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Plantwide Control of a Cumene Manufacture Process

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Abstract

This work describes the application of the plantwide control design procedure of Skogestad (Skogestad, 2004) to the cumene production process. A steady state "top down" analysis is used to select the set of "self-optimizing" primary controlled variables which when kept constant lead to acceptable economic loss without the need to reoptimize the process when disturbances occur. Two modes of operation are considered: (I) given feed rate and (II) optimized throughput.

Keywords: cumene production, control structure design, self-optimizing control

1. Introduction

Cumene is an important industrial intermediate in the manufacture of phenolic and polycarbonate resins, nylon and epoxy and is conventionally produced by the Friedel Crafts alkylation of benzene with propylene. (Concentration unit: kmol/m^3).

Main reaction: $C_6H_6 + C_3H_6 \rightarrow C_9H_{12}$ (Cumene) *(k=2.8E7, E= 104174 kJ/kmol)*

Side reaction: $C_9H_{12} + C_3H_6 \rightarrow C_{12}H_{18}$ (DIPB) *(k=2.32E9, E= 146742 kJ/kmol)*

Some research has already been done over the past few years which discusses the various aspects of operation, design and control of a cumene production plant. [1, 2] But none of them address the issue of control structure design in a systematic manner. In this work we try to address this by applying a part of Skogestad's plantwide procedure of (Skogestad, 2004). The main steps of this procedure are as follows:

- Degree of freedom analysis.
- Definition of optimal operation (cost and constraints).
- Identification of important disturbances
- Identification of candidate controlled variables c.
- Evaluation of loss for alternative combinations of controlled variables
- Final evaluation and selection (including controllability analysis)

Two modes of operation are considered for the process: Mode 1: Given Throughput. Mode 2: Optimized/Maximum Throughput. (feed rate is also a degree of freedom).

2. Base Case Design

The base case design parameters and kinetics data and cost correlations were taken from Luyben (2010). Figure 1 provides a schematic of the conventional process. The fresh benzene and fresh C_3 (95% propylene and 5% n-propane) streams are mixed with the recycle benzene, vaporized in a vaporizer, preheated in a feed effluent heat exchanger (FEHE) using the hot reactor effluent, before being heated to the reaction temperature in a furnace. The heated stream is fed to a cooled packed bed reactor. The hot reactor effluent loses sensible heat in the FEHE and is further cooled using cooling water. The cooled stream is sent to a light out first distillation train. The inert n-propane and small amounts of unreacted propylene are recovered as vapour distillate from column 1.The bottom stream is further distilled in the recycle column to recover and recycle unreacted benzene as the distillate. The recycle column bottom stream is sent to the product column to recover 99.9% cumene as the distillate and the heavy DIPB as the bottoms.

2.1. Determination of column 1 pressure

The flash tank in the Luyben design has been replaced with a distillation column (column 1) to reduce the loss of benzene and hence increase the plant operating profit. A column operating pressure of 5 bar with a benzene loss of 0.12 kmol/h was found to be near optimal. Table 1 provides an economic comparison of the base case design with the original Luyben design (with a flash tank instead of column 1) for the same operating conditions. The yearly operating profit of the base-case design is noticeably higher than the Luyben design due to the reduction in the loss of precious benzene in the fuel gas stream. For completeness, economic / operating condition details of Mode I and Mode II optimum solutions, where the plant operating profit (defined later) is optimized, are also provided in Table 1.

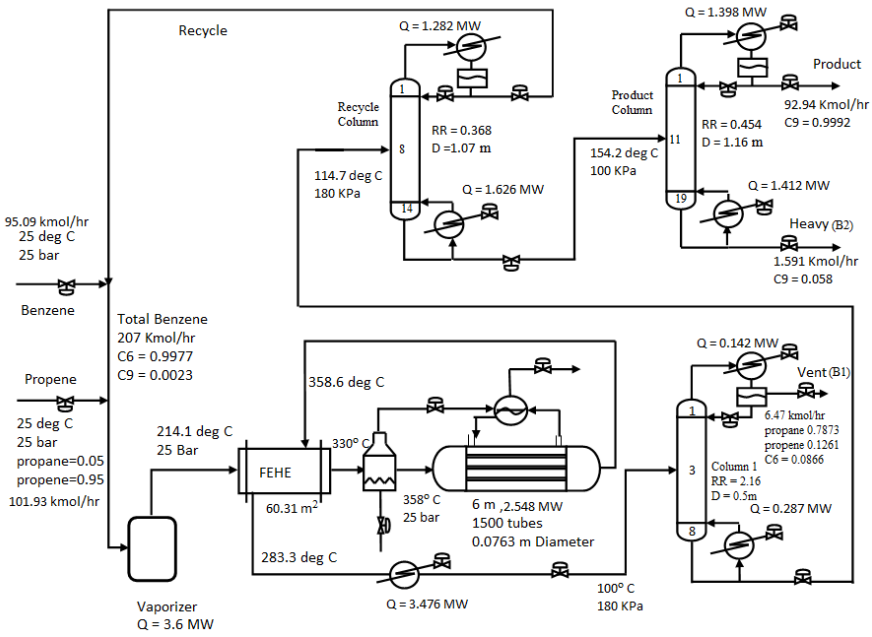

Figure1: Base-case cumene process flowsheet

3. Economic optimization of the base case design

3.1. Definition of objective function (J) and constraints

Total operational profit per year (365 days) was chosen as the objective function *J* which is to be maximized with

J = Product revenue – reactant cost + DIPB credit + vent gas credit + reactor steam credit – preheater electricity cost – steam cost in reboilers and vaporizer

Since the plant is already built, it has certain physical limitations associated with the unit operation equipment. Moreover it is always optimal to have the most valuable product at its constraint to avoid product give-away. The steady state degrees of freedom to maximize the Mode I / Mode II operating profit are noted in Table 2. Note that since *J* does not have a strong relationship with cooler outlet temperature it is fixed at 100 °C.

Table 1. Economic comparison of base-case design with original Luyben design

	Unit	*Luyben*	*Base case*	*Mode I*	*Mode II*
Reactor inlet temp	$^{\circ}$C	358	358	361	346.99
Total benzene flow	kmol/h	207	207	245	269.7
Hot Spot temp	$^{\circ}$C	430	421.60	417.50	411.3
Benzene recycle	kmol/h	207	207	245	269.70
Vent	kmol/h	9.98	6.47	6.02	19.04
Heavy Bottom	kmol/h	1.55	1.59	1.20	2.99
Fresh Propene	kmol/h	101.93	101.93	101.93	175.02
Fresh Benzene	kmol/h	98.78	95.09	95.00	153.87
Product	kmol/h	92.86	92.94	93.67	150.47
Total Capital Cost	$ 10^6	4.11	4.26	4.26	4.26
Total Energy Cost	$ 10^6/year	2.23	2.35	2.68	3.43
Benzene cost	$ 10^6/year	59.36	57.14	57.09	92.47
Propylene cost	$ 10^6/year	30.63	30.63	30.62	52.59
Reactor steam credit	$ 10^6/year	0.40	0.54	0.53	0.86
Vent (B1) credit	$ 10^6/year	1.59	0.70	0.59	1.84
Heavy (B2) credit	$ 10^6/year	0.71	0.48	0.38	0.95
Product revenue	$ 10^6/year	107.74	107.87	108.72	174.64
Total operational cost	$ 10^6/year	89.52	88.40	88.89	144.88
Total operational profit (J)	**$ 10^6/year**	**18.23**	**19.47**	**19.83**	**29.76**

Price Data: HP steam $9.83/GJ, Steam generated $6.67/GJ, Electricity cost $16.8/GJ, Benzene price $68.6/kmol, Propylene price $34.3/kmol, Cumene price $132.49/kmol.

Table 2. Steady state degrees of freedom

Process variables			*DOF*
Fresh propene flow rate		101.93 kmol/h$^{\#}$	0/1*
Total benzene flow rate		Variable	1
Furnace outlet temperature		Variable	1
Reactor cooler temperature		Fixed	0
Column 1	Condenser Temperature	32.25 ^{0}C	1
	$x_{C3,B}$	Variable	
Column 2	$x_{C9,D}$	Variable	2
	$x_{C6,B}$	Variable	
Column 3	$x_{C9,D}$	0.999	1
	$x_{C12,B}$	Variable	

#: Fixed for Mode I. *: Degree of freedom for Mode II

3.2. Optimization results

Ideally all dofs in Table 1 should be simultaneously optimized. However, to overcome convergence issues in UniSim, the separation section is optimized first followed by the rest of the plant (see e.g. Araujo et al, 2007). The optimization results obtained are summarized in Table 3.

For Mode I operation, none of the constraints are active while in Mode II operation (optimal throughput), the maximum furnace duty and product column boilup constraints are active. From an economical point of view, it is optimal to increase the Mode I feed rate without violating the constraints of the plant. As the propylene feed rate is

increased the profit increases due to higher production. The first constraint to become active is maximum furnace heating. However this is not the real bottleneck as feed rate can be further increased by lowering the reactor inlet temperature and/or recycle benzene flow and hence increasing the profit. As the throughput is further increased, the maximum product column boilup constraint becomes active for a fixed DIPB mol fraction in the product column bottoms. This mol fraction may be decreased to further increase the throughput and profit with the boilup constraint active. The DIPB mol fraction can however not be decreased too much as the profit decreases due to cumene product loss in the heavy fuel stream. The reported column 3 $x_{C12,\,B}$ value in Table 3 corresponds to this limit of maximum operating profit.

Table 3. Summary of Mode I and Mode II Optimization Results

Process variables		*Mode I*		*Mode II*	
		Type	*Value*	*Type*	*Value*
Fresh propene		Fixed	101.93 kmol/h	Variable	175.02 kmol/h
Total benzene		Variable	245 kmol/h	Variable	269.7 kmol/h
Rxr inlet temperature		Variable	361 $^{\circ}$C	Max furnace duty*	346.99 $^{\circ}$C
Cooler temperature		Fixed	100 $^{\circ}$C	Fixed	100 $^{\circ}$C
Column 1	Top T	Fixed	32.25 $^{\circ}$C	Fixed	32.25 $^{\circ}$C
	$x_{C3,B}$	Variable	0.01	Variable	0.01
Column 2	$x_{C9,D}$	Variable	$5.5\text{x}10^{-3}$	Variable	0.0012
	$x_{C12,B}$	Variable	$2.7\text{x}10^{-4}$	Variable	$3.5\text{x}10^{-4}$
Column 3	$x_{C9,D}$	Fixed	0.999	Fixed	0.999
	$x_{C12,B}$	Variable	0.9542	Max boil up*	0.9628

*: Variable is fixed by this constraint

4. Self-optimizing Controlled Variables

Skogestad (2004) states that self-optimizing control is when one can achieve an acceptable economic loss with constant setpoints for appropriately chosen / designed controlled variables without the need to re-optimize for disturbances. In this work, four disturbances are considered as in Table 3.

Table 4. Set of disturbances considered

SN.	*Disturbance variable*	*Nominal Value*	*change*
d1	Propylene flow rate	101.93 kmol/h	- 10 kmol/h
d2	Column 1 condenser temperature	32.25 ^{0}C	+3 ^{0}C
d3	Inert composition in the propylene feed	5% propane	+3 %
d4	Propylene flow rate	101.93 kmol/h	+10 kmol/h

4.1. Mode I Self Optimizing Controlled Variables

For each of the four disturbances, the plant is sequentially reoptimized for all 6 unconstrained dofs (see Table 2). We also reoptimize the process keeping the distillation column mole recoveries constant (i.e. using 6 – 4 = 2 degrees of freedom). The difference in the objective function for the two cases was observed to be very small for all the disturbances (< 0.07%). Hence we choose to use distillation column mole recoveries as controlled variables for two reasons: First, resulting loss values are very small. Second, it reduces the number of self-optimizing variables to be determined and simplifies the further analysis to a great extent as we are left with only 2 input variables instead of 6.

To choose the remaining two self-optimizing controlled variables, we use the “exact local method” (Halvorsen et al., 2003) which minimizes the worst case loss due to

suboptimal self-optimizing control policy. The branch and bound algorithm of Kariwala (2007) is used for the evaluation of the loss. Seven candidate controlled variables, namely, reactor inlet temperature, preheater duty, fresh benzene flow rate, total benzene flow rate, reactor feed benzene to propane ratio, reactor feed benzene mol fraction and vaporizer outlet temperature, are evaluated. The best set of two self optimizing variables for Mode I operation are thus found to be the reactor inlet temperature and the reactor feed benzene to propylene ratio.

4.2 Mode II Self Optimizing Controlled Variables

The maximum furnace duty and maximum product column boil up are the two active constraints in Mode II. This leaves 5 (7 dof – 2 active constraints) unconstrained dof for which we need to find 5 self optimizing controlled variables. Similar to Mode I, the column purity specifications, namely, column 1 $x_{C3,B}$, column 2 $x_{C9,D}$ and $x_{C6,B}$ when kept at their optimized nominal values with no disturbance result in negligible loss for the set of disturbances considered (note that column 3 $x_{C12,B}$ is fixed by its maximum boilup constraint).

As in Mode I, the exact local method is used to select the best self optimizing variables for the remaining two unconstrained dof. The best set was found out to be fresh benzene flow rate and the reactor inlet propylene mol fraction. The economic loss for the next best set, which is total benzene flow and the reactor feed benzene to propylene is only slightly higher. Since the latter variable is a self-optimizing variable also in Mode I, we select this set as our choice of controlled variables in Mode II to simplify the transition from Mode I to Mode II. The transition would only require replacing the reactor inlet temperature controller with the total benzene flow controller.

5. Conclusion and future work

In this work, a cumene production plant has been systematically analyzed for economically optimal operation at given throughput (Mode I) and optimum throughput (Mode II). Results show that in Mode I operation, the optimized unconstrained column product purities are self optimizing along with the reactor inlet temperature and the reactor feed benzene to propylene ratio. In Mode II, the maximum furnace duty and product column boilup constraints are active. The self-optimizing variables are again the unconstrained column product purities along with the total benzene flow to the reactor and the reactor feed benzene to propylene ratio. Further work would focus on developing a plantwide control structure for the process and its dynamic validation.

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