

# Semibatch Reactive Distillation for Isopropyl Acetate Synthesis

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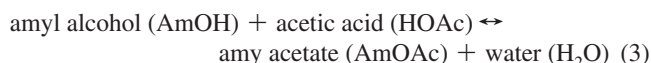
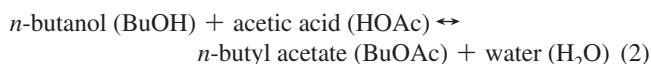
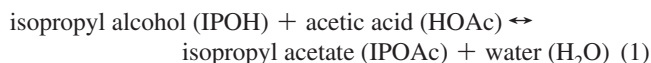
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Batch reactive distillation, which combines the flexibility of batch process with the advantages of reactive distillation, can be an effective alternative to conventional batch processing. For instance, acetate esters such as *n*-butyl acetate and amyl acetate can be produced using batch reactive distillation. Previous studies have shown that isopropyl acetate can also be produced in batch reactive distillation with the addition of chloroform as an entrainer and using a large reflux ratio and number of stages. This paper compares the vapor–liquid and liquid–liquid features of these acetate ester systems, and shows the similarities and differences among them. We show why the isopropyl system is more difficult than the others and how semibatch reactive distillation without an additional entrainer can result in a feasible and more efficient process for the production of isopropyl acetate than has been previously known. In a semibatch reactive distillation, the loss of isopropyl alcohol can be substantially decreased, the purity of water byproduct can be improved, and the total reflux or recycle of the organic distillate phase can be avoided. The semibatch reactive distillation can provide 20% higher production efficiency than batch reactive distillation.

## 1. Introduction

Acetic acid (HOAc) esterification is a common application<sup>1</sup> of reactive distillation, effective because it circumvents the reaction equilibrium limitation by removing one or more of the products from the reaction zone. Yu and colleagues<sup>2</sup> studied continuous reactive distillation processes for the esterification of acetic acid with different alcohols, ranging from C<sub>1</sub>–C<sub>5</sub>. They established qualitative relationships between possible process flowsheets and phase equilibria and also proposed a systematic design procedure to optimize the possible designs for minimum total annual cost (TAC). Their results provide excellent insights for the conceptual design of continuous reactive distillation systems for these acetate esters.

For the isopropyl acetate (IPOAc), *n*-butyl acetate (BuOAc) and amyl acetate (AmOAc) systems, binary mixtures of water and the acetate product form two liquid phases, in which a high purity of water (99.6 mol % at 50 °C, 99.9 mol % at 91 °C, and 99.9 mol % at 25 °C for IPOAc,<sup>3</sup> BuOAc<sup>4</sup> and AmOAc<sup>5</sup> systems, respectively, at 1 atm) can be obtained in the aqueous phase.



Each of these three systems has a ternary minimum-boiling heterogeneous azeotrope composed of various amounts of the alcohol, ester, and water. These azeotropes have the lowest boiling points in their quaternary mixtures, so each can be collected as a distillate product from a rectification section. For both BuOAc and AmOAc systems, like the binary mixtures of H<sub>2</sub>O and acetate products, the ternary azeotropes naturally

provide a relatively high purity (>99.5 mol %<sup>4,5</sup>) of H<sub>2</sub>O in the aqueous phases resulting from a liquid–liquid split. As a result, batch reactive distillation (BRD) can work very well for the BuOAc and AmOAc systems by decanting the H<sub>2</sub>O from the distillates. This shifts the reaction in the desired direction, and acetate products can be collected in the bottoms via a total reflux of the organic distillates. Venimadhavan et al.<sup>4</sup> showed that a BRD process can produce high purity BuOAc and high purity H<sub>2</sub>O without any additional separation steps. On the basis of the research of Yu and colleagues,<sup>6</sup> we can expect similar results for the AmOAc system. However, for the IPOAc system, in contrast to a binary mixture of IPOAc and H<sub>2</sub>O, the ternary azeotrope does not yield a high purity of H<sub>2</sub>O in the aqueous phase, which makes it significantly more difficult to use a BRD process for the IPOAc synthesis.<sup>7</sup>

Isopropyl acetate (IPOAc) is an important material with a wide variety of manufacturing uses in the chemical industry. It is described as an effective solvent for many synthetic resins, such as ethyl cellulose, nitrocellulose, methacrylic resin, and epoxy resins, and for many natural resins such as kauri and manila gums, rosin, and dammar.<sup>8</sup> It also can be found as an important component in printing inks,<sup>9</sup> especially gravure inks,<sup>8</sup> because of its fast evaporation and low hygroscopicity. It is also used as a solvent in the production of adhesives, flavoring agents, and perfumes.<sup>8</sup>

Chin et al.<sup>7</sup> investigated a BRD process for the IPOAc synthesis. They showed that the distillate is heterogeneous and splits into an aqueous phase and an organic phase, and that by removing the aqueous phase, the reaction can be shifted in the desired direction. However they pointed out a challenge arising from a significant solubility of a reactant (IPOH) in the aqueous phase as noted above. This challenge also exists in steady-state designs of the continuous IPOAc reactive distillation process.<sup>2,9</sup> Unlike the case for methyl acetate production,<sup>10</sup> using HOAc as an entrainer to extract pure IPOAc is infeasible.<sup>7</sup> To reduce the loss of IPOH in the aqueous phase and improve the purity of H<sub>2</sub>O, Chin et al.<sup>7</sup> introduced an external heterogeneous entrainer. They showed that a BRD using chloroform as an entrainer, together with a large number of theoretical stages (60) and high reflux ratios (>80) can produce high purity H<sub>2</sub>O in a

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**Table 1.** Comparison between the Measured Azeotropes and UNIQUAC Model Prediction at 1 atm

	IPOH/IPOAc/H <sub>2</sub> O (heterogeneous)	IPOAc/H <sub>2</sub> O (heterogeneous)	IPOH/H <sub>2</sub> O	IPOH/IPOAc
UNIQUAC prediction (mol %)	(19.36, 42.62, 38.02)	(59.24, 40.76)	(67.02, 32.98)	(66.08, 33.92)
measured value <sup>14</sup> (mol %) <sup>a</sup>	(13.77, 49.38, 38.85)	(59.82, 40.18)	(68.75, 31.25)	(65.08, 34.92)
UNIQUAC prediction (boiling point)	75.6 °C	76.8 °C	80.2 °C	80.7 °C
measured value <sup>14</sup> (boiling point)	75.5 °C	76.6 °C	82.5 °C	80.1 °C

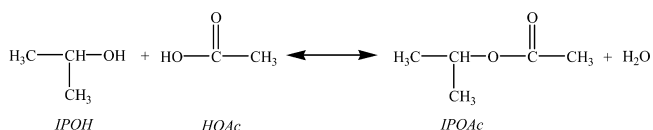
<sup>a</sup> Converted to mol % from the weight % values reported in the literature.<sup>14</sup>

distillate, and eventually a mixture of IPOAc along with the entrainer will be left in the still pot.

In this paper, we develop an alternative to the use of chloroform, or another entrainer not naturally present in the mixture. Instead of using HOAc to extract IPOAc, we consider the use of HOAc as an entrainer to eliminate the presence of IPOH in distillate. We show that in a semibatch reactive distillation (SBRD) system with a continuous HOAc feed, the presence of IPOH in distillate can be substantially reduced, leading to a relatively sharp liquid–liquid split, thereby reducing the IPOH loss in the aqueous phase of the distillate and relatively high purity H<sub>2</sub>O as a byproduct. Furthermore, the organic phase of the distillate becomes predominantly a binary mixture of IPOAc–H<sub>2</sub>O, so that IPOAc can be essentially fully recovered from that mixture using a stripper and a decanter.

## 2. Reaction and Phase Equilibria

**2.1. Reaction Equilibrium.** We consider the following liquid-phase reaction in the limit of reaction equilibrium with a coexisting vapor.<sup>11</sup>



Over the temperature range from 80 to 120 °C and at 1 atm pressure, the reaction equilibrium constant has an approximately constant value of  $K_{\text{eq}} = 8.7$ .<sup>12</sup>

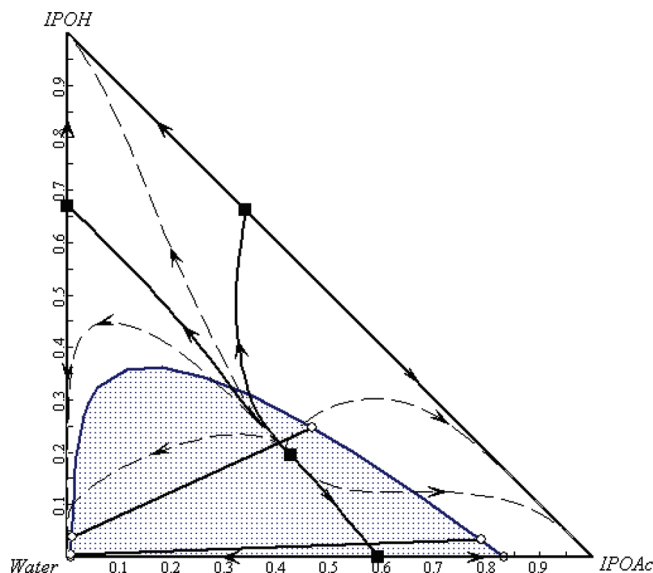
**2.2. Phase Equilibrium.** The UNIQUAC model is used to describe nonidealities in the liquid phases, and vapor phase dimerization of HOAc is taken into account by the Hayden–O’Connell model; we use parameters from the Aspen Plus<sup>13</sup> database for these VLE calculations. The model predicts three binary minimum-boiling azeotropes and one ternary minimum-boiling azeotrope in this quaternary system and is consistent with experimental data as shown in Table 1.

The IPOH/IPOAc/H<sub>2</sub>O ternary azeotrope has the lowest boiling point in the mixture, and, as shown in Figure 1, this azeotrope is in the liquid–liquid region of the IPOH–IPOAc–H<sub>2</sub>O ternary system.

## 3. Batch and Semibatch Column Configuration

A schematic of the process is given in Figure 2. For the BRD process, all reactants are fed at the start of the process. The reaction occurs in the reboiler and near the bottom of the column, and the overhead vapor is removed via the rectifier. Because the ternary azeotrope is the lightest boiler, that is, the unstable node in Figure 1, the overhead vapor entering the condenser/decanter has a composition near this azeotrope. The overhead vapor condenses into an organic phase and an aqueous phase in the condenser and is then decanted.

One challenge for the BRD process is that there is a significant amount of IPOH in aqueous phase, and as we remove



**Figure 1.** Calculated residue curve map for the IPOH–IPOAc–H<sub>2</sub>O ternary system (mole fraction coordinates) at 1 atm pressure: (■) azeotrope; arrows indicate increasing time or temperature; dashed lines represent residue curves; the shaded region indicates a liquid–liquid split at the normal boiling temperature and the solid straight lines represent tie lines for liquid–liquid splits.

the H<sub>2</sub>O, we will also lose IPOH. This is due to the nature of the phase equilibrium; for compositions close to the ternary azeotrope, a liquid–liquid split is not very sharp. Taking a tie-line (Figure 1) near the ternary azeotrope as an example, there is a significant amount of H<sub>2</sub>O in the aqueous phase; however, there is still 3.7 mol % IPOH.

A larger challenge for a BRD process is that the organic distillate is a ternary mixture. For instance, there is about 25 mol % IPOH in the organic phase for the tie-line (Figure 1) near the ternary azeotrope. To recover the IPOH in the organic distillate, we can reflux all of the organic distillate, or we can use an additional stripper to recover some IPOAc from the organic distillate,<sup>2,9</sup> then recycle IPOH, H<sub>2</sub>O and the rest of the IPOAc. In either case, there are significant amounts of H<sub>2</sub>O and IPOAc sent to the reboiler/reactor, which makes separation inefficient and may also cause a backward reaction.

Finally, as the BRD proceeds we separate the IPOH from the reaction zone, which will cause the loss of ingredients and inefficiency in the process.

If we can reduce or eliminate IPOH in the distillate, for example, with a distillate at the lower tie line (Figure 1) approaching the IPOAc–H<sub>2</sub>O edge, the purity of H<sub>2</sub>O can be improved and the organic phase will predominantly be a binary mixture of IPOAc–H<sub>2</sub>O, which can be separated completely by a stripper and a decanter. In that case, total reflux or recycling of the organic distillate is unnecessary. However, in the BRD process, the ternary azeotrope prevents a distillate composition from approaching the IPOAc–H<sub>2</sub>O edge.

An alternative to reduce the presence of IPOH in the distillate is to use an entrainer to extract IPOH from the ternary mixture

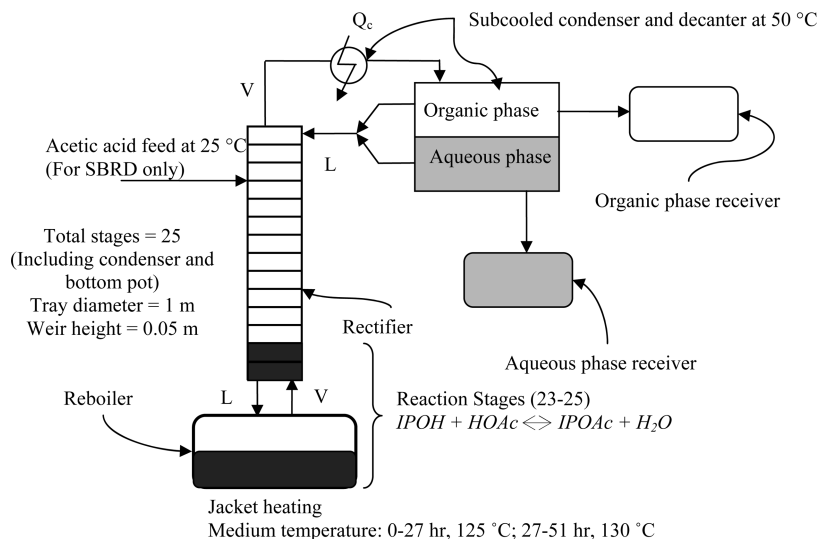


Figure 2. Schematic of BRD/SBRD process (stage numbers decrease up the column).

of IPOH–IPOAc–H<sub>2</sub>O leaving the reactor/reboiler and bring IPOH back to the bottom. As in many instances, a preferred first choice for an entrainer is one of the components already in the system, if that is feasible. Here, HOAc is the heaviest component, it does not form any azeotrope with the other three components, and each of the ternary residue curve maps for (1) HOAc–IPOH–IPOAc, (2) HOAc–IPOH–H<sub>2</sub>O and (3) HOAc–IPOAc–H<sub>2</sub>O are the so-called “extractive” maps.<sup>15</sup> These characteristics make HOAc a possible entrainer; however, we still need a further investigation to ensure the practicality of using HOAc as an entrainer in this case, which specifically requires the entrainer to (1) extract IPOH to the bottom with high recovery, and (2) simultaneously allow IPOAc and H<sub>2</sub>O to pass upward into the distillate. We emphasize that we are *not* trying to extract IPOAc from the distillate, which has been proven infeasible.<sup>7</sup> Instead, we are trying to extract IPOH from the vapor and direct it back to the reboiler/reactor, where the reaction occurs.

Figure 2 also shows the concept of using HOAc as an entrainer in a SBRD. In analyzing this SBRD, we assume that the holdup in the column is small compared to that in the reboiler/reactor. Because the column is then in a quasi-steady state, we first conduct a steady-state simulation of the corresponding *continuous* extractive distillation in Aspen Plus<sup>13</sup> to test the feasibility and practicality of using HOAc as an entrainer. The continuous process is shown in Figure 3.

As shown in Figure 4, the results from these simulations show that the recovery of IPOH at the bottom, the recovery of IPOAc and H<sub>2</sub>O in the distillate, and the mole fraction of IPOAc + H<sub>2</sub>O in the distillate all increase to significantly higher levels as the feed ratio of HOAc to the ternary mixture increases. As the feed ratio of HOAc to the ternary mixture approaches 1, the recovery of IPOH in the bottom can reach >99.5%. Simultaneously, this process also allows us to recover most of the IPOAc (>70 mol %) and H<sub>2</sub>O (>80 mol %) in the distillate with the combined mole fractions of IPOAc + H<sub>2</sub>O in distillate greater than 99.5%. Thus, the simulation results show that acetic acid is both feasible and practical (a large excess above the reaction requirement is not needed).

A SBRD model was built in Aspen BatchSep,<sup>16</sup> along with a BRD model for a comparison, according to the schematic in Figure 2. In both models, the reaction occurs in the reboiler and in two stages above it to allow for the potential entrainment of catalysts. (The results are not very sensitive to the number

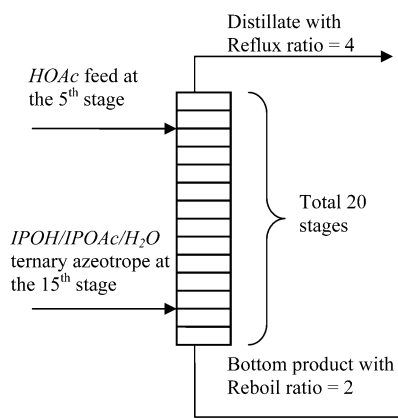


Figure 3. Steady-state schematic for HOAc as an entrainer for IPOH/IPOAc/H<sub>2</sub>O ternary mixture at 1 atm.

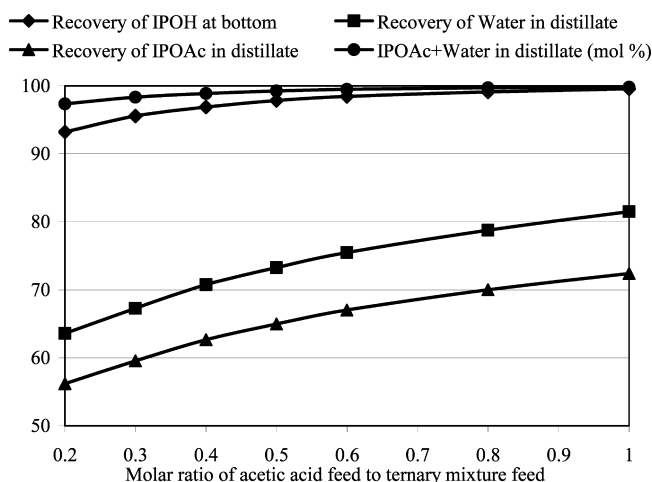


Figure 4. Simulation results for a continuous system using HOAc as an entrainer for IPOH/IPOAc/H<sub>2</sub>O ternary mixture in a steady-state process.

of reactive stages.) The overhead vapor condenses into an organic phase and an aqueous phase.” Two receivers are used to collect distillate products, one for the organic phase, and the other for the aqueous phase. In the SBRD process, HOAc is fed to the column continuously during the process; while in the BRD process, all reactants are fed to the reactor/reboiler at the start of the process. For the SBRD and BRD simulations,

**Table 2. Operating Parameters of SBRD and BRD at 1 atm Pressure**

	SBRD	BRD I	BRD II	BRD III
initial charge	9 kmol IPOH 1 kmol HOAc	9 kmol IPOH 9 kmol HOAc	9 kmol IPOH 9 kmol HOAc	9 kmol IPOH 9 kmol HOAc
feed stage	6th	N/A	N/A	N/A
HOAc feeding rate (kmol/h)	0–2 h, 2.4 2–8 h, 1.8 8–15 h, 0.95 15–27 h, 0.35 27–51 h, 0.05	N/A	N/A	N/A
reflux ratio of aqueous phase	0–2 h, 15 2–27 h, 6 27–51 h, 15	same as SBRD	15	20
reflux ratio of organic phase	0–2 h, total reflux 2–27 h, 5 27–51 h, 35	same as SBRD	0–2 h, total reflux; 2–51 h, 35	total reflux

we use the same piece of equipment. The differences are only in operating parameters as summarized in Table 2.

For the SBRD process, HOAc is fed near the top of the column, and we use a HOAc feed policy with a decreasing rate during the batch. The HOAc feed serves as an entrainer to extract IPOH from the ternary vapor containing IPOH, IPOAc, and H<sub>2</sub>O, and returns IPOH to the reactor/reboiler in the liquid. At the beginning of the process, the amount of IPOH in the system is at its peak, which requires the highest feed rate of HOAc to prevent IPOH from escaping from the top. As the process proceeds, the reaction consumes IPOH, so that the HOAc feed rate can decrease with time. The feed rate of HOAc can be optimized continuously for certain targets; however, for practical implementation, we change feed rates from one constant value to another over discrete time periods. During each time period, we calculate the amount of HOAc feed required to keep the composition of IPOH in the aqueous product at or below 0.05 mol %.

For the SBRD process, we use high reflux ratios initially to build up the compositions of IPOAc and H<sub>2</sub>O inside the column, and to prevent freshly charged IPOH from escaping. Subsequently, we decrease the reflux ratios in order to collect products from the distillate. Later in the process, as the amounts of IPOAc and H<sub>2</sub>O decrease, we increase reflux ratios to maintain the purities of products. In BRD I, we use the same values of reflux ratios for comparison. We also compare the SBRD to BRD II with higher reflux ratios for both organic and aqueous phases, and BRD III with a higher reflux ratio for the aqueous phase and a total organic reflux.

The composition of the aqueous distillate should ideally approach pure H<sub>2</sub>O, so that we will not lose any ingredients. As shown in Figure 5, for the SBRD, the H<sub>2</sub>O composition in

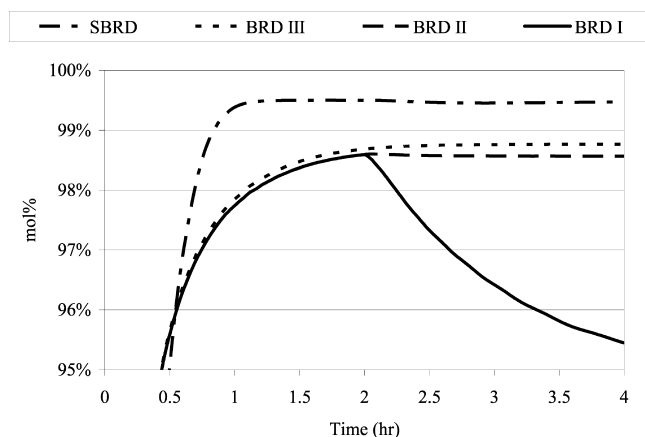
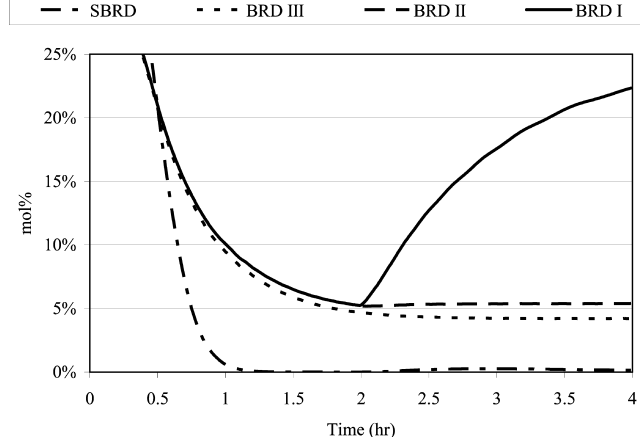
the aqueous phase of the distillate reaches about 99.4 mol % after 1 h, and remains at or near that purity even when we decrease the aqueous reflux ratio at  $t = 2$  h. For BRD III, with the higher aqueous reflux ratio, the H<sub>2</sub>O composition in the aqueous phase of distillate reaches about 98.7 mol % after about 2 h. Unlike the SBRD, as we decrease the aqueous reflux ratio in the BRD process (e.g., BRD I), the H<sub>2</sub>O purity decreases dramatically.

The organic distillate, in the ideal situation, should contain a negligible amount of IPOH which should stay at the bottom of column in the reaction zone. Figure 6 shows that the IPOH composition in the organic phase of distillate for SBRD is below 0.3 mol % after about 1 h, and remains low even when we decrease the organic reflux ratio at  $t = 2$  h. For BRD III, even with the total organic reflux, we still have about 5 mol % IPOH in the organic distillate after about 2 h. Unlike the SBRD, as we decrease the organic reflux ratio in the BRD process (e.g., BRD case I), the IPOH composition increases dramatically.

These results show that SBRD not only reduces the IPOH losses, but also retains IPOH in the reaction zone throughout the process while BRD does not.

The results in Table 3 show that compared to all the BRD cases, the SBRD provides significantly lower compositions of IPOH in the both aqueous and organic products, that is, 0.04 mol % IPOH in the aqueous product, and 0.12 mol % IPOH in the organic product versus much larger values for all of the BRD cases. SBRD also offers a lower composition of IPOAc in the aqueous product: 0.5 mol % IPOAc for the SBRD versus 0.6 mol % IPOAc for the best case of BRD (BRD III). Consequently, SBRD can provide highest purity of H<sub>2</sub>O.

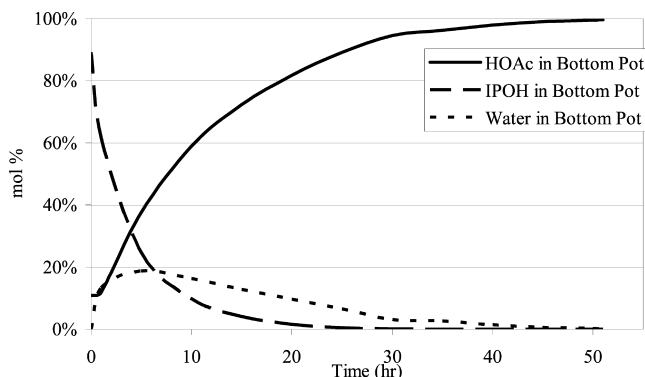
For the SBRD and the BRDs with organic distillate product (BRD I and II), pure IPOAc can be obtained from the organic

**Figure 5.** H<sub>2</sub>O composition in the aqueous phase of distillate.**Figure 6.** IPOH composition in the organic phase of distillate.



**Table 3. Comparison between the SBRD and BRDs for a 51-h Operation**

	composition of the aqueous product (mol %) (IPOH, IPOAc, H <sub>2</sub> O, HOAc)	product collected in the aqueous receiver (kmol)	composition of the organic product (mol %) (IPOH, IPOAc, H <sub>2</sub> O, HOAc)	product collected in the organic receiver (kmol)
SBRD	(0.04, 0.50, 99.46, 0.00)	7.53	(0.12, 85.97, 13.91, 0.00)	10.28
BRD Case I	(2.45, 0.70, 96.85, 0.00)	4.52	(17.49, 60.48, 22.03, 0.00)	11.08
BRD Case II	(1.24, 0.62, 98.14, 0.00)	6.83	(11.65, 68.72, 19.63, 0.00)	5.68
BRD Case III	(0.93, 0.60, 98.47, 0.00)	6.96	(14.04, 66.17, 1.80, 17.99) <sup>a</sup>	10.28 <sup>a</sup>

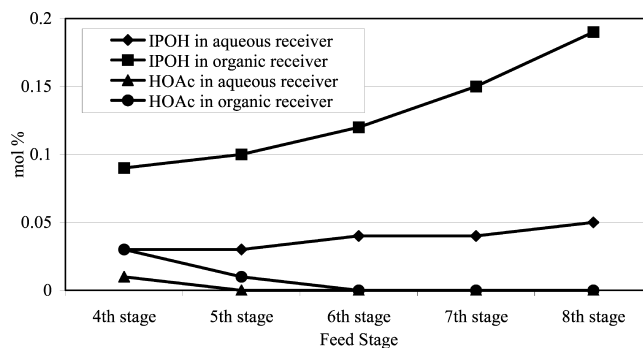
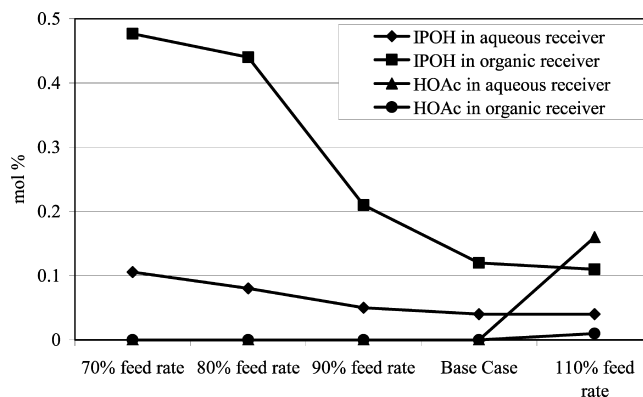
<sup>a</sup> Organic product is collected in the bottom pot.**Figure 7.** Compositions in the bottom pot during 51 h of operation. The composition of IPOAc is not shown because it overlaps with H<sub>2</sub>O composition.**Table 4. Percentage of Theoretical Production of Products Collected in Receivers for a 51 h Operation**

	% of theoretical H <sub>2</sub> O production collected in the aqueous receiver	% of theoretical IPOAc production collected in the organic receiver
SBRD	83.3	98.2
BRD I	48.6	74.5
BRD II	74.5	43.4
BRD III <sup>a</sup>	76.2	75.6

<sup>a</sup> IPOAc is collected in the bottom pot.

product via a stripper.<sup>2,9</sup> However, even with a higher organic reflux, BRD II, the organic product in the BRD is a ternary mixture with a significant amount of IPOH, which makes high recoveries of IPOAc and H<sub>2</sub>O from the organic product infeasible without additional expensive processing of the ternary azeotrope. As we recycle the IPOH reactant to BRD, significant amount of products (IPOAc and H<sub>2</sub>O) will also be recycled to BRD, which will cause back-reaction and lower separation efficiency. In contrast, for the SBRD, the organic product is predominantly the IPOAc–H<sub>2</sub>O binary mixture (IPOAc + H<sub>2</sub>O > 99.87 mol %), which can be separated completely by a stripper and a decanter, so that recycling reactant is unnecessary. For the SBRD operation, in order to reuse HOAc, we continue the operation until a high purity of HOAc is achieved in the bottom pot. Figure 7 shows that after 51 h operation, excess HOAc is left in the bottom pot with 99.59 mol % purity and can be recycled for use as an entrainer/reactant in the next SBRD operation. For the BRD with a total organic reflux, BRD III, the IPOAc is collected in the reboiler/reactor with significant amounts of IPOH and HOAc.

Besides the improvements in compositions of the products, SBRD also provides higher process efficiency. As shown in Table 4, during the same operating time (51 h), 98.2% of the theoretical maximum production of IPOAc can be collected in the organic receiver of the SBRD, compared to the best case of BRD with 75.6% of the theoretical maximum production of IPOAc collected in the bottom pot. For the aqueous phase product, 83.3% of the theoretical maximum production of H<sub>2</sub>O

**Figure 8.** Impacts of HOAc feed location on compositions of IPOH and HOAc in products.**Figure 9.** Impacts of the HOAc feed rate on compositions of IPOH and HOAc in products.

can be collected in the aqueous receiver of SBRD, while the best case of BRD collects 76.2% of the theoretical production of H<sub>2</sub>O in the aqueous receiver.

We also studied the impacts of the HOAc feed location on the SBRD process. As shown in Figure 8, when the HOAc feed location is moved toward the bottom of the column, the compositions of IPOH in the both aqueous and organic products increase. As we move the HOAc feed location toward the bottom of the column, we decrease the extraction region for IPOH. Consequently, the compositions of IPOH in the both aqueous and organic products increase. However, moving the HOAc feed location toward the top of the column decreases the rectification section for HOAc, which can lead to larger presence of HOAc in the product. As shown in Figure 8, when the feed enters the fourth stage, there are 0.01 mol % and 0.03 mol % HOAc in the aqueous product and the organic product, respectively.

Figure 9 shows that we can decrease the usage of HOAc at the expense of increasing the compositions of IPOH in the both aqueous and organic products. As we decrease the HOAc feed rate to 70% of the base case (HOAc feed rate in Table 2), the compositions of IPOH in the aqueous and organic products increase to 0.11 mol % and 0.48 mol %, respectively. Figure 9 also shows that increasing the HOAc feed rate from the base

case can exacerbate the presence of HOAc in both the aqueous and organic products. Obviously, the feed rate can be further optimized by implementing an economic cost model.

We note that a more detailed model for the best conceptual designs(s) may be appropriate to develop a more fully optimized final design, for example, to include heat and mass transfer limitations,<sup>17</sup> to revise the HOAc feed schedule, and to refine reflux ratio values and catalyst levels, etc. However, we emphasize that these detailed models are expensive to develop and typically less useful for conceptual design or process development studies.

#### 4. Conclusions

Unlike its use in the BuOAc and AmOAc systems, BRD is difficult to use for the IPOAc system because of the nature of the phase equilibrium. We have shown that in a SBRD process, a continuous HOAc feed can perform as an entrainer to improve the desired aqueous–organic split. In SBRD, we can reduce the loss of IPOH and improve the purity of the H<sub>2</sub>O byproduct without any external entrainer. Furthermore, in the SBRD with HOAc as an entrainer, IPOAc can be obtained in the organic phase of the distillate as an IPOAc–H<sub>2</sub>O binary mixture instead of an IPOH–IPOAc–H<sub>2</sub>O ternary mixture which is obtained in BRD. Unlike the ternary mixture, the IPOAc–H<sub>2</sub>O binary mixture can be separated completely by a stripper and a decanter. Therefore, recycling the reactant IPOH from the organic product or total reflux of organic phase distillate can be avoided in the SBRD. We have also shown that, compared to a BRD, SBRD can provide 20% higher production efficiency.

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#### Nomenclature

AmOAc = amyl acetate  
AmOH = amyl alcohol  
BuOAc = butyl acetate  
BuOH = *n*-butanol  
HOAc = acetic acid  
H<sub>2</sub>O = water  
IPOAc = isopropyl acetate

IPOH = isopropyl alcohol

$K_{eq}$  = reaction equilibrium constant

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