carried out and click “Next”.
5. Drag and drop Material stream available at right and rename stream as Feed. Serves as input stream.
6. Double click the Feed stream. Information about stream will be displayed on right side of screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams.
7. Add two more Material streams.
8. Add an energy stream from the object palette to the flowsheet section.
9. Locate Conversion Reactor block. Drag and drop into the flowsheet.
10. Conversion reaction for the given problem. A dialogue box will appear in which name of the equation and description about the equation can be mentioned. Give the stoichiometry of the reaction and choose appropriate base component. Once base component is selected.
11. Click on Conversion Reactor block in flowsheet section. Information about the block is displayed on the right. Under “connections” tab, for all streams click the dropdown button and select the appropriate streams.
12. Run the simulation by pressing “Solve flow sheet” button on the top corner of the screen.

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13. To analyze/display the results, select on “Master property table” icon on the tool bar. The property table will be opened showing all the results as shown in the figure below.

Stepwise Procedure for CSTR Simulation

1. Start a new DWSIM Simulation.
2. Simulation configuration window will be opened.
3. Ensure all components added from same property package. Click “Next” button.
4. Select and add property package and click Next.
5. Flow sheeting section simulation window open.
6. On clicking Feed block, general information about block will displayed on left of screen.
7. Specify feed compositions, flow rate, temperature and pressure for inlet streams.
8. Add one more Material stream and rename as Product. Serves as output stream.
9. Add energy stream which is available in object.
10. Locate Continuous Stirred Tank Reactor CSTR block. Drag and drop into the flow sheet.
11. Choose the type of reaction A dialogue box will appear. Give an appropriate name and description about the reaction.
12. Select checkboxes adjacent to component names which to be included in reaction. Give the stoichiometry of the reaction.
13. Once base component, stoichiometry is specified, a text “OK” appears in the stoichiometry tab. Specify the rate constant of the reaction.
14. Default basis is activity and liquid phase chosen. This case has to be changed to Molar concentration and specify the phase as liquid.
15. Specify rate constant of reaction and click OK.
16. Click on CSTR-REC block general information about the block is displayed on the right. If all connections given correctly blocks will turn blue.
17. Run the simulation by pressing “Solve flow sheet” button on top corner of the screen.
18. To analyze/display the results select on “Master property table” icon on the tool bar. The property table will be opened showing all the results as shown in the figure below.

III. CONCLUSIONS

DWSIM is the open media simulators use to simulate various unit operations and processes like reactors, distillation, heat exchangers, adsorption column etc. There various types of reactors give the outlet property of reactions by simulating them in to simulators. Like DWSIM lot of chemical simulators are available some paid version and some of open media like DWSIM. Conversion reactor are used for calculating conversion of reaction. Similarly, Gibbs and equilibrium reactors are used to calculate equilibrium constant. Reactors are usually the heart of the chemical processes in which relatively cheap raw materials are converted to more economically favourable products. Reactions play essential safety and environmental protection roles. Process simulation is a successful tool for design, optimization and control of chemical processes.

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