

Case Study & Performance Analysis of Reactive Distillation Unit Operation for Phenol Synthesis Relative to Conventional Hock Process

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Highlights

- The reactive distillation column achieved 99.99% conversion of CHP to phenol/acetone
- With 99.99% separation of phenol (distillates) & acetone (bottoms) using 46,871 kW condenser duty
- The Thermodynamic nature of CHP to phenol/acetone reaction eliminates the need for the reboiler
- Smaller feed streams led to lower CHP concentration & desired phenol output of 663 kmol hr⁻¹

1. Introduction

Distillation is one of the most widely employed separation processes in the chemical industry. However, conventional distillation columns in the current political & energy climate is growing prohibitively costly, impeding economic gains & supply chain security. Process intensification, specifically reactive distillation columns (RDC) offer a mean to improve process optimization through energy utilization. RDC combines conventional distillation with chemical reaction into a single unit. This paper will adjust the conventional Hock process, typically consisting of a series of packed-bed reactors followed by a succession of distillation columns. It is also perturbed by azeotrope & maximum conversion constraints by incorporating RDCs assessing the benefits & limitations of this process intensification method.

2. Methods

Aspen Plus V12.1 & MATLAB will be employed to be the primary analysis software tools for this design. A simulation of the RDC as a RadFrac under identical conditions to the conventional Hock Process to achieve a preliminary comparison in the field of energy utilization & economic sustainability. For the reactive section design heuristics, the Langmuir isotherm was adopted to formulate the catalytic reaction occurring within the RDC. Furthermore, using the site balance eqn & inputting species' concentration will yield a reaction rate equation for the main reaction:

$$-r_s = \frac{k_{sr} w_{cat} \rho_{liq} \left(\gamma_{CHP} x_{CHP} - \frac{(\gamma_{ph} x_{ph})(\gamma_{ace} x_{ace})}{K} \right)}{1 + K_{CHP} \gamma_{CHP} x_{CHP} + K_{ph} \gamma_{ph} x_{CHP} + K_{ace} \gamma_{ace} x_{CHP}} \quad (1)$$

Through this the catalyst weight needed for the design section can be calculated. As for the separation section design heuristics, to achieve the minimum number of stages that allow the realization of desired level of separation, the Fenske equation is needed. Accounting for the characteristics of the RDC, the typical procedure had to be modified & pseudo binary mol fractions have to be calculated in terms of the key components, phenol and acetone.

3. Results and discussion

The modified Hock process with RDC was able to achieve the set goal of 663 kmol hr⁻¹ of phenol and acetone as the traditional process with less unit operations & less utility use with a catalyst weight of W = 2800 kg, as can be seen in figure 1.

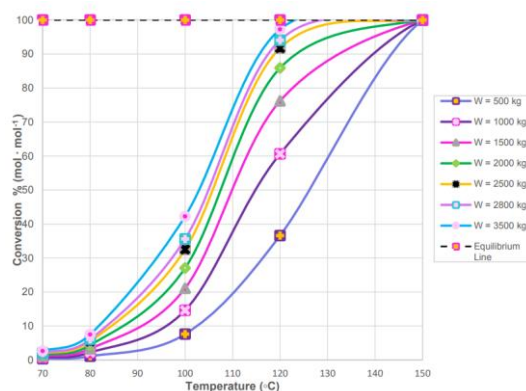


Figure 1. Conversion-temperature diagram (CTD) for an isothermal PFR mimicking the reactive section of the RDC

This was done by utilizing the exothermic nature of the reaction, the latter tray stages see an increase in temperature due to reaction which can give further insight into placing future streams into the RDC. To make the reaction more favorable to phenol & acetone synthesis, splitting the feed stream into smaller streams (see figure 2) will be considered particularly close to the reaction location as recommended by literature to reduce the concentration of phenol & acetone at feed stages relative to cumene hydroperoxide (CHP).

After concluding the optimization process, the reboiler duty was 44 kW, signaling the ability to remove it & save further capital, operational & maintenance costs.

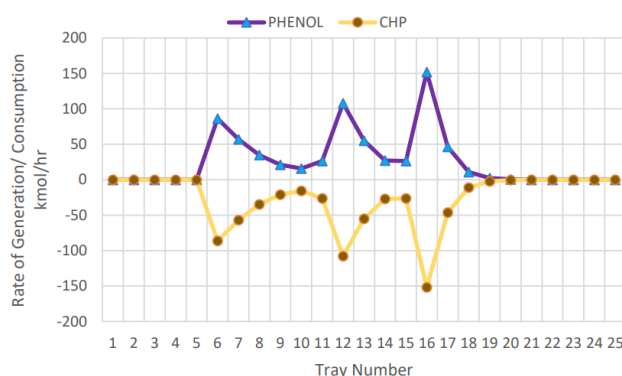


Figure 2. The tray stages exhibiting phenol/acetone reaction generation & CHP consumption

4. Conclusions

Incorporating a reactive distillation column into the traditional Hock Process has shown capability in reducing utility & capital costs by maintaining excellent product conversion & separation of acetone byproduct while eliminating the need for reboilers & other units, signifying RDC's as a very prospective method of process intensification. However, for other processes, catalyst cost and availability as well as the thermodynamic nature of the main & side reactions will also play a role in the viability of the chosen methods.

References

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Keywords

Process Intensification; Reactive Distillation Column; Simulation; Optimization

