Plantwide Control Design of the Monoisopropylamine Process

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Abstract: Plantwide regulatory control system design for a monoisopropylamine (MIPA) process is presented from the perspective of plantwide transient variability propagation. The process consists of a hot reaction section followed by a cold separation section with three columns and a decanter with two liquid recycles. Two control structures with the throughput manipulator (TPM) at, respectively, the limiting reactant fresh feed (CS1) and the decanter feed (CS2) are evaluated. The decanter level control scheme dramatically affects the overall plantwide response speed. The response is extremely sluggish when total decanter hold-up is regulated using the organic outflow (Scheme 1) and is significantly speeded-up (> 3 times) when the total (organic + aqueous) outflow (Scheme 2) is manipulated instead. The reason is traced to Scheme 2 effectively propagating water imbalance transients out of the plant to the water by-product stream and not to the organic recycle stream, which disturbs the side-product recycle-to-extinction balance. The case-study affirms the heuristic of structuring the plantwide control system to propagate transients out of a recycle loop for improved dynamic performance.

Keywords: Plantwide control, control structure design, control configuration, regulatory control.

1. INTRODUCTION

In the design of plantwide regulatory control systems for complete integrated chemical plants, the propagation of transients through recycle loops is a key consideration dictating control structure design decisions (Downs, 2012; Kanodia and Kaistha, 2010). In reactor-separator systems, the recycle loop component inventories behave like integrators with respect to any mismatch in the plant overall component material balance. For effective dynamic performance, a key heuristic is to configure the control structure to propagate component imbalances out of the recycle loop. This is the basis for Luyben's rule (Luyben, 1998) of fixing a flow inside a recycle loop. It forces the upstream inventory control system to be in the reverse direction of process flow, thereby bringing in the fresh reactant feed(s) as a make-up stream(s). Recycle variability is then effectively transformed to the fresh feed flow for smooth plant regulation. By contrast, in the conventional approach, a fresh feed is fixed (Skogestad, 2004; Buckley, 1964) and the inventory control system must allow the recycle inventory to float appropriately to close the overall plant material balance.

In this work, we present an interesting application of control structure design to propagate component imbalances out of the recycle loop for achieving dramatic improvement in plantwide dynamic regulatory performance. The same is crucial as it sets performance limits on the higher supervisory and real-time optimization layers that adjust the regulatory layer setpoints for economic process operation.

The particular process considered here continuously manufactures monoisopropyl amine (MIPA) via amination of isopropyl alcohol (IPA) with ammonia (NH_3) and recycles the diisopropylamine (DIPA) side product to extinction. The process consists of a hot reaction section and a cold separation section of three columns plus a decanter, and includes two liquid recycle streams. Two control structures, namely, a conventional structure with the throughput manipulator (TPM) at a fresh feed (CS1), and a control structure with the TPM inside the liquid recycle loop (CS2), in line with Luyben's recommendation, are considered. We particularly focus on the impact of decanter level control scheme on the overall plantwide response. Two possible manipulated variables for the decanter organic layer level (total hold-up) controller, viz., decanter organic layer outflow and total (aqueous+organic) outflow, are considered.

In the following, the MIPA process is briefly described along with the two control structures, CS1 and CS2, plus the two "local" decanter level control schemes. Rigorous closed loop dynamic simulation results for principal disturbances are then presented and interpreted from the point of view of the settling time of the plantwide transients and its relation to plantwide variability propagation. The main findings are finally summarized to conclude the article.

2. MIPA PROCESS

2.2 Reaction Chemistry and Thermodynamic Package

MIPA is produced via the gas-phase irreversible catalytic amination of isopropyl alcohol (IPA) with ammonia (NH_3) in an adiabatic packed bed reactor (PBR) as
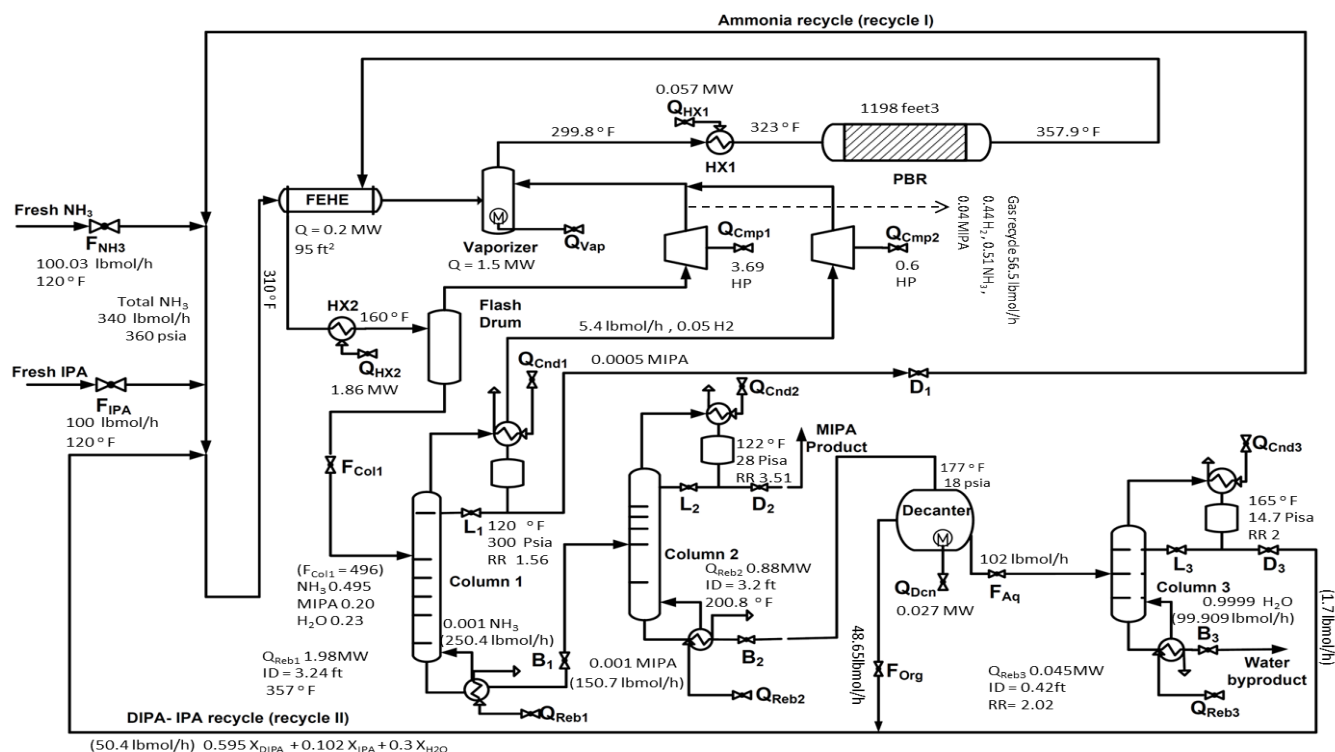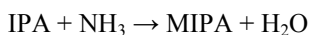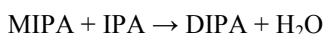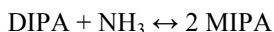
Fig. 1. MIPA process flowsheet

$$IPA + NH_3 \rightarrow MIPA + H_2O$$

The series irreversible side reaction forming diisopropyl amine (DIPA) as

$$MIPA + IPA \rightarrow DIPA + H_2O$$

also occurs in the PBR. The DIPA reversibly adds to NH_3 to give back MIPA as

$$DIPA + NH_3 \leftrightarrow 2\ MIPA$$

The reaction kinetics have been taken from Luyben (2009). Note that with the third reaction, DIPA can be recycled to extinction by letting it build-up in the recycle loop to such an extent that the DIPA formation by the side reaction is exactly balanced by the DIPA consumption in the third reaction.

The system contains 3 binary minimum boiling azeotropes (DIPA-H_2O, DIPA-IPA and IPA-H_2O) along with liquid-liquid DIPA-H_2O phase split. To model the process, Aspen Plus is used as the simulation platform. The UNIFAC method is for the liquid phase activity coefficients along with the ESRK equation for the vapour phase.

2.2 Process Description

A schematic of the MIPA process is shown in Fig. 1. It consists of a reaction section followed by a separation section. In the reaction section, fresh IPA and fresh ammonia are mixed with recycle ammonia (Recycle I) and the IPA-DIPA-H_2O recycle stream (Recycle II) followed by preheating in a feed-effluent heat exchanger (FEHE). The preheated stream is vaporized and further heated in a high pressure steam heater to the reaction temperature before being fed to a catalytic vapor-phase high conversion PBR. The PBR is operated in excess NH_3 environment to suppress DIPA formation. Also, the single-pass PBR conversion is high to ensure feasibility of

the downstream separation-cum-recycle scheme. The reactor effluent vapor loses sensible heat in the FEHE and is then partially condensed in a flash drum. The NH_3 rich flash drum vapor is compressed and recycled to the vaporizer.

The liquid from the flash drum is sent to the separation section, which consists of three columns and a decanter. The first column (ammonia column), recovers and recycles ammonia as liquid distillate while its bottoms is distilled in the product (second) column to recover nearly pure MIPA as liquid distillate. Its bottoms is a ternary IPA-DIPA-H_2O mixture with the binary azeotropes partitioning the composition space into three distinct distillation regions with a liquid-liquid phase split envelope as in Fig. 2.
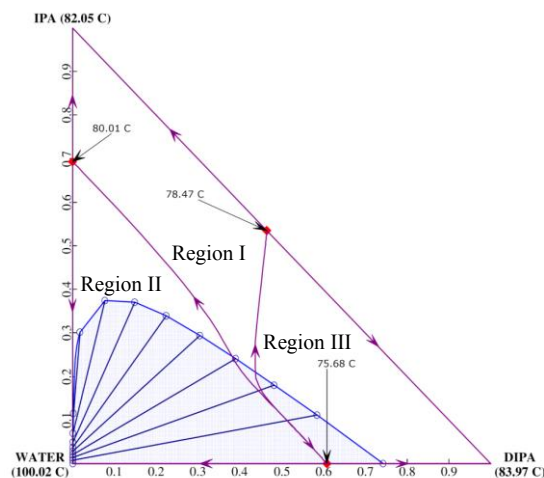

Fig. 2. IPA-DIPA-water distillation regions and liquid-liquid envelope

A high single pass reactor conversion forces the product column bottom ternary composition close to the DIPA-H_2O edge (low unreacted IPA) in distillation Region II. A liquid-liquid phase split in a decanter would then give an aqueous layer composition close to the pure water vertex and a water lean DIPA rich organic layer. The product column bottoms is therefore subcooled and decanted. The aqueous layer draw is distilled in a small column that recovers nearly pure water with negligible IPA leakage as the bottoms. Its distillate and the decanter organic layer draw are mixed and recycled to the reaction section, through the FEHE.

3. PLANTWIDE CONTROL SYSTEM

Two plantwide control structures, CS1 and CS2, are evaluated in this work and are briefly described in the following.

3.1 Control Structures

CS1 is a conventional structure with the TPM at the fresh IPA (limiting reactant) feed. In CS2, the decanter feed is chosen as the TPM. Figure 3 depicts the two control structures. Both
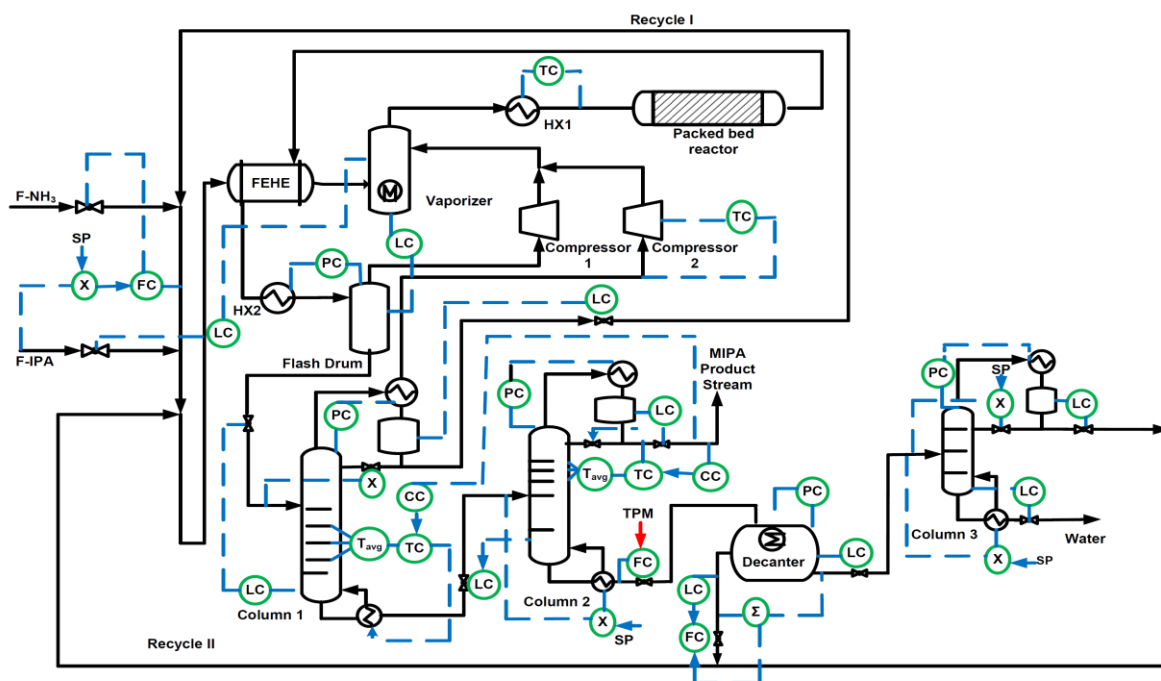

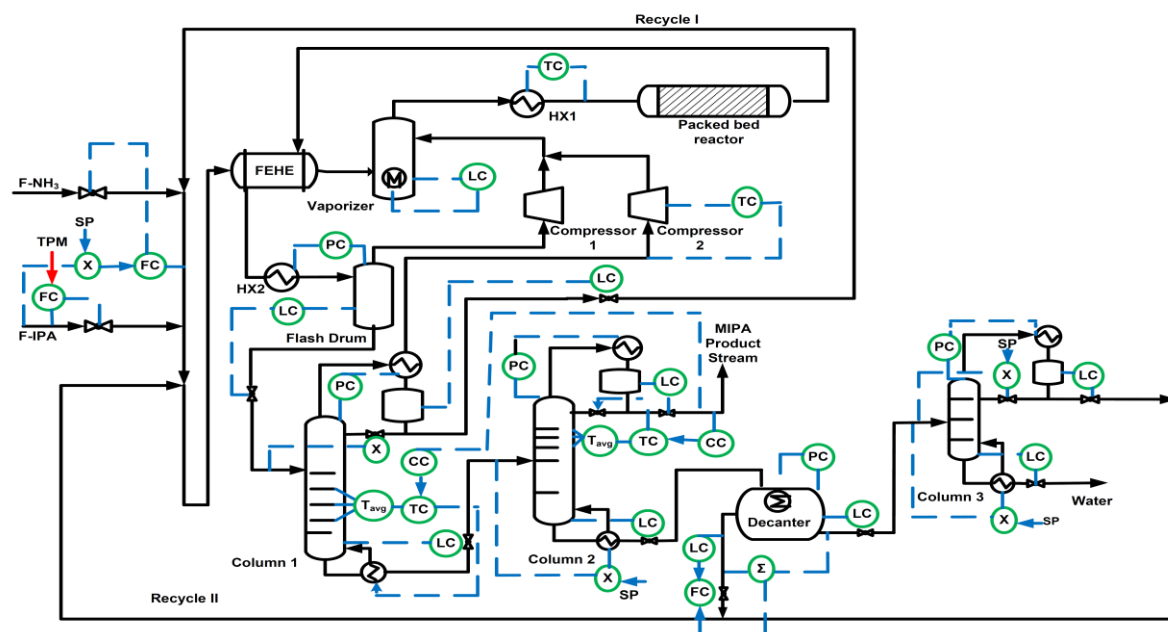Fig. 3 (b). Control Structure 2 (CS2)

Fig. 3 (a). Control Structure 1 (CS1)

structures have the same set of controlled variables for closing the material / energy balances on each of the individual units.

The differences in the pairings are due to the TPM location. In CS1, all the levels to be controlled are downstream of the TPM. The level controllers then adjust the immediate downstream flows. In CS2, since the TPM is at the decanter feed, the upstream level controllers adjust immediate upstream flows. In both structures, the total (fresh + recycle) NH_3 is maintained in ratio with the fresh IPA. This ensures reactor operation in appropriate excess ammonia environment for suppressing DIPA formation. Also, single-ended temperature control is implemented on all the columns. In the product column, the average temperature of three sensitive rectifying trays (T^R_{Col2}) is controlled using the reflux (L_2) while the reboiler duty (Q_{Reb2}) is kept in ratio with the column feed (B_1). The temperature setpoint is adjusted by a main product DIPA impurity (x^{D2}_{DIPA}) controller. On the ammonia column, the average temperature of three sensitive stripping trays (T^S_{Col1}) is controlled using the reboiler duty (Q_{Reb2}) with the reflux (L_1) in ratio to the column feed. The temperature setpoint is adjusted to maintain the main product NH_3 impurity (x^{D2}_{NH3}) composition. Note that in CS2, the bottom sump levels of columns upstream of the decanter (V^{Bot}_{Col2} and V^{Bot}_{Col1}) are controlled using the respective column feeds (B_1 and F_{Col1}). The flash drum level (V_{FD}) is controlled using the vaporizer duty (Q_{Vap}) while the vaporizer level (V_{Vap}) is maintained by adjusting the fresh IPA feed (F_{IPA}).

Two alternative "local" decanter level control schemes are considered as in Fig. 4. In Scheme 1, the organic and aqueous layer levels are controlled using their respective outflow valves (F_{Org} and F_{Aq}). Note that the organic layer level reflects the total decanter hold-up ($V_{Tot}=V_{Org}+V_{Aq}$) and is not the same as the organic hold-up (V_{Org}). For Scheme 1 then,

$$\Delta F_{Aq} = K_{C1}\Delta V_{Aq}$$

$$\Delta F_{Org} = K_{C2}\Delta V_{Tot} = K_{C2}(\Delta V_{Org}+\Delta V_{Aq})$$

One way interaction occurs with changes in V_{Aq} affecting V_{Tot} and hence F_{Org}.

(a) Scheme 1   (b) Scheme 2

$$\Delta F_{Aq} = K_{C1}\Delta V_{Aq}$$
$$\Delta F_{Org} = K_{C2}\Delta V_{Tot}$$

$$\Delta F_{Aq} = K_{C1}\Delta V_{Aq}$$
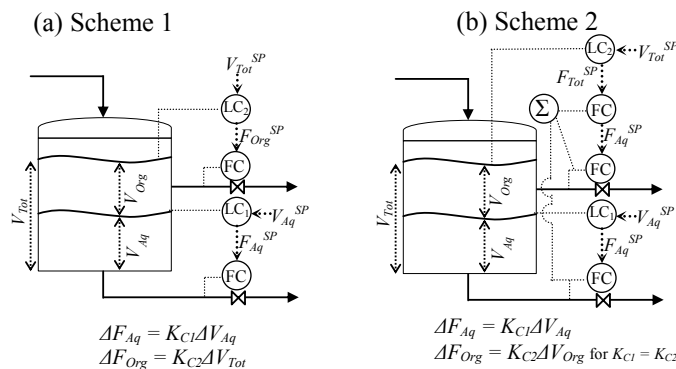$$\Delta F_{Org} = K_{C2}\Delta V_{Org} \text{ for } K_{C1} = K_{C2}$$

Fig. 4.   Alternative decanter level control schemes.

In Scheme 2, V_{Tot} is controlled by adjusting the decanter total outflow ($F_{Tot} = F_{Org} + F_{Aq}$). As before, $\Delta F_{Aq} = K_{C1}\Delta V_{Aq}$ with the organic layer level controller equation changing to

$$\Delta F_{Tot} = K_{C2}\Delta V_{Tot}$$

or $$\Delta F_{Aq} + \Delta F_{Org} = K_{C2}(\Delta V_{Org}+\Delta V_{Aq})$$

or $$\Delta F_{Org} = K_{C2}\Delta V_{Org}+(K_{C2}-K_{C1})\Delta V_{Aq}$$

If we choose $K_{C2} = K_{C1}$, the above equation simplifies to

$$\Delta F_{Org} = K_{C2}\Delta V_{Org}$$

Scheme 2, proposed originally by Buckley, then effectively eliminates one-way interaction between the two level controllers.

3.2 Controller Tuning

A consistent tuning procedure is applied to tune the different controllers in CS1 and CS2. All flow controllers are PI with a reset time of 0.3 mins and gain of 0.5. Similarly, all pressure controllers use a reset time of 0.5 mins with the gain chosen high for tight control. All level controllers are P only with a gain of 2. To tune the temperature / composition controllers, the relay feedback test is applied and the Tyreus-Luyben settings are appropriately tweaked for a slightly underdamped servo response. The salient controller parameters used in the rigorous dynamic simulations are noted in Table 1.

Table 1: Salient controller parameters[*]

CV	K_c	τ_i min	PV Range[&]	MV Range[&]	Sensor dead time / lag min
T^S_{Col1}	2	4.0	125-175°C	3.95MW	0/1
x^{D2}_{NH3}	0.35	60	0.0052	132-172°C	5/5
T^R_{Col2}	0.85	6.6	40-90°C	5.24kg/s	0/1
x^{D2}_{DIPA}	0.35	70	0.0036	56-76°C	5/5
T^{Cnd}_{Col1}	0.8	60	26-71°C	0.9kW	0/1
T_{Rxr}	16.9	4.0	135-190°C	0.11MW	0/1

[*]: All level loops use $K_C = 2$ unless otherwise specified
[&]: Minimum value is 0, unless specified otherwise

4. RESULTS AND DISCUSSION

The two control structures are tested via rigorous dynamic simulations for two principal load disturbances, a TPM step change and a fresh IPA feed composition step change. The TPM setpoint is changed to effect a ±10 lbmol/hr change in the steady MIPA production rate. The water impurity in the IPA feed changes as a step from 0 mol% to 5 mol%.

Fig. 5 plots the dynamic response of salient process variables to a throughput change (Fig. 5a) and the IPA feed composition disturbance (Fig. 5b). The transient responses for decanter level control using Scheme 1 and Scheme 2 is shown in the plot. The dynamic results show that both structures achieve tight product purity control to within a very small band, during the transients for the two principal disturbances. The CS2 plantwide response completes somewhat quicker than CS1, for both disturbances.

This is likely due to CS2 being a control structure that is in accordance with Luyben's rule of holding a flow inside a recycle loop constant. The upstream level control system then ends up bringing in the fresh feed IPA as a make-up stream.

In CS2 on the other hand, the IPA feed is fixed and the liquid recycle must float to the appropriate value to close the DIPA recycle-to-extinction balance. The inventory control system then transforms transients into the recycle loop, which slows down the plantwide response.

Referring back to Fig. 5, very significant differences in the plantwide transients are evident for both CS1 and CS2, depending on the decanter level control strategy. For decanter level control using Scheme 1, the overall plantwide response is extremely sluggish particularly for the fresh IPA feed composition disturbance. Decanter level control using Scheme 2 significantly speeds up the plantwide response and the overall response completes much quicker in ~100 hrs compared to more than 300 hrs for Scheme 1.

The dramatic difference in the speed of the plantwide response due to a seemingly innocuous change in the "local" level control scheme of a unit operation may be explained as follows. As discussed earlier (Fig. 4), in Scheme 1, one way

interaction occurs with change in the decanter aqueous level affecting organic outflow. Thus, if only the water inflow to the decanter is changing to cause an aqueous layer level change, the action of the organic layer level controller would necessarily manipulate the organic outflow. This adjustment in the organic outflow alters the DIPA recycle rate to the reactor disturbing its recycle-to-extinction balance. Rebalancing the same is necessarily slow with the imbalance (cause) propagating through the downstream units to manifest in the DIPA recycle rate (effect) till the reactor net DIPA generation rate self-regulates to zero. Instead of propagating the "local" water imbalance transients only towards the water by-product stream for closing the overall plant water balance, Scheme 1 thus ends up (partially) propagating the transients to the slow plantwide DIPA component balance. The significantly slow overall plantwide response for both CS1 and CS2 with Scheme 1 decanter level control is then not-at-all surprising.
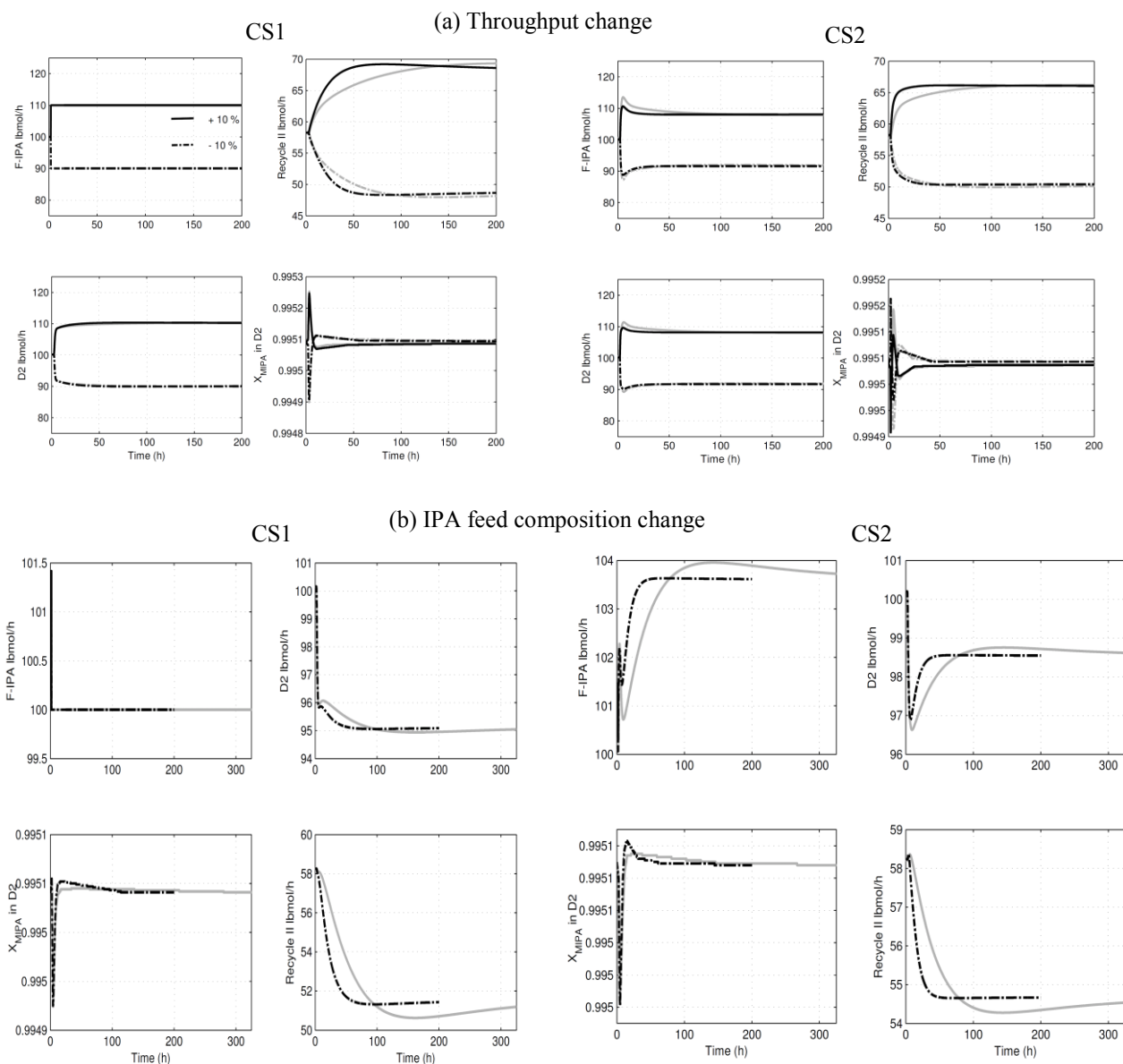

Fig. 5. Dynamic response of salient process variables to principal disturbances
Grey line: Decanter level control scheme 1
Black line: Decanter level control scheme 2

In Scheme 2, on the other hand, the organic layer outflow is not affected by changes in the aqueous level, as the organic layer level controller manipulates the total (organic + aqueous) decanter outflow. This decoupling ensures "local" decanter water imbalance transients are not propagated into the liquid recycle loop through the organic outflow. Scheme 2 then effectively propagates the decanter water imbalance transient to the water by-product stream, as it should, without disturbing the DIPA recycle-to-extinction balance. Propagating the component imbalance transients out of the recycle loop thus helps to effectively close the overall plant component balances. This naturally leads to a dramatically faster overall plantwide dynamic response for decanter level control using Scheme 2, compared to Scheme 1.

To lend credence to the above, Fig. 6 compares the transient response of the decanter component flow imbalance (outflow – inflow) for CS1 for the two decanter level control schemes. The disturbance is a change in IPA feed composition which causes water input into the process, causing the water balance on the decanter to be disturbed. This can be observed as the large initial water imbalance transient in the plot. This transient is followed by a transient imbalance in the DIPA, which is particularly severe for decanter control Scheme 1. Scheme 2 significantly mitigates this imbalance for a dramatic speed-up in the overall plantwide response.
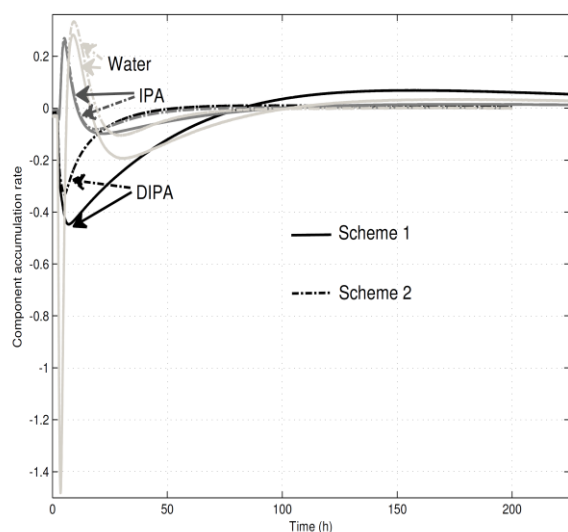

Fig. 6. Transient decanter component imbalance

To end the discussion, we highlight the need to consider plantwide control structure design in conjunction with the function of the unit operation. In the present case, the decanter separates the DIPA rich organic material, which is recycled, from water, which is discharged from the plant. An increasing organic layer hold-up indicates increasing DIPA inventory and hence the need to increase organic recycle rate in order to recycle the accumulating DIPA to extinction. Scheme 2 level control accomplishes precisely this by adjusting the organic outflow in proportion with the organic hold up. Scheme 2 is thus naturally aligned with the decanter function and hence gives the best dynamic performance.

5. CONCLUSIONS

In conclusion, this work demonstrates that plantwide regulatory control system design for dynamic performance must duly consider the propagation of component material imbalance transients inside the plant. The control system must be structured to propagate the component imbalances out of the recycle loop. For the specific MIPA process, the decanter level control scheme dramatically affects the overall plantwide response settling time. The proper scheme holds the total decanter hold up by adjusting the total decanter outflow (Scheme 2) and not the organic layer outflow (Scheme 1). Rigorous dynamic simulations for two alternative plantwide control structures show that the overall plantwide response settling time for both structures is more than 3 times faster

when decanter inventory is regulated using Scheme 2. This strategy ensures propagation of water component imbalance transients out of the plant to the water by-product stream and not into the organic recycle stream, which disturbs the DIPA side-product recycle-to-extinction balance.

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