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Design and Control of Heat Pump Assisted Distillation Processes for Flexible E-methanol Production

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ABSTRACT

This study investigates control strategies for the flexible operation of heat pump-assisted distillation processes, focusing on the heat integrated distillation column configuration. The methanol/water separation system was selected as a case study and modelled to achieve 99.9 wt% AA-grade methanol purity. A limiting piece of equipment for flexible operation of heat pump assisted distillation is the compressor. To assess its impact on flexible operation, dynamic simulations in Aspen Dynamics were conducted for two heat integrated distillation column control strategies: one using fixed compressor duty and one using variable compressor duty. The control performance for a 20% throughput disturbance, as well as for a 50% turndown ratio scenario was investigated. Results show that fixed-duty operation maintains robust stability and rapid disturbance recovery even at 50% turndown, while variable-duty operation delivers higher efficiency for moderate load changes but cannot sustain low-load stability. This work supports the electrification of distillation by enhancing the operational flexibility of heat pump-assisted distillation, enabling better integration with intermittent renewable electricity grids.

Keywords: Distillation, Energy Efficiency, Dynamic Modelling, Aspen Dynamics, Methanol

INTRODUCTION

E-methanol produced from green hydrogen and captured CO_2 can be used as a versatile chemical building block, transportation fuel, and steel carburizing agent, making it central to the transition toward circular economy [1]. Heat pump assisted distillation (HPAD) enables fully electric purification using compressor shaft work, while significantly lowering energy consumption compared to conventional distillation. A common used HPAD configuration is mechanical vapor recompression (MVR) [2]. Here, the pressure of the overhead vapor of the column is increased such that its latent heat can be used to drive the reboiler. However, the application of MVR is limited to separations of close boiling point mixtures (ΔT_b = 20 °C), as large compression ratios are needed to overcome the entire temperature lift over the column [2]. Due to the large boiling point difference for methanol-water (ΔT_b = 34.7 °C) the heat-integrated distillation column (HIDiC) becomes an attractive HPAD technology. HIDiC reduces the required temperature lift and compression ratio by coupling the whole rectifying and stripping sections via internal heat exchange [3]. Nevertheless, very few HIDiC configurations exist at plant scale due to its complex design and structure [3]. Wakabayashi et al. [4] proposed a discretely heat-integrated distillation column (D-HIDiC), removing the need for impractical continuous heat exchange between stripping and rectifying section of HIDiC. This resulted in the first commercial HIDiC. Commercial operation has shown that D-HIDiC can increase control robustness of HIDiC, while maintaining high energy efficiency [4]. Cui et al. have investigated the design of a fully electrified D-HIDiC for the separation of methanol-water [5]. Previous studies on HIDiC process control proposed control structures based on expensive online composition analysers [6]. Cui et al. proposed a single end inferential composition control strategy based on temperature control for D-HIDiC [7]. This strategy manipulates compressor duty for control and showed robust performance under ±20% disturbances in throughput and feed composition. Recently, flexible operation of electrified processes to accommodate variations in electricity prices has gained increased attention, but this has not been investigated for HIDiC.

PROBLEM STATEMENT

E-methanol plants could operate flexibly to reduce costs by adapting to fluctuating electricity prices, as green hydrogen production is the main cost driver. To prevent the need for large hydrogen holdups, downstream processes could be operated flexibly. In this work, D-HIDiC is chosen as a technology of interest for full electrification of e-methanol purification due to its significant energy savings of up to 80%. Flexible operation of D-HIDiC is challenging, as D-HIDiC's strong thermal integration introduces complex process dynamics: disturbances in feed throughput or composition cause rapid, system-wide shifts in temperature, pressure, and composition profiles [8]. These tightly coupled responses challenge conventional control strategies, especially under flexible operation with frequent turndowns of up to 50%. While Cui et al. demonstrated control with variable compressor duty [7], their strategy requires the compressor to operate over a wide range when operating flexibly (e.g. 50-120% of design capacity), which is often infeasible due to compressor surge/stall limits. They mention that the modular nature of compressor systems could be used to enhance flexibility, but using this approach would increase CAPEX as well as control complexity. Therefore, this study aims to explore an alternative control strategy for D-HIDiC using fixed compressor operation, which is capable of operation at high turndown ratios of up to 50% to enable flexible operation.

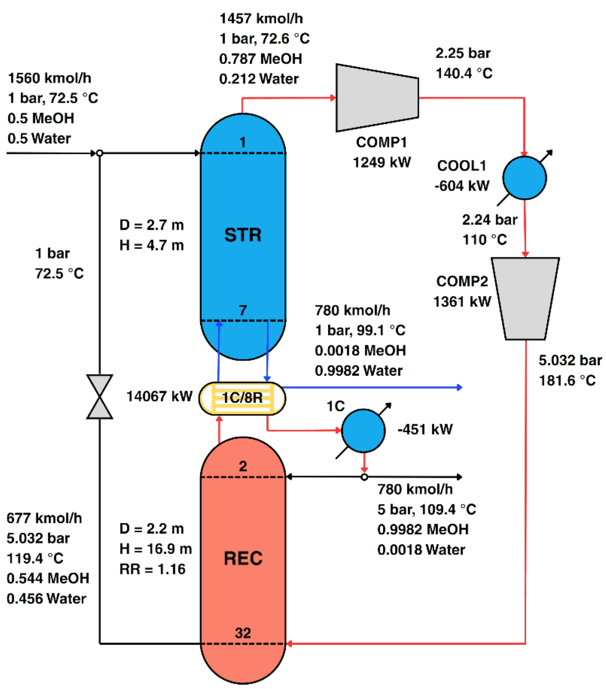

Figure 1. D-HIDiC configuration studied

METHODOLOGY

Process description

The HIDiC studied in this paper is shown in Figure 1 and is a modified version of the design proposed by Cui et al [5]. The following thermodynamic and hydrodynamic models are used for the process simulations in Aspen Dynamics, based on the work of Cui et al.:

- The thermodynamic model used is non-random two-liquid (NRTL), which is suitable and validated for the methanol water system [9].
- Column pressure drop was based on rigorous calculations using Aspen Plus column internals. To ensure high energy efficiency, low pressure drop Mellapak 350Y packing is used for the column internals.
- The hydrodynamic model is based on equilibrium stage, which is used in various process dynamics studies [10]. It is therefore assumed that each stage reaches vapor liquid equilibrium.
- Liquid holdup is estimated based on design heuristics by Luyben, ensuring a 5 minute holdup time at 50% full [10].

This design is a D-HIDiC, which features heat integration between the reboiler of the stripping section and the condenser in the rectifying section to realize full electrification of the column. Instead of utilizing the compressor interstage cooling duty for heat integration with the column, an interstage cooler is used for improved dynamic performance at a slight decrease in energy efficiency. Still, this design reduces the primary energy consumption compared to a conventional distillation column (CDiC) by 81.6% and has a heat pump coefficient of performance (COP) of 5.39. The D-HIDiC is designed to separate the effluent of an e-methanol reactor consisting of equimolar amount of methanol and water up to an AA grade methanol purity of 99.85 %wt [11]. Due to the maximum allowed mass fraction of water in AA grade methanol, the final purity was set at 99.9 %wt. A 200 kt/y methanol capacity is chosen based on the capacities of planned hydrogen electrolysers in Europe [12].

The D-HIDiC consists of 40 stages, split into an 8-stage low pressure stripping column (STR) and a 32-stage high pressure rectifying column (REC). A compression ratio of 5 was chosen to raise the boiling point of methanol in the high-pressure rectifying column, ensuring a minimum ΔT of 10 °C in the reboiler/condenser heat exchanger. A packed height of 0.5 meter per stage is used. A 20% column cross-section increase is applied to account for factors such as liquid holdup for surge capacity, based on recommendations by Luyben [10]. Furthermore, isentropic compressors with an isotropic

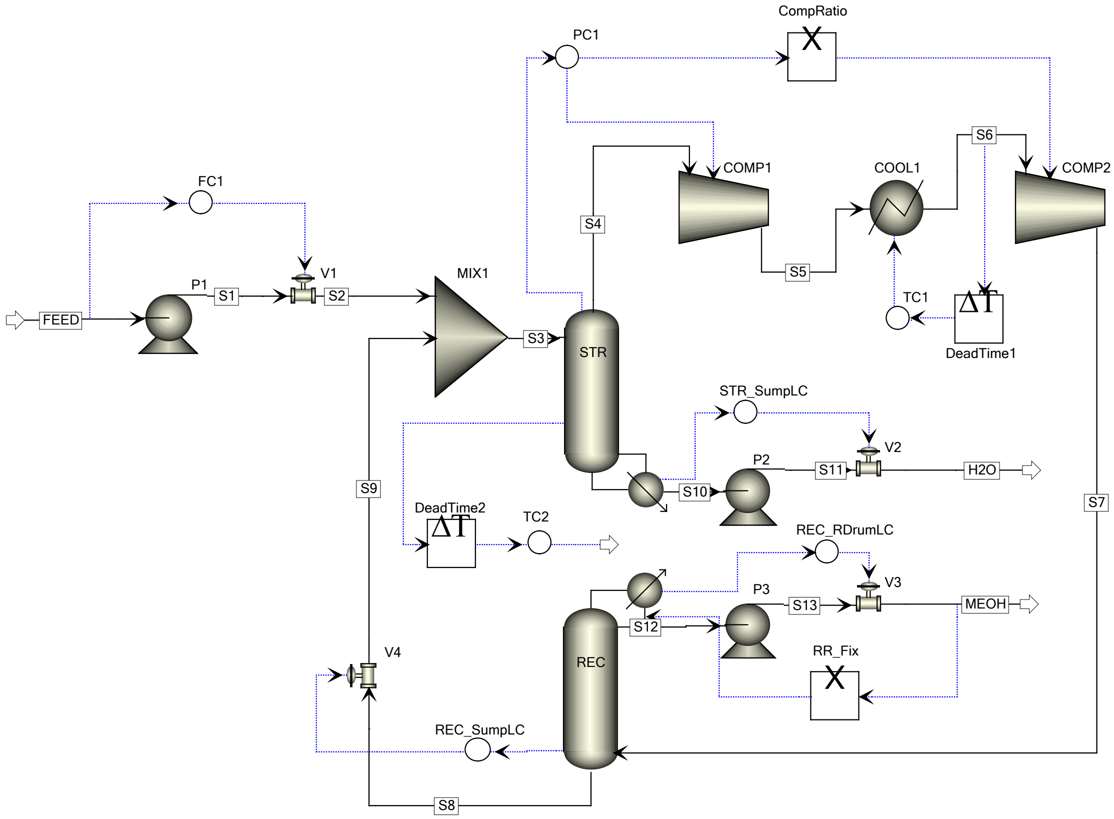

Figure 2. Process control structure 1 (PCS 1) utilizing variable compressor duty

efficiency of 80% were used.

Dynamics and control

Two control structures were evaluated in this work: one employing variable compressor duty based on the work by Cui et al. [7], and one novel control structure utilizing fixed compressor duty. The dynamic performance of both control structures was evaluated for ±20 % throughput disturbances, typical for industrial operation [10]. Composition disturbances were not investigated, as the effluent of a CO_2 hydrogenation methanol reactor typically has minor variations in composition. A sensitivity study was done on compressor mass throughput, since compressors have a limited range of operation. The sensitivity study was done for turndown ratios up to 50%, to account for a scenario with high energy prices and/or reduced availability of hydrogen to produce methanol.

Control basis

The process control structures were modelled using pressure driven simulations in Aspen Dynamics V14. Control valve pressure drops are 3 bar with the valve half open at design flow rates. PI controllers are used, with flow controllers having a K_c of 0.5 and τ_i of 0.3 min, the level controllers a K_c of 2 and τ_i of 9999 min based on recommendations by Luyben [10]. The other controllers were tuned using Tyreus-Luyben tuning rules. Temperature controllers are set at a 1 minute deadtime. Stage 5 of the stripper is identified as the most temperature sensitive stage based on the slope criterium [10]. Condenser and reboiler heat integration is done using flowsheet equations (Figure 4 & 5). Reboiler duty is calculated using (1), and then total condenser duty is calculated by adding auxiliary condenser duty to the reboiler duty (2). UA is kept constant. Condenser and reboiler duties then have to be changed from 'fixed' to 'free' in Aspen Dynamics.

$$Q_{reb} = UA(T_{cond} - T_{reb}) \tag{1}$$

$$Q_{cond} = -Q_{reb} + Q_{aux\,cond} \tag{2}$$

Process control structure 1 (PCS 1) is shown in Figure 2 and uses the following control loops:

- Fresh feed is flow controlled (FC1).
- L_{sump} is controlled using bottoms flowrate for both columns (STR_SumpLC & REC_SumpLC).
- $L_{refluxdrum,\,REC}$ is controlled using distillate flowrate (REC_RDrumLC)
- $T_{interstage}$ is controlled by manipulating duty of interstage cooler 'COOL1' (TC1).

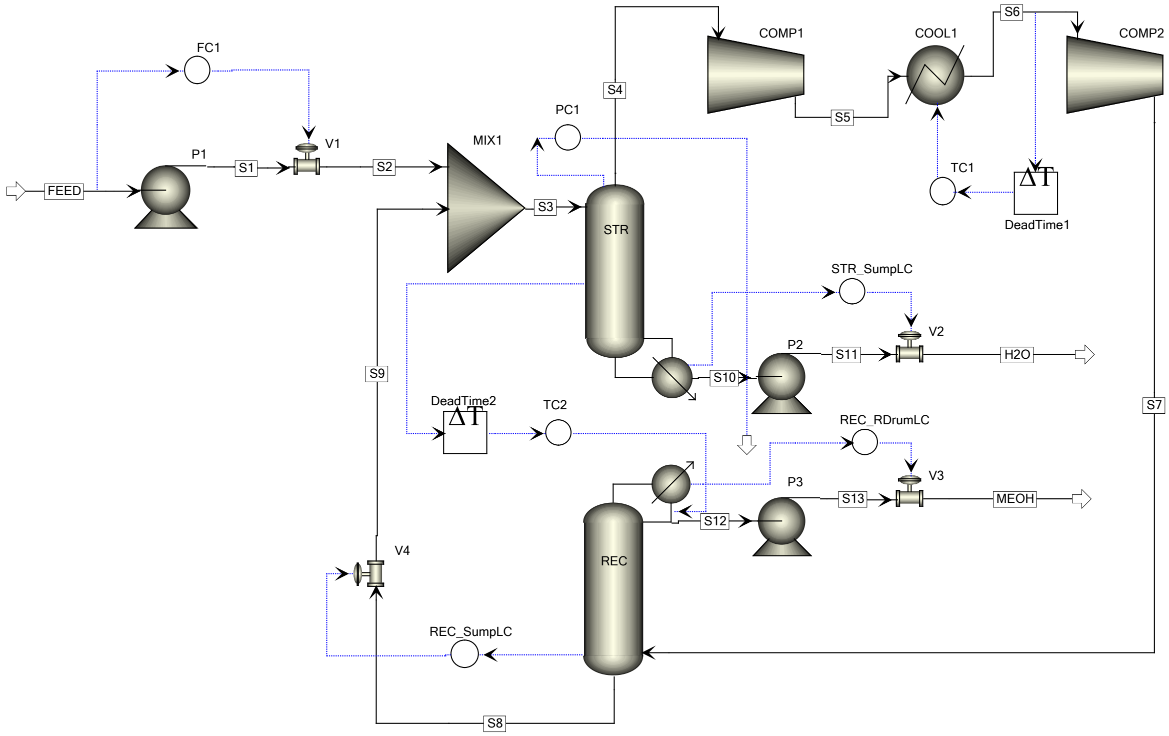

Figure 3: Process control structure 2 (PCS 2) utilizing fixed compressor duty

Constraints - Flowsheet

```
CONSTRAINTS
  // Flowsheet variables and equations...
  blocks("STR").Qreb = 4.944989695 * (blocks("REC").Stage(1).T-blocks("STR").Stage(8).T);

  blocks("REC").Condenser(1).Q = -blocks("STR").QReb + blocks("TC2").op;

```

Figure 4. Flowsheet equations PCS 1

Constraints - Flowsheet

```
CONSTRAINTS
  // Flowsheet variables and equations...
  blocks("STR").Qreb = 4.944989695 * (blocks("REC").Stage(1).T-blocks("STR").Stage(8).T);

  blocks("REC").Condenser(1).Q = -blocks("STR").QReb + blocks("PC1").op;

```

Figure 5: Flowsheet equations PCS 2

- $T_{\text{stage 5, STR}}$ is controlled by manipulating auxiliary condenser duty, see Figure 4 (TC2).
- $P_{\text{stage 1, STR}}$ is controlled by manipulating compressor duty, using a ratio controller to evenly change both compressor duties (PC1).
- P & T in the rectifier floats to allow for effective heat integration between rectifier and stripper
- Reflux ratio is kept constant using a ratio controller setting reflux flow as a ratio of distillate flow.

Process control structure 2 (PCS 2) in Figure 3 uses the same flow, interstage temperature, and level control loops, but has different control loops for stripper T and P:

- $T_{\text{stage 5, STR}}$ is controlled by manipulating reflux flow (TC2).
- $P_{\text{stage 1, STR}}$ is controlled by manipulating auxiliary condenser duty, see Figure 5 (PC1).

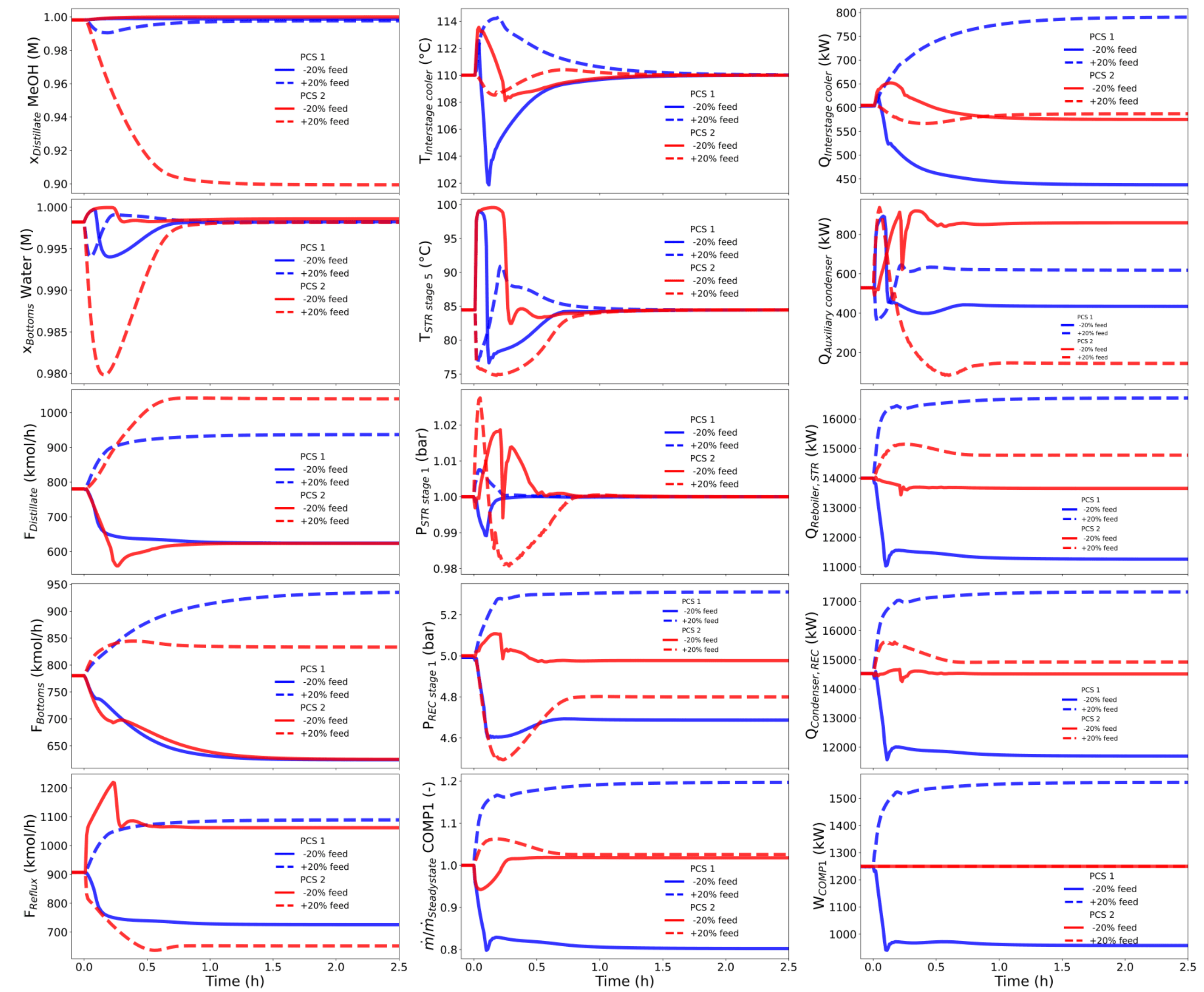

Figure 6. Control responses of PCS 1 and PCS 2 for ±20 % feed throughput disturbances

- Reflux ratio is no longer fixed, but instead compressor duty is kept constant.

The closed-loop system is continuously disturbed after 0.1 hr, for a total of 2.5 hr. The results are shown in Figure 6.

Compressor sensitivity analysis

A compressor feed disturbance sensitivity analysis was done by finding the maximum change of corrected mass throughput for the compressor for step change feed disturbances ranging from 0.5 feed fraction to 1.2 feed fraction. For each step change feed disturbance, a separate simulation run in Aspen Dynamics was done using a continuous disturbance for 2.5 h, after which the maximum change of corrected compressor mass throughput was found. The compressor mass throughput is corrected based on (3) to account for the effect of inlet temperature and pressure changes:

$$\dot{m}_{corr} = \dot{m}\sqrt{\frac{T_{in}}{T_{ref}}} * \frac{P_{ref}}{P_{in}} \tag{3}$$

The results can be seen in Figure 7. An open source high efficiency centrifugal compressor (HECC) map from NASA was included (Figure 8) as an example for surge margins [13]. The data for a vaneless diffuser with 0.018 inch tip clearance was used, as this was the largest dataset with larger surge margin.

RESULTS AND DISCUSSION

System control responses

Figure 6 shows that both control structures achieve stable control for feed throughput disturbances, with fast responses and settling times of about 1 hr, due to short liquid holdup times of the packed columns. PCS 1 shows faster pressure control than PCS 2, while temperature control settling times are similar. For both strategies, a large auxiliary condenser operating range is recommended for fast and robust control. The studied D-HIDiC has an auxiliary condenser duty to total condenser duty ratio of only 4.3%. A feed preheater or higher compressor interstage temperature could be used to increase this ratio, improving control robustness at an efficiency cost.

PCS 2 is a material balance-based control strategy and therefore cannot maintain product purity at increased feed throughput, as the reflux ratio must decrease to keep compressor flow constant. For a 20% feed throughput increase, the reflux ratio changes from 1.16 to 0.63, decreasing distillate purity by 10 mol% and dropping methanol below fuel grade (95 wt%, max 1 wt% water). Because the steady-state reflux ratio is close to 1, the absolute changes in reflux and distillate flow produce a large relative change in reflux ratio; for high reflux ratio columns, this effect would be smaller. Conversely, feed decreases cause over-purification at the same energy expenditure as steady-state production, meaning a 50% turndown ratio results in twice the energy cost per unit of purified methanol compared to steady state.

Despite these disadvantages, PCS 2 has one significant merit: compressor mass throughput is stabilized and step-change feed disturbances are substantially damped at the compressor. PCS 2 is therefore suitable for processes where the economic benefits of flexible operation of electricity-intensive upstream processes outweigh the increased purification cost per unit during turndown. For e-methanol production, about 90–95% of all electric power is consumed by water electrolysis [14], making the cost savings from electrolyzer turndown during electricity price spikes larger than the increased purification costs per unit of methanol incurred by PCS 2.

In general, PCS 2 should only be applied for turndown and the subsequent return to steady-state production, as product purity is maintained during these transient periods. Ramping above design capacity with PCS 2 should be avoided; a different strategy such as PCS 1 should be used instead to prevent distillate purity loss.

Compressor sensitivity analysis

PCS 1 shows a proportional change of the corrected compressor mass throughput for feed rate changes (Figure 7). This is expected, as the compressor duty is altered to maintain stripping column pressure, matching the change of feed inflow. For PCS 2, the change in compressor mass throughput is damped (Figure 7). For example, a -20% feed step change causes a -5.7% change in compressor mass throughput. Figure 8 shows that for any given operating point, if the pressure ratio is maintained constant and the corrected mass flow rate is halved, the new operating point is beyond the surge limit. Based on this compressor map, PCS 1 is incapable of a 50% turndown ratio. This shows the potential of PCS 2 for flexible operation, especially when using feed ramp changes. Ramp time could be chosen such that the compressor experiences minimal changes in mass throughput. Nevertheless, it should be mentioned that a compressor map is unique for every compressor. Choices can be made in compressor design to increase surge margin at a decrease in efficiency and pressure ratio.

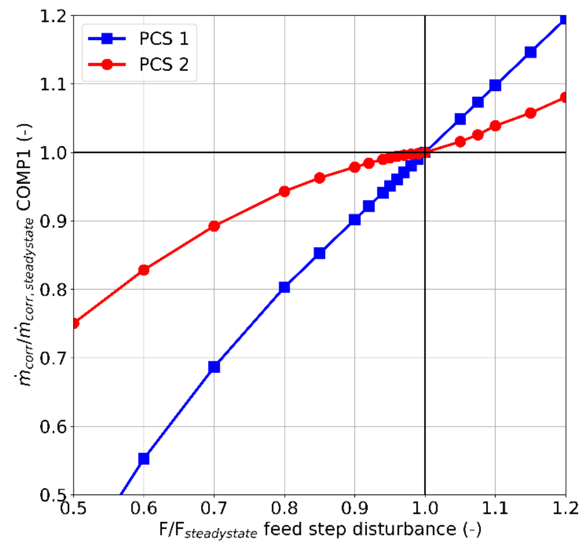

Figure 7. Compressor sensitivity analysis

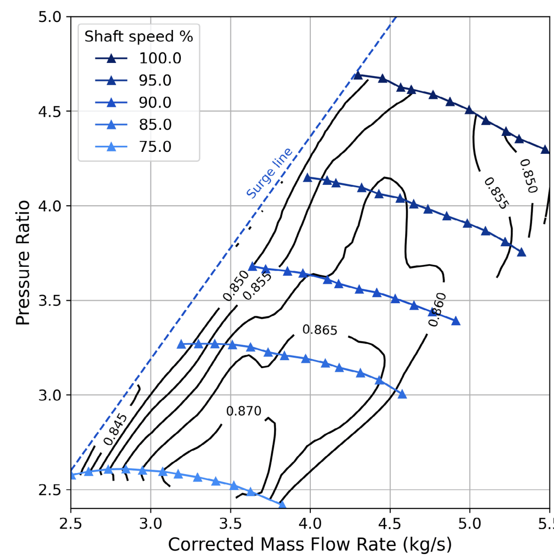

Figure 8: HECC compressor map

CONCLUSIONS

This study has provided a thorough analysis of a control structure based on variable compressor duty (PCS 1) and for a control structure based on fixed compressor duty (PCS 2) for D-HIDiC. Both control structures are based on inferential temperature control and show robust performance for ±20 % feed throughput disturbances. Compressor sensitivity analysis has shown that

PCS 2 damps throughput disturbances for the compressor. PCS 2 can maintain stable compressor operation at 50% turndown ratio, whereas PCS 1 requires a compressor capable of operating at 50% capacity. PCS 2 enables high turndown, but at the cost of losing purity control during production increases and incurring an energy efficiency penalty during turndown. Its application is therefore best suited for scenarios where the economic value of flexibility outweighs these drawbacks.

These findings highlight the potential application of D-HIDiC technology in flexible chemical production systems. This work contributes to further electrification of distillation processes by making D-HIDiC compatible with variations in power availability.

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