



Synthesis of Iso-butane from n-butane

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Background:

The use of the isomerisation process to transform normal paraffin into their isomers will increase the octane numbers of the LSR naphtha (C5-82°C). The catalytic isomerisation of n-butane to iso-butane is an industrially significant reaction owing to the growing need for iso-butane in the manufacture of synthetic rubber and the alkylation of isoparaffins, which are considered an option for octane boosters instead of oxygenate and aromatic compounds, all of which are subject to stringent environmental restrictions.

A large portion of the iso-butane used in alkylation is generated in refineries by hydrocrackers and catalytic crackers, but it is also obtained from catalytic reformers, crude distillation, and natural gas processing. Normal butane is isomerised to generate additional iso-butane for alkylation unit feed in refineries that do not have hydrocracking facilities to provide iso-butane for alkylation unit feed.

Only iso-paraffins with tertiary carbon atoms, such as iso-butane or iso-pentane, react with the olefins during the alkylation process. In reality, only iso-butane is used because iso-pentane has a high enough octane number and low vapour pressure to be blended directly into finished gasoline.

Description of Flowsheet:

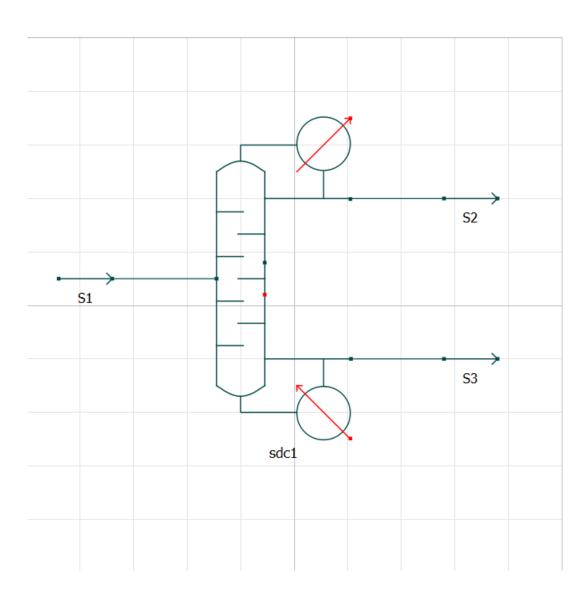
The thermodynamic property package Raoult's Law is included.

A fresh feed stream S1 of propane, iso-butane, n-butane and isopentane is delivered to the distillation column "sdc1". A vapour side stream S2 is drained and fed to an isomerisation reactor R1 in the stripping section of the column, where some of the n-butane is transformed to iso-butane. In the rectifying portion, the reactor effluent is recycled into the column. Isopentane is extracted from the bottoms, and moderate-purity iso-butane is obtained from the distillate.



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Flowsheet:



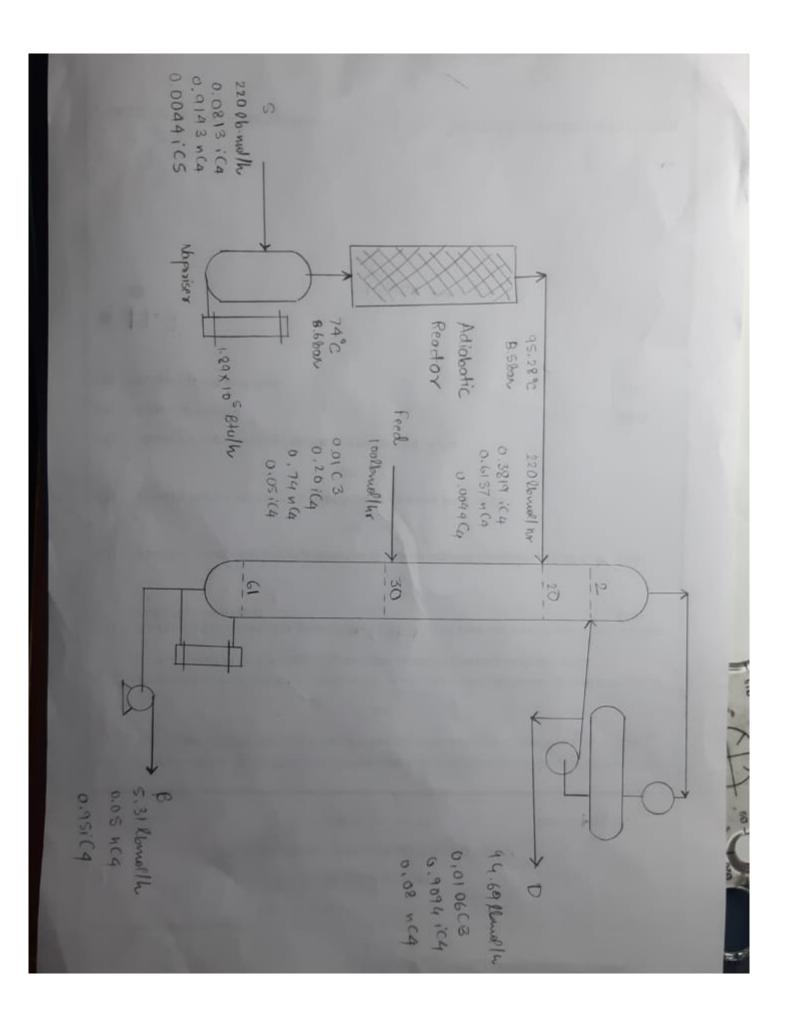
Results:

Problem faced during simulation of flowsheet in Open Modelica:

I faced an issue to take the side stream output at the 45th stage in Distillation column "sdc1" and thus I wasn't able to proceed further with the Adiabatic reactor. If an extended time for submission is provided, I might be able to find the solution and stimulate the flowsheet in the following manner:



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Reference: Control of an Isomerization Column/Reactor Process