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SIMULATION OF CUMENE PRODUCTION

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ABSTRACT

The Cumene production process has seen an immense rise in prospects and so better ideas and studies should be continued so that the production cost is reduced .With the modernization of technology like computers and simulating processes such as DWSIM, it is possible to design and optimize the given process. Production cost can be reduced severely by designing it in the most effective way possible hence reducing environment hazards and maintaining proper safety protocols.

AIM

To Simulate the production of Cumene using DWSIM software.

OBJECTIVE

1. To prepare the flow sheet for production of cumene
2. To optimize the contents of the flow sheet for minimization of loss of material along with a greater production of cumene and low requirement of energy
3. To stimulate the process to get a higher yield.

INTRODUCTION

● Cumene also known as Isopropyl benzene is the principal chemical used in the production of phenol and its co-product acetone on an industrial scale.

● Physically, cumene is a colorless, volatile liquid with a gasoline-like odor and it is a natural component of coal tar and crude oil, and also can be used as a blending component in gasoline.

● Cumene is the starting material in the production of acetophenone, methyl styrene, diisopropyl benzene and dicumyl peroxide.

● Minor uses of cumene include as a thinner for paints, enamels, and lacquers. It is also a good solvent for fats and resins and has been suggested as a replacement for benzene in many of its industrial applications.

CATALYST ANALYSIS

Cumene is produced by the alkylation of benzene with propylene over an acid catalyst. Catalysts like aluminum chloride, boron trifluoride, hydrogen fluoride and solid phosphoric acid (SPA) are normally used. Over the years these catalysts have given way to zeolite based catalysts. There are some inherent problems associated with conventional acid catalysts.

1. Disadvantages of using solid phosphoric acid (SPA) Process:- a)The presence of side reactions limits the production of cumene to 95% b)The catalyst is not regeneratable hence it must be replaced with a new amount in each cycle

2. Disadvantages of using Aluminum chloride as catalyst
a)Pretreatment of feeds are essential. b)The occurrence of corrosion.

3. Advantages of using the zeolite based catalyst:
a)Less needed for regeneration which means the process can run for months without worrying about affecting the

selectivity or yield. b)No corrosions. c) More profitable in terms of the capital cost and operating cost since the temperature required is lower, which can also increase the lifetime of the reactors.

CHEMICAL EQUILIBRIUM

One of the challenges is how to minimize the side reaction which forms DIPB to maximize the fraction of cumene in the outlet stream.

The selectivity of cumene can be enhanced greatly by increasing the molar ratio of benzene/propylene. Which means more molecules of benzene are available to react with propylene.

This can be achieved by recycling a great amount of benzene to the reactor. If no recycling is used either the selectivity of cumene will be poor or a larger amount of fresh benzene is needed and then dumping the excess amount after separation which is illogical.

SIMULATION

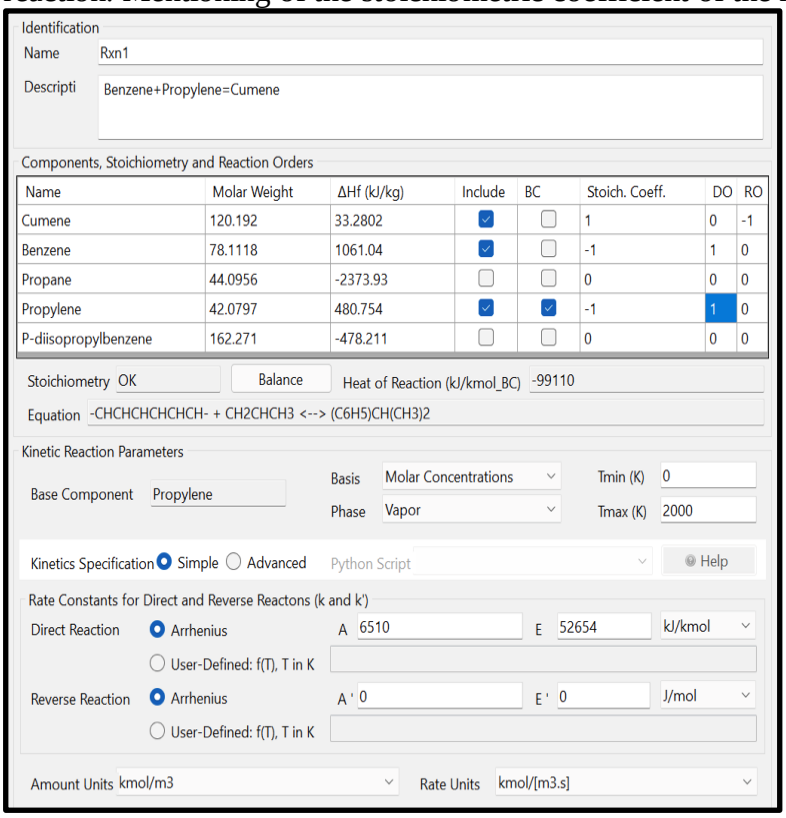
For the synthesis of Cumene, DWSIM was used for simulating the process. DWSIM is an open-source CAPE-OPEN compliant chemical process simulator. It allows us to conduct experiments and analyze data using advanced models and operations. DWSIM allows chemical engineering students and practicing engineers to model process plants by using rigorous thermodynamic and unit operations models. Since DWSIM is free and open-source, one can see how the calculations are actually being done by inspecting the code behind during execution using free tools available elsewhere.

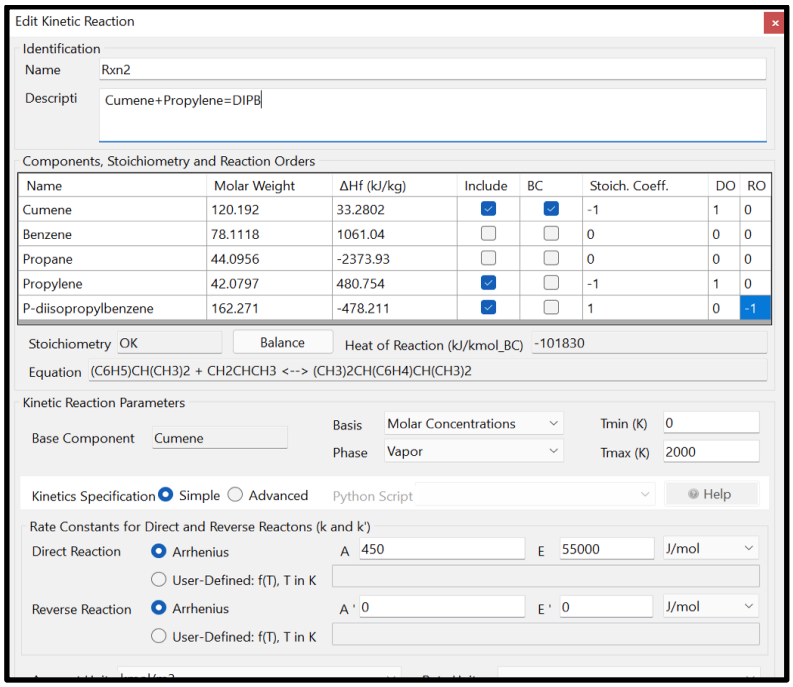
Steps involved

1.Addition of the components required from the component library and pure components were added for the synthesis of CUMENE , add the property package required (Here Peng- Robinson was used)and select the system of units.

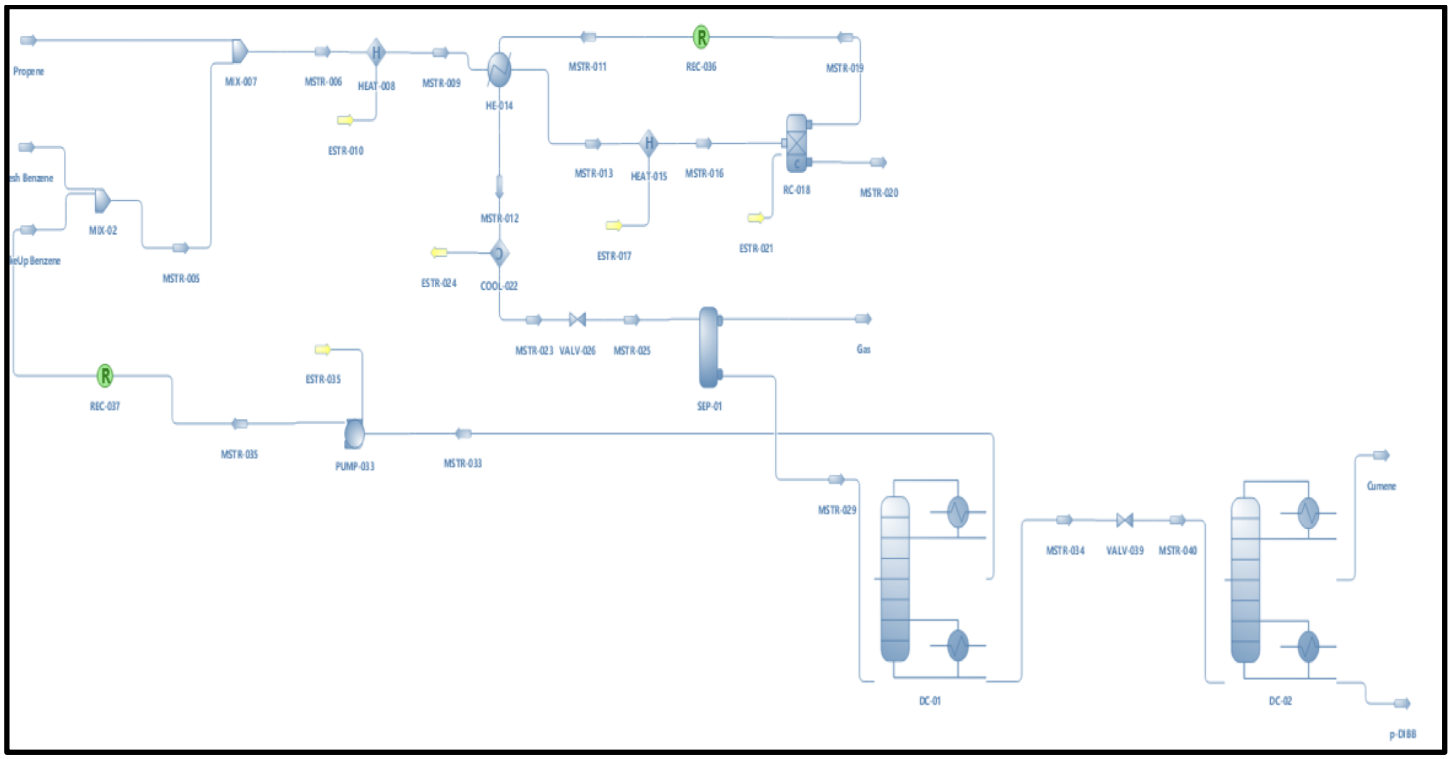
Added	Name	CAS Number	Formula	Source Database
☑	Cumene	98-82-8	(C6H5)CH(CH3)2	ChemSep
☑	Benzene	71-43-2	-CHCHCHCHC...	ChemSep
☑	Propylene	115-07-1	CH2CHCH3	ChemSep
☑	Propane	74-98-6	CH3CH2CH3	ChemSep
☑	P-diisopropylbenzene	100-18-5	(CH3)2CH(C6H...	ChemSep
☐	Carbon dioxide	124-38-9	CO2	ChemSep
☐	Carbon monoxide	630-08-0	CO	ChemSep
☐	Argon	7440-37-1	Ar	ChemSep
☐	Bromine	7726-95-6	BrBr	ChemSep
☐	Carbon tetrachloride	56-23-5	CCl4	ChemSep
☐	Chlorine	7782-50-5	Cl2	ChemSep
☐	Hydrogen iodide	10034-85-2	HI	ChemSep

2. Addition of reaction set involved in the process in the settings and choosing the base component of the reaction. Mentioning of the stoichiometric coefficient of the reactants and products.



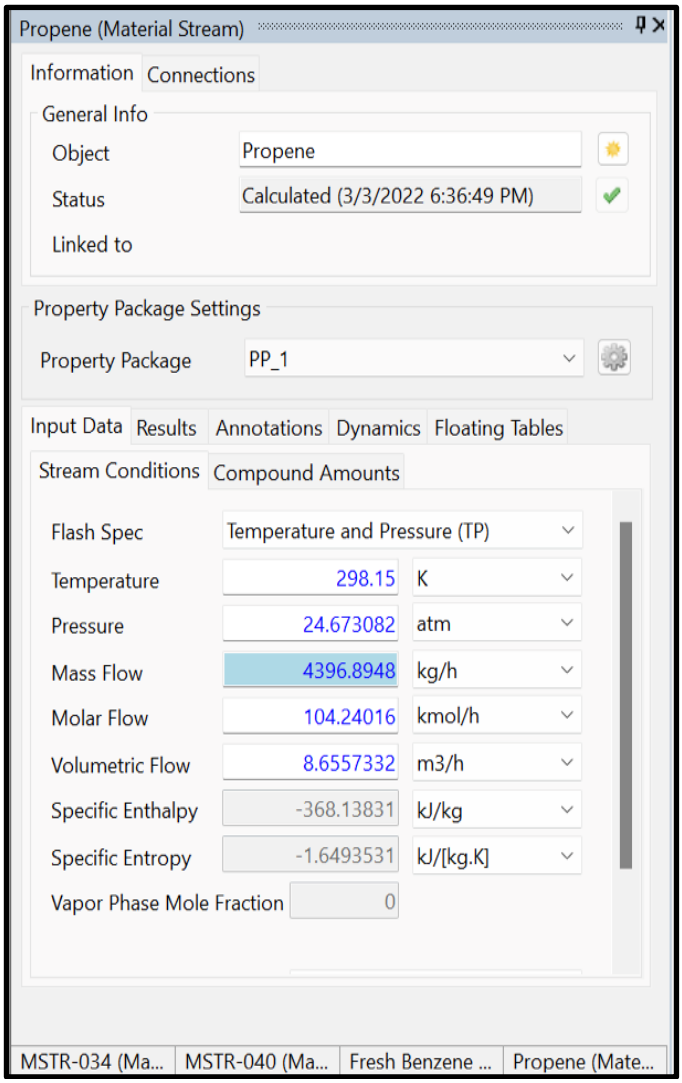


3. Enter the simulation environment. Add all the required equipment to the flowsheet from the object palette. Addition and defining of inlet and outlet material and energy streams.

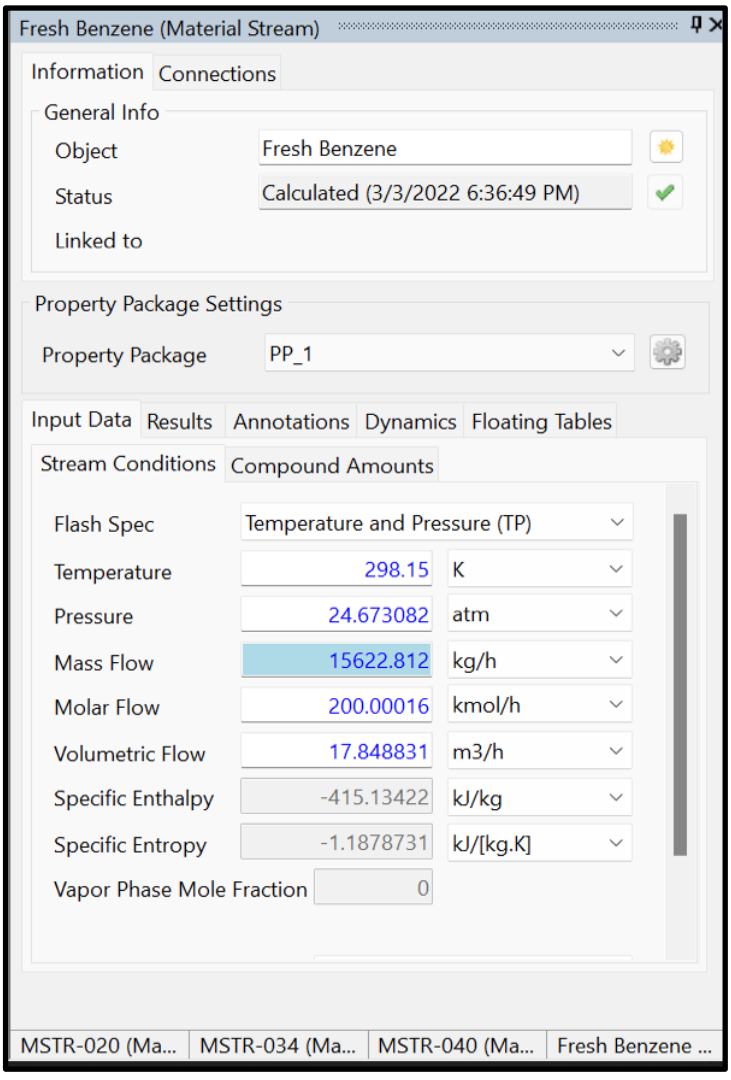


4. Defining the properties of the inlet stream.

Propene :

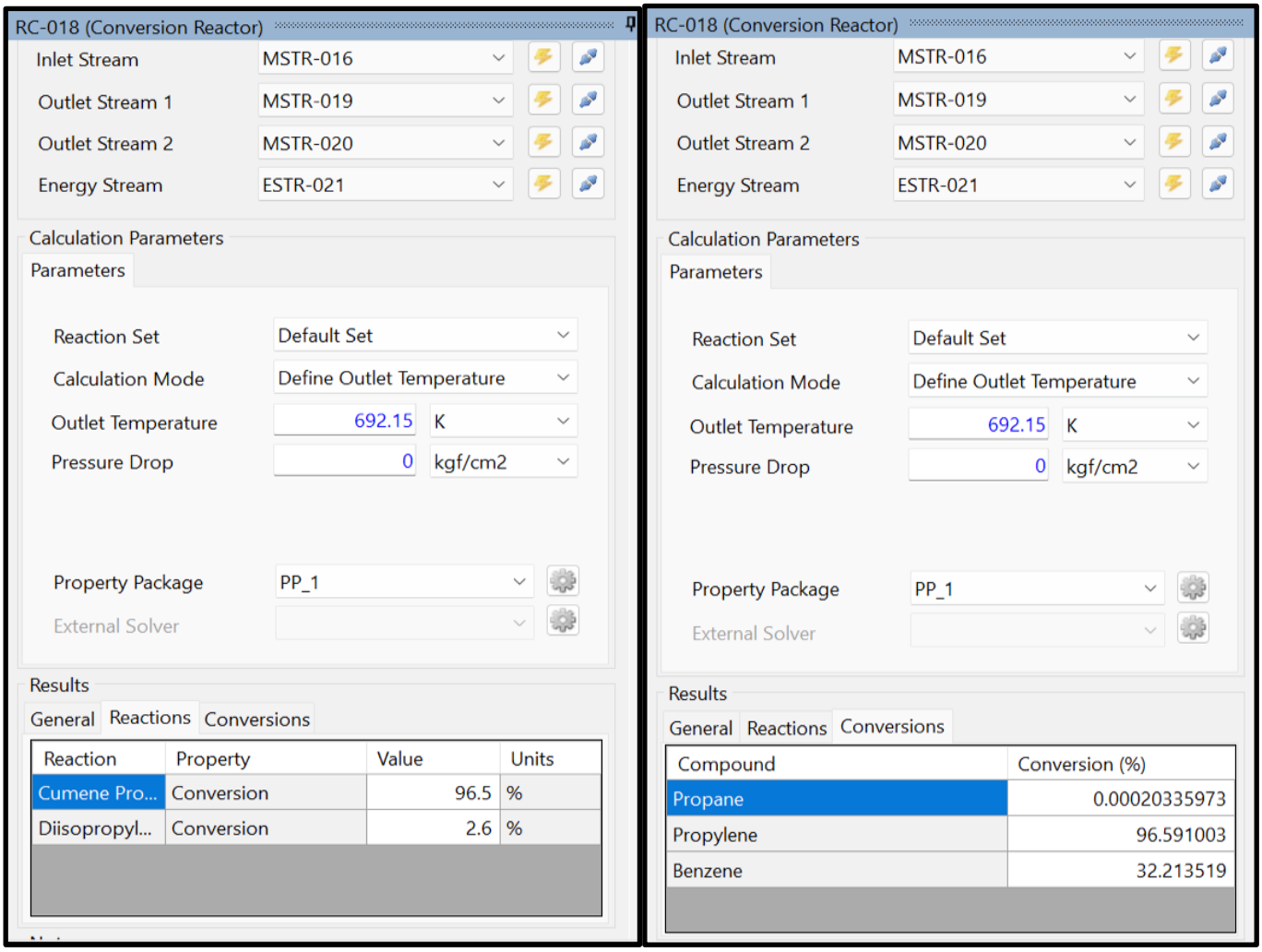


Benzene :



RESULTS AND DISCUSSION

Conversion reactor :



Stream wise results of the simulation

Stream wise Results								
Object	p-DIB	MakeUp Benzene	MSTR-020	Gas	Fresh Benzene	Excess Benzene	Cumene	
Temperature	474.17212	323.91588	692.15	363.15151	298.15	281.49104	424.87021	K
Pressure	0.98692327	24.673098	24.673082	2.3320705	24.673082	24.673082	0.98692327	atm
Mass Flow	14.538979	8316.2754	0	586.32718	15622.812	7796.8958	11516.62	kg/h
Molar Flow	0.089605966	109.06435	0	10.199988	200.00016	99.81432	95.833402	kmol/h
Volumetric Flow	0.022300383	10.318883	0	125.6549	17.848831	8.7457649	22.296875	m3/h
Molar Fraction (Mixture) / Propane	0	0.045223425	0	0.46655797	0	0	1.9930759E-13	
Molar Fraction (Mixture) / Propylene	4.6437046E-20	0.015689235	0	0.16467123	0	0	4.1746403E-14	
Molar Fraction (Mixture) / Benzene	3.3982516E-14	0.93336474	0	0.3408777	1	1	0.00050046751	
Molar Fraction (Mixture) / Cumene	0.00039010455	0.0057225977	0	0.027890776	0	0	0.99949009	
Molar Fraction (Mixture) / P-diisopropylbenzene	0.9996099	3.620992E-11	0	2.3206056E-06	0	0	9.4409417E-06	

CONCLUSION

Cumene is an organic compound that is widely used as a chemical intermediate in the production of phenol and acetone. In our project we have studied the industrial method of production of cumene by the alkylation of benzene and propylene. The simulation of production of cumene will be carried out using DWSIM Software. We will be using a zeolite based catalyst to cut down production cost and also minimize environmental impacts.

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