Isophorone reactor: Modelling and performance enhancement

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HIGHLIGHTS

► Production of isophorone incorporating multiple reactions was modelled.
► A dynamic non-equilibrium model of reactive distillation was developed.
► The model was used to understand influence of various parameters on a key mass ratio.
► Simulated results will be useful for improving performance of isophorone reactor.

ARTICLE INFO

ABSTRACT

The production of isophorone in a reactive distillation column was modelled. Mass transfer and heat transfer accompanied by chemical reactions were incorporated in a dynamic non-equilibrium multistage model. A base case simulation was identified and established. The base case simulation showed the value of key performance indicator that is mass ratio of acetone consumed to isophorone produced as 1.54. The computational model was then used to understand and to evaluate influence of various key design and operating parameters on this key performance indicator. Influence of reactor volume, mass transfer coefficient and feed composition, location and temperature was evaluated. The simulated results indicate that the key performance indicator can be improved (reduce acetone consumed per isophorone produced) by manipulating acetone content in the feed and location of the feed. The presented results will be useful for realising performance enhancement of isophorone and other similar reactors.

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1. Introduction

Isophorone is an important industrial chemical having applications in inks, paints, lacquers, adhesives, vinyl resins, copolymers, coatings, finishes, and pesticides. It is also used as a chemical intermediate for organic synthesis. Isophorone is commercially produced [1] by alkali catalysed condensation of acetone at high pressure and high temperature. Aldol condensation of acetone is a complex reaction [2–8] involving the feedstock: acetone, water and hydroxide catalyst; several intermediate products (diacetone alcohol, mesityl oxide), byproducts (oxylitone and heavies) and the desired product of the reaction–isophorone. Acetone condensation for isophorone production can be commercially feasible, if the specificity of the reaction is controlled to achieve a high selectivity towards isophorone. One of the key indicators of the plant performance in isophorone production is the overall mass ratio of acetone consumed to isophorone produced. In this work, a mathematical model of isophorone reactor is developed and used for

evolving guidelines for enhancing performance of isophorone reactors.

Isophorone is usually produced by carrying out acetone condensation in single or multiple distillation columns. The reactive distillation facilitates formation and separation of isophorone and intermediate products of the reaction including diacetone alcohol, mesityl oxide and xylitones. It is essential to understand the key aspects of isophorone production process and of reactive distillation for manipulating selectivity towards isophorone and reducing the acetone consumption. In this section we address the issues pertinent to isophorone production via reactive distillation from a process perspective.

Issues relevant to isophorone production have been addressed in various patents, which describe the reactor configuration, reaction conditions and nature of contacting among various reactants for catalysed condensation of acetone. Walton and Yeomans [1] outline a process for isophorone production using a potassium hydroxide catalyst in multiple distillation columns consisting of a reaction and a hydrolysis column (Fig. 1). The temperature in the reaction and hydrolysis columns is in the range of 150–250 °C and pressure is in the range of 10–55 bar. The feed consisting of 65–85% w/w acetone, 35–15% w/w water and 0.7–0.3% w/w potassium hydroxide is

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Nomenclature

Total and component molar balance

$M_{(j)}^{L}$	total number of liquid phase moles on stage j (kmol)
$M_{(j)}^{V}$	total number of vapour phase moles on stage j (kmol)
$M_{(i,j)}^{L}$	total number of liquid phase moles of ith component on stage j (kmol)
$M_{(i,j)}^{V}$	total number of vapour phase moles of ith component on stage j (kmol)

Initial molar holdup and stage accumulation ratios

$\Im_{(j)}^{L}$	total initial number of liquid phase moles on stage j (kmol)
$\Im_{(j)}^{V}$	total initial number of vapour phase moles on stage j (kmol)
$f_{(t)}^{V}$	time dependent functional multiplier for ratio of liquid phase molar output flow to molar accumulation rate (function of time)
$f_{(t)}^{L}$	time dependent functional multiplier for ratio of vapour phase molar output flow to molar accumulation rate (function of time)
$LRatio_{(j)}^{Output/Accumulation}$	ratio of output liquid molar flow to molar accumulation rate on stage j (–)
$VRatio_{(j)}^{Output/Accumulation}$	ratio of output vapour molar flow to molar accumulation rate on stage j (–)
$LRatio_{(j)}^{MaxVol/InitialVol}$	ratio of maximum liquid stage volume to initial volume on stage j (–)
$VRatio_{(j)}^{MaxVol/InitialVol}$	ratio of maximum vapour stage volume to initial volume on stage j (–)
t	simulation time (h)

Molar flows

$L_{(j)}$	total liquid phase molar flow originating from stage j (kmol h^{-1})
$L_{(j-1)}$	total liquid phase molar flow originating from stage $j-1$ (kmol h^{-1})
$V_{(j)}$	total vapour phase molar flow originating from stage j (kmol h^{-1})
$V_{(j+1)}$	total vapour phase molar flow originating from stage $j+1$ (kmol h^{-1})
$F_{(j)}^{L}$	total molar flow of liquid feed entering stage j (kmol h^{-1})
$F_{(j)}^{V}$	total molar flow of vapour feed entering stage j (kmol h^{-1})
R	reflux ratio (–)

Gas liquid mass transfer

$A_{(i)}^{diff}$	parameter A corresponding to component i (–)
$B_{(i)}^{diff}$	parameter B corresponding to component i (–)
$H_{(i)}^{diff}$	parameter H corresponding to component i (–)
$W_{(i)}^{diff}$	parameter W corresponding to component i (–)
$MW_{(i)}$	molecular weight of component i (kg kmol^{-1})
$T_{(i)}^{Critical}$	critical temperature of component i (K)
$T_{r(i,j)}$	reduced temperature of component i on stage j (–)
$D_{L(i,j)}$	liquid phase diffusion coefficient of component i on stage j (m^2 s^{-1})
a	packing area for structured packing/interfacial area per unit liquid volume (m^2 m^{-3})
C_E	factor for structured packing (–)
$holdup_{L(j)}$	fractional liquid phase holdup on stage j (–)
$S_{(j)}$	characteristic length: side dimension of the corrugation cross section (m)
$U_{LE(j)}$	effective liquid velocity in the column on stage j (m s^{-1})

$U_{LS(j)}$	superficial liquid velocity in the column on stage j (m s^{-1})
ε	void fraction of the structured packing (–)
θ	channel flow angle of the structured packing (°)
$\mu_{(j)}^{L}$	liquid phase viscosity on stage j (Pa s)
$Mass\ Flow_{(j)}^{L}$	liquid phase mass flow on stage j (kg h^{-1})
$Mass\ Flow_{(j)}^{V}$	vapour phase mass flow on stage j (kg h^{-1})
$\rho_{(j)}^{L}$	liquid phase density on stage j (kg m^{-3})
$\rho_{(j)}^{V}$	vapour phase density on stage j (kg m^{-3})
$A_{(j)}^{bubbling}$	bubbling area of the tray on stage j (m^2)
$heightw_{(j)}$	exit weir height of stage j (m)
$pitch_{(j)}$	hole pitch of stage j (m)
$A_{(j)}^{hole}$	hole area of the sieve tray on stage j (m^2)
$height_{(j)}^{L}$	clear liquid height on stage j (m)
$u_{SV(j)}$	superficial vapour velocity on stage j (m s^{-1})
$\sigma_{(j)}$	surface tension of the liquid phase on stage j (N m^{-1})
$ah_{f_{(j)}}$	interfacial area per unit bubbling area on stage j (m^2 m^{-2})
$K_{(i,j)}^{Distribution}$	gas–liquid distribution coefficient of component i on stage j (–)
$\gamma_{(i,j)}^{L}$	liquid phase activity coefficient of component i on stage j (–)
$k_{L(i,j)}$	liquid side mass transfer coefficient of component i on stage j (m s^{-1})
$k_L a_{(i,j)}$	overall liquid side mass transfer coefficient of component i on stage j (h^{-1})
$N_{(i,j)}^{GL}$	molar gas–liquid mass transfer rate of component i on stage j (kmol h^{-1})

Reaction parameters

$z_{(i,k)}$	stoichiometric coefficient of component i in the kth reaction (–)
$b_{(k)}$	base stoichiometric coefficient for the kth reaction (–)
$k_{0(k)}$	pre-exponential factor of the kth reaction ((m^3 kmol^{-1})$^{(order\ of\ reaction-1)}$ h^{-1})
$E_{(k)}$	activation energy of the kth reaction (kJ kmol^{-1})
$o_{(i,k)}$	order of the kth reaction for component i (–)
$k_{(k)}$	rate constant of the kth reaction ((m^3 kmol^{-1})$^{(order\ of\ reaction-1)}$ h^{-1})
$K_{(k,k+1)}$	equilibrium constant of the $k/k+1$ reaction (–)

Mole fractions

$x_{(i,j)}$	liquid phase mole fraction of component i on stage j (–)
$x_{(i,j-1)}$	liquid phase mole fraction of component i on stage $j-1$ (–)
$x_{(i,j)}^{Interface}$	interface liquid phase mole fraction of component i on stage j (–)
$x_{(i,j)}^{initial}$	initial liquid phase mole fraction of component i on stage j (–)
$y_{(i,j)}$	vapour phase mole fraction of component i on stage j (–)
$y_{(i,j+1)}$	vapour phase mole fraction of component i on stage $j+1$ (–)
$y_{(i,j)}^{Interface}$	interface vapour phase mole fraction of component i on stage j (–)
$y_{(i,j)}^{initial}$	initial vapour phase mole fraction of component i on stage j (–)
$z_{(i,j)}^{L}$	liquid phase mole fraction of component i fed to stage j (–)
$z_{(i,j)}^{V}$	vapour phase mole fraction of component i fed to stage j (–)