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Dynamics and control of discretely heat integrated distillation columns

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ABSTRACT

This study investigates the dynamics and control of discretely heat integrated distillation columns, focusing on two configurations: one utilizing a liquid pumparound loop and the other employing liquid injection for waste heat recovery in a multi-stage vapor recompression cycle. These innovative designs eliminate the need for vapor splitters, simplifying operation and enhancing control robustness. As case study, the methanol/water separation process was modelled to achieve 99.99 mol % purity for both products. Dynamic simulations were conducted in Aspen Dynamics to evaluate the control performance for $\pm 20\%$ throughput and composition disturbances. Results demonstrated that the proposed control structures, which rely on inferential temperature-based strategies, effectively maintain product specifications and ensure stable operation. This work provides valuable insights into the practical implementation of discretely heat integrated distillation columns, offering a pathway toward energy-efficient and operationally flexible distillation systems.

1. Introduction

Distillation is the cornerstone of thermal separation processes and is widely regarded as the most mature and indispensable technology in the chemical industry (Kiss, 2013). It is widely used in various fields such as petroleum fractionation, gas processing, and the production of petrochemicals, pharmaceuticals, and fine chemicals (Cui et al., 2022, 2017). Despite its critical importance, distillation remains one of the most energy-intensive processes, accounting for 90–95 % of the total energy used in fluid separation operations (Mathew et al., 2022). This energy intensity poses significant economic and environmental challenges, especially in a world increasingly focused on reducing carbon emissions and enhancing energy efficiency (Kiss and Smith, 2020; Li et al., 2023).

As industries move toward sustainability, the electrification of distillation processes has emerged as a promising strategy (Cui et al., 2024a, 2024b). Electrification enables the integration of renewable energy sources, reduces reliance on fossil fuels, and facilitates innovative separation technologies that were previously constrained by traditional steam-driven mechanisms. Heat pump assisted distillation (HPAD) exemplifies this paradigm shift, offering a means to reduce energy consumption and carbon emissions simultaneously (Kiss et al., 2012; Kiss and Infante Ferreira, 2016). Within this context, the heat integrated distillation column (HIDiC) has attracted growing interest. Unlike traditional columns, HIDiC leverages pressure differentials

between rectifying and stripping sections to enable efficient internal heat exchange, providing a highly energy-efficient alternative to conventional setups (Jana, 2014; Kiss and Olujić, 2014).

While HIDiC technology has demonstrated significant potential in reducing energy requirements, its adoption is very challenging. Effective operation requires precise control strategies to manage the complex interactions between pressure, temperature, and composition within the column. Research efforts have thus focused on developing dynamic models and control systems tailored to HIDiC configurations. Huang et al. (1996) pioneered HIDiC dynamic modeling by developing a simplified stage model that assumes ideal vapor-liquid equilibrium relationship, along with a control structure for an ideal HIDiC (i-HIDiC) featuring a preheater. Their proposed control structure regulates the bottoms composition through the feed preheater, while the distillate composition is controlled by adjusting the distillate flow rate. Due to the significant time delay associated with online composition measurement instruments, soft sensing techniques were used to estimate the product composition. This estimation was achieved using nonlinear multivariable regression methods with easily measurable temperature and pressure variables, resulting in generally satisfactory control performance. In subsequent work, Huang et al. (2007) introduced a novel temperature control scheme for an i-HIDiC without condenser and reboiler, while adding a feed preheater to regulate the energy balance of the whole system. The focus of this study was on using tray temperature or

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temperature differentials to infer product compositions, thereby circumventing the need for online composition analyzers. A comprehensive review of HIDiC startup, dynamics and operation studies is provided by Nakaiwa et al. (2003). Based on an i-HIDiC designed for separating propylene/propane (Olujic et al., 2006), Ho et al. (2009) analyzed the control degree of freedom (DOF) in various configurations, including an i-HIDiC, a HIDiC with a preheater, and a HIDiC with a reboiler. They found that adding a reboiler to the i-HIDiC increased the DOF, resulting in improved control flexibility. Bisgaard et al. (2017) presented a systematic control configuration design procedure for the HIDiC with a reboiler. Using a decentralized control scheme, they achieved stable and economically efficient performance by controlling the pressures in both column sections and managing the temperature profile within one of the sections. Economic variables were further optimized through cascade control loops, with guidelines provided for both regulatory and supervisory control layer designs. The above literature review indicates the significant progress made in developing effective control strategies for HIDiC systems, particularly those employing whole-section internal heat integration. However, such configurations often involve complex design and operational requirements, which limits their practical applicability in industrial scenarios.

To address these challenges, a new class of HIDiC systems has emerged, characterized by discretized heat integration (Wakabayashi and Hasebe, 2013). The world's first commercial application of such a discretely HIDiC (D-HIDiC) was introduced by Wakabayashi et al. (2019). Designed for separating a multicomponent mixture, which mainly includes methyl-ethyl-ketone and sec-butanol, this D-HIDiC

strategically positions a finite number of external heat exchangers at specific points along the column sections, as shown in Fig. 1. From an operational perspective, the authors highlighted that increasing the number of heat exchangers enhance the flexibility of process control by enabling the vapor flow rates to these exchangers to serve as manipulated variables. By adjusting the vapor flow rate from the top of the high-pressure rectifying section, the heat duty at each heat exchanger can be finely tuned, offering precise thermal management across the column. Despite these advantages, controlling vapor streams poses great challenges compared to liquid streams due to the less predictable nature of vapor flow. For instance, as demonstrated in studies on dividing wall columns, vapor splitters often introduce complexities in maintaining stable operation (Kang et al., 2017). To mitigate these difficulties, it is preferable to avoid vapor splitting and instead adopt alternative strategies that rely on liquid-based control, which is typically more stable and easier to implement.

Recognizing these challenges, our recent work proposed a novel design methodology for D-HIDiC, leveraging column grand composite curves to identify heat integration options (Cui et al., 2025). Two innovative configurations were introduced: one employing a liquid pumparound loop and the other utilizing liquid injection. These designs aim to recover waste heat within a multi-stage vapor recompression cycle, offering a practical and efficient approach to heat integration. Unlike traditional vapor-based control strategies, these configurations avoid the need for vapor splitters, thus simplifying operation and improving control robustness. However, the dynamics and control strategies specific to these D-HIDiCs remain underexplored. Therefore,

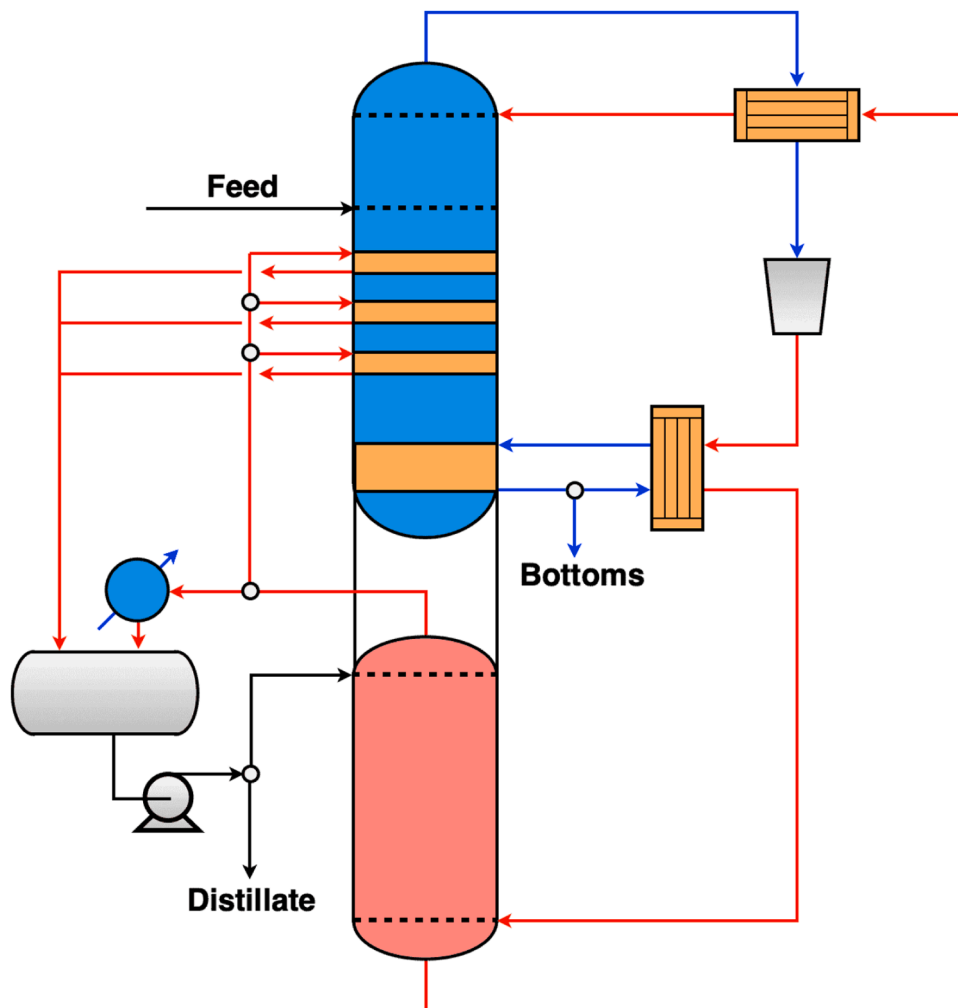


Fig. 1. Modified D-HIDiC proposed by Wakabayashi et al. (2019).

this study aims to bridge this research gap by investigating the dynamic behavior of D-HIDiC configurations and proposing effective control structures to overcome potential disturbances.

2. Process description

Fig. 2 illustrates the process studied, which closely resemble the double-effect heat integration configuration commonly used in air separation units (Qi et al., 2022). The steady-state design is based on our previous work (Cui et al., 2025). The following thermodynamic and hydrodynamic models are used in the process simulations:

- The thermodynamic model used is non-random two-liquid (NRTL), which has been widely validated for the methanol/water distillation and is considered suitable for this system (Kiss et al., 2016).
- The hydrodynamic model is based on equilibrium stage, which assumes that each stage reaches vapor-liquid equilibrium. This assumption has been widely used in various process dynamics and control studies (Luyben, 2013).
- Pressure drop across stages is based on rigorous calculation using Aspen Plus column internals. In this work, Mellapak 350Y is selected for the packed column internals.
- Liquid holdup is estimated based on design heuristics, ensuring that the reflux drum and column sumps provide 5 min of holdup at 50 % full (Luyben, 2013).

Design #1 is the D-HIDiC with a pumparound loop to recover compression inter-stage cooling duty, while **Design #2** is further built on this by utilizing a liquid injection method. Notably, in both designs, the entire overhead vapor from the high-pressure rectifying section is used to drive the reboiler in the low-pressure stripping section. This eliminates the need for vapor splitters, making the systems inherently simpler to control.

Note that in terms of energy savings, a key metric for assessing the balance is the coefficient of performance (COP). For the proposed D-HIDiC configurations, the COP exceeds a value of 5, indicating that for every unit of energy consumed by the compressors more than five units

of heat are effectively recovered. This suggests highly favorable energy utilization. For example, **Design #2** achieves a net energy reduction of approximately 80 % compared to a conventional distillation column (CDiC). Given the high COP and substantial energy savings, D-HIDiC presents a strong incentive for industrial applications, particularly in scenarios favoring process electrification and sustainable energy integration.

For each process, the feed is 1000 kmol/hr equimolar methanol/water mixture in a saturated liquid state. Both the methanol and water product purities are targeted at 99.99 mol %.

Fig. 3 shows the temperature and composition profiles. These column profiles are important in determining the temperature sensitive stages for the dynamic control structure design.

The D-HIDiC design features an 8-stage low-pressure stripping section (including the reboiler) and a 32-stage high-pressure rectifying section (including the condenser). Sulzer standard Mellapak 350Y is selected for the packed column internals, with a packed height of 0.5 meters per stage, resulting in a total packed height of 19 meters for 38 stages. To account for additional factors such as liquid holdup for surge capacity and the necessary net positive suction head requirements for pumps, a 20 % height oversizing is applied, following design heuristics recommended by Luyben (Luyben, 2013).

3. Dynamics and control

This section develops robust control structures developed for **Design #1** and **Design #2** of the D-HIDiC configurations. The dynamic performance of these designs is evaluated when ± 20 % disturbances occur in throughput and feed composition, which is a typical range for industrial operation and process upsets e.g., 80–120 % of design capacity (Luyben, 2013). Note that startup and shutdown procedures are beyond the scope of this work, as the current study focuses on process dynamics and control. However, the review paper by Nakaiwa et al. (2003) has already demonstrated practical startup and shutdown procedures for HIDiC.

In terms of controllability, traditional HIDiCs rely on continuous stage-by-stage heat exchange, which creates strong interactions between

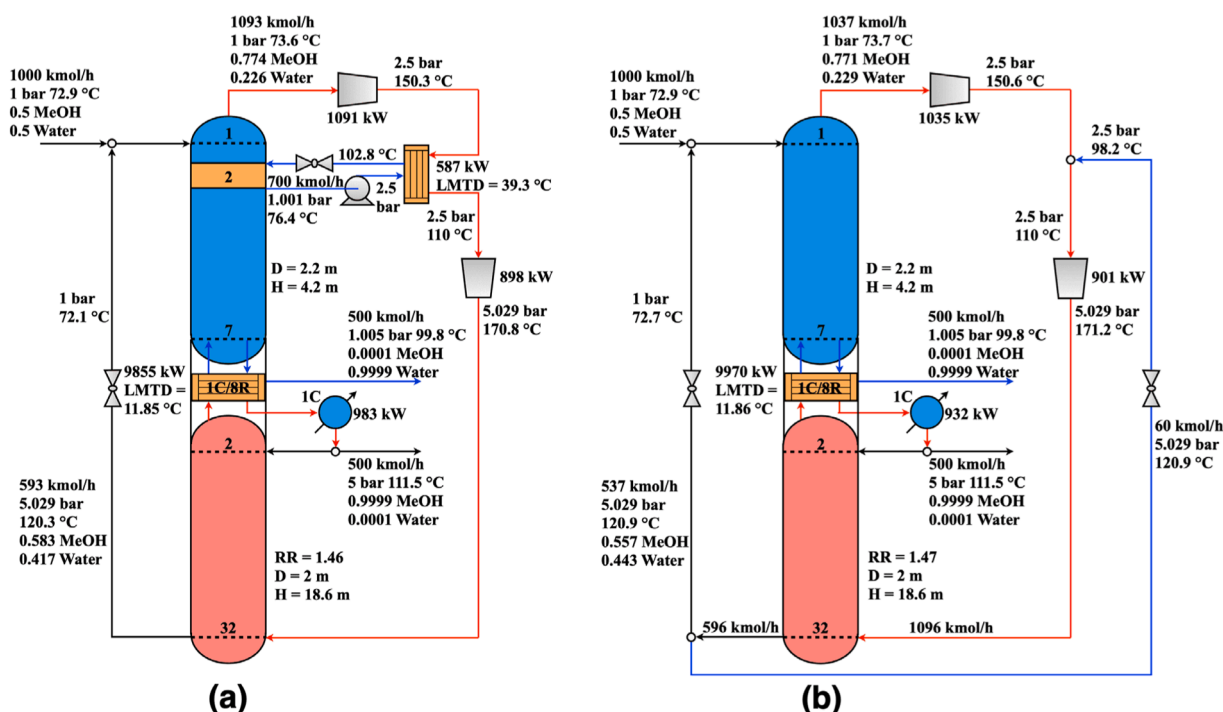


Fig. 2. (a) D-HIDiC with pumparound loop (Design #1); (b) D-HIDiC with liquid injection (Design #2).

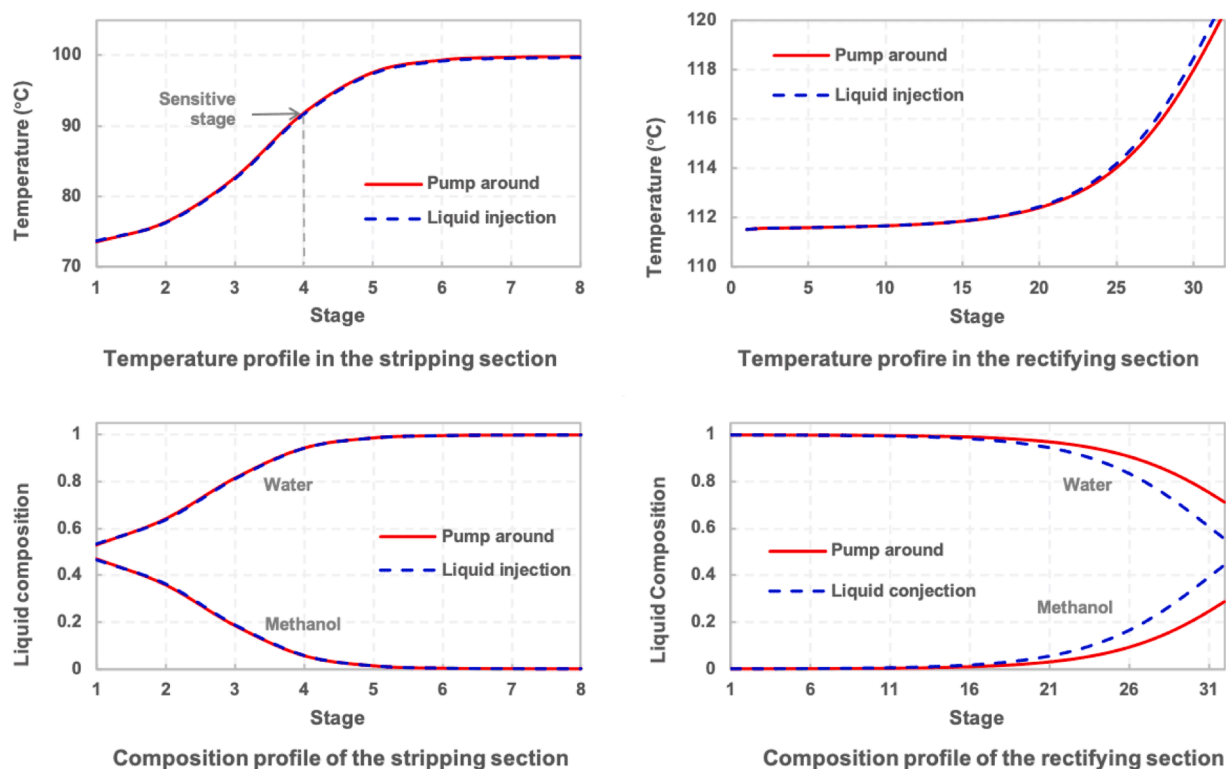


Fig. 3. Steady-state temperature and composition profiles.

pressure, temperature, and composition throughout the column. These coupled heat and mass transfer effects make process control more challenging, as disturbances in one section can propagate rapidly, requiring complex control strategies to maintain stability. The D-HiDiC proposed here eliminates stage-by-stage heat exchange by integrating the main reboiler and main condenser, thereby reducing internal process interactions. This structural modification decouples pressure and temperature control, so it is easy to control compared to traditional HiDiCs.

The control structures are limited to inferential composition control, which relies solely on temperature measurements. This approach avoids the need for online composition analyzers, which are often avoided in industrial applications due to their cost and maintenance complexity (Zhang et al., 2021, 2019).

In this study, we focus on demonstrating the feasibility of the inferential temperature-based control approach. Therefore, integral error metrics (IAE, ISE) are not introduced. Additionally, measurement noise is not explicitly considered, as the objective is to evaluate the general dynamic behavior of the system under disturbances. Also, the case study presented in this paper is an idealized binary system (without impurities or other minor components), primarily intended to introduce and evaluate the proposed D-HiDiC design and control strategy.

3.1. Control basis

Pressure-driven dynamic simulations in Aspen Dynamics V14 are used to develop the process control structures. Pump heads and valve pressure drops are selected to give reasonable rangeability so that 20 % increases in throughput can be handled without valve saturation. All reflux drums and column sumps are sized to provide 5 min of holdup when 50 % full at steady-state conditions. Typical design control valve pressure drops are 3 bar with the valve half open at design flow rates. The conventional proportional-only (P-only) controller with the gain $K_c = 2$ and integral time $\tau_I = 9999$ min is employed in level control loops. For flow, pressure, and temperature controls, proportional-integral (PI)

controllers are used. Flow controllers are tuned with parameters $K_c = 0.5$ and $\tau_I = 0.3$ min, while pressure and temperature loops are tuned using Tyreus-Luyben tuning rules. Each temperature controller has a 1 min deadtime in the loop. The temperature sensitive stage locations are identified by using the slope criterion (Luyben, 2013). As shown in Fig. 3, stage 4 of the stripping column section exhibits the steepest temperature slope in both **Design #1** and **Design #2**, making it the most suitable choice for the controlled variable.

3.2. Control structure of Design #1

A significant challenge in applying HiDiC systems lies in managing the complex process dynamics they introduce. Early studies, such as those by Huang et al. (1996), relied on using either the rectifying or stripping section pressure as a manipulated variable to regulate product composition in i-HiDiC. However, this approach often leads to operational instability, particularly under large disturbances in throughput or feed composition.

In the control structure proposed here (Fig. 4), the pressure in the low-pressure stripping section is tightly controlled, while the pressure in the high-pressure rectifying section is floating to achieve heat integration. Owing to the continuous pressure variations in the rectifying section, simple temperature control cannot work as effectively as in a conventional distillation column. Although a dual-end control strategy with pressure-compensated temperature measurement was investigated, its control performance was unsatisfactory because of the great magnitude in pressure variations and thus the high degree of process nonlinearity incurred. To address these issues, a single-end temperature control strategy is utilized. The reflux ratio is maintained constant, ensuring operational stability and simplifying control complexity. Meanwhile, the stable pressure in the stripping section allows the use of a direct temperature controller for regulating the bottom product.

Dynamic simulation that accurately capture the heat integration of liquid pumparound loop and the condenser/reboiler require the use of



Fig. 4. (a) Control structure of Design #1; (b) Aspen Dynamics layout of Design #1.

Flowsheet Equations in Aspen Dynamics. For the liquid pumparound loop, by default, the inter-stage cooler heat duty "QR" and the pumparound heat duty "PumpAround(1).QR" are set as "fixed" variables. However, for the intended dynamic operation, these variables must be set as "free" to ensure that all inter-stage cooling duty can be effectively transferred to the stripping section. To achieve this, flowsheet equation (1) (refer to Fig. 5) is introduced, and the "QR" variable in INT-COOL unit is redefined as "free".

Additionally, the cold pumparound loop stream outlet vapor fraction is set to be zero, as specified in flowsheet equation (2). This measure prevents the stream from vaporizing, which is critical for maintaining stability and avoiding fluctuations in dynamic control (Luyben, 2020). Consequently, the "PumpAround(1).QR" variable is also set as "free". For heat integration between the condenser and reboiler, two critical conditions must be maintained dynamically. First, the heat transfer in the condenser/reboiler must be equal to the product of the area, the overall heat transfer coefficient, and the current temperature difference. As the compositions and pressures vary, these temperatures change dynamically, with the pressure in the high-pressure rectifying section floating intentionally to support heat integration. This relationship is governed by flowsheet equation (3). Second, the auxiliary condenser duty must satisfy the overall energy balance, as defined by flowsheet equation (4). This duty is controlled by the PC2 controller, serving as the output signal. Under these conditions, the reboiler heat in the low-pressure column section and the condenser duty in the high-pressure column section are dynamically determined. Thus, "QRebR" and "Condenser(1).QR" are also defined as "free" variables to enable dynamic simulation of heat integration.

The basic control loops are the following:

1. Fresh feed is flow controlled.
2. Base level of the stripping column section is controlled by the bottoms flow rate.
3. Reflux drum level is controlled by the distillate flow rate.
4. Base level of the rectifying column section is controlled by the bottoms flow rate.

5. Reflux ratio (RR) is kept constant to achieve single-end control. This is achieved by using a multiplier (RR), in which the first input is connected from the mass flowrate of the distillate using a *ControlSignal* stream type. The second input is the constant reflux ratio, while the output is connected to the mass flowrate of reflux in the column.
6. Overhead pressure of the stripping column section is controlled by manipulating the compressor powers (PC1). Note that a multiplier (CompRatio) is added, whose input is the compressor power of Comp1 and whose output sets the compressor power of Comp2.
7. Overhead pressure of the rectifying column section is not controlled but floats (PC2).
8. The compressor inter-stage temperature is controlled by manipulated liquid pumparound flow rate (TC1).
9. The 4th stage temperature of the low-pressure stripping column section is controlled by manipulated the auxiliary condenser duty (TC2). This is similar to control reboiler duty, because the increase in auxiliary condenser duty will increase the pressure of the rectifying section thus increase the temperature difference in condenser/reboiler, providing more heat to the stripping section.

The closed-loop system is continuously disturbed after 0.5 hr, and the test is completed after 10 hr. The responses of the system to $\pm 20\%$ step change in feed throughput are shown in Fig. 6. The temperature controllers respond fast and the target product purities are maintained closed to their required specifications. Meanwhile, responses for feed composition disturbances from 50 to 60 mol % (+ 20 %) methanol and 50 to 40 mol % (- 20 %) methanol are shown in Fig. 7. In all cases, stable regulatory control is achieved for these large composition disturbances.

3.3. Control structure of Design #2

Liquid injection is another way to utilize the compression inter-stage duty. **Design #2** is slightly modified from **Design #1** so their control structures are similar, as shown in Fig. 8.

The only difference is the temperature controller TC1, which is used

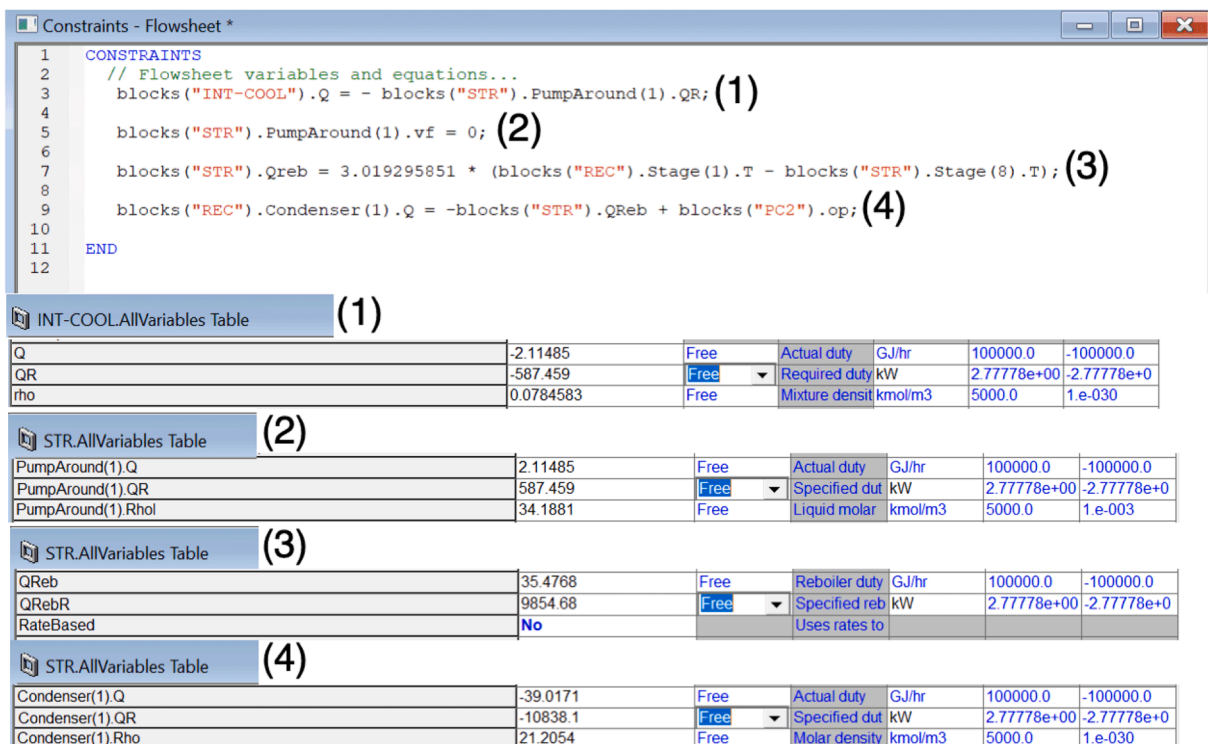


Fig. 5. Flowsheet equation and changing "fixed" variables to "free" variables.

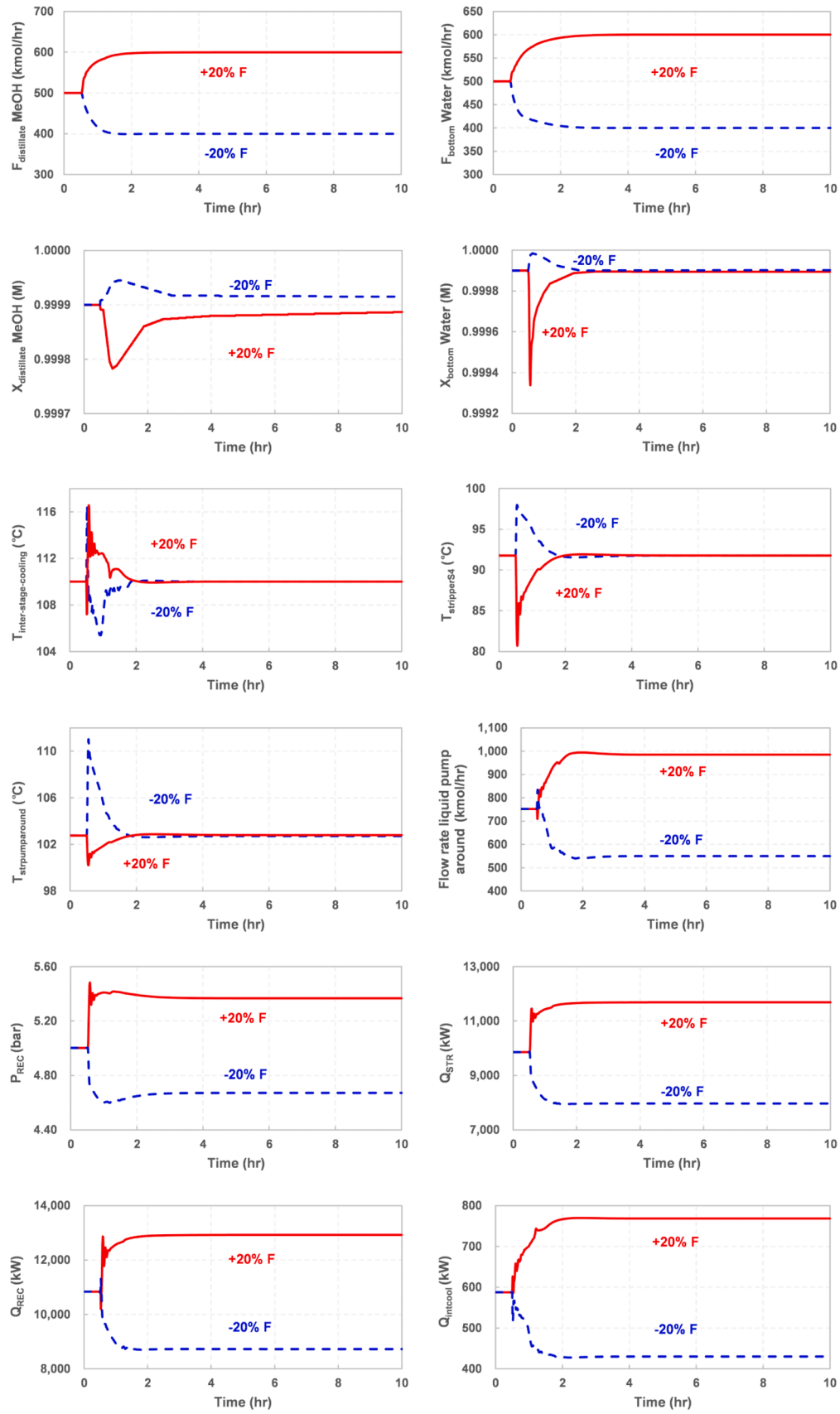


Fig. 6. Dynamic responses of control structure for Design #1 under $\pm 20\%$ throughput disturbance.

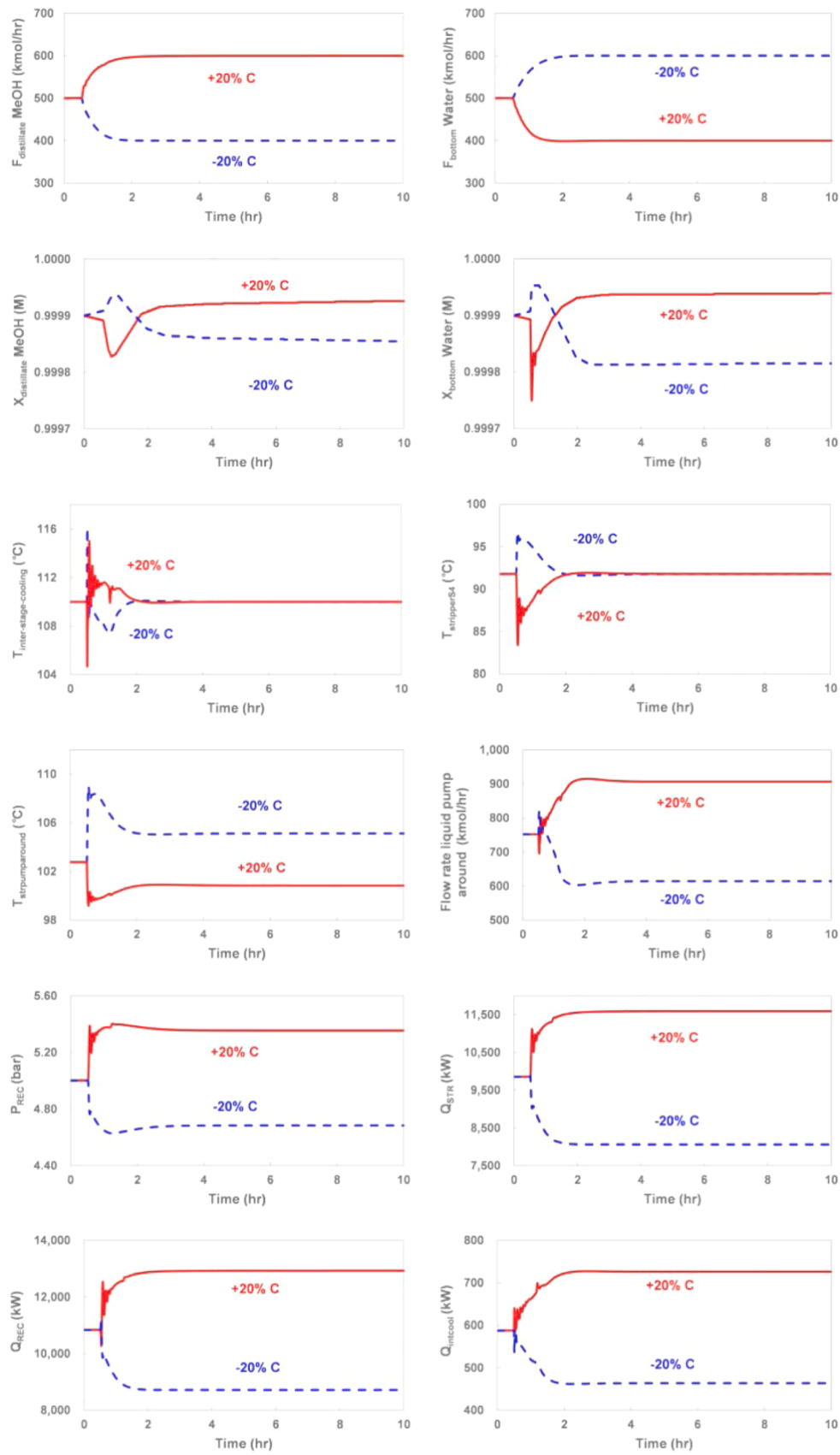


Fig. 7. Dynamic responses of control structure for Design #1 under $\pm 20\%$ methanol composition disturbance.

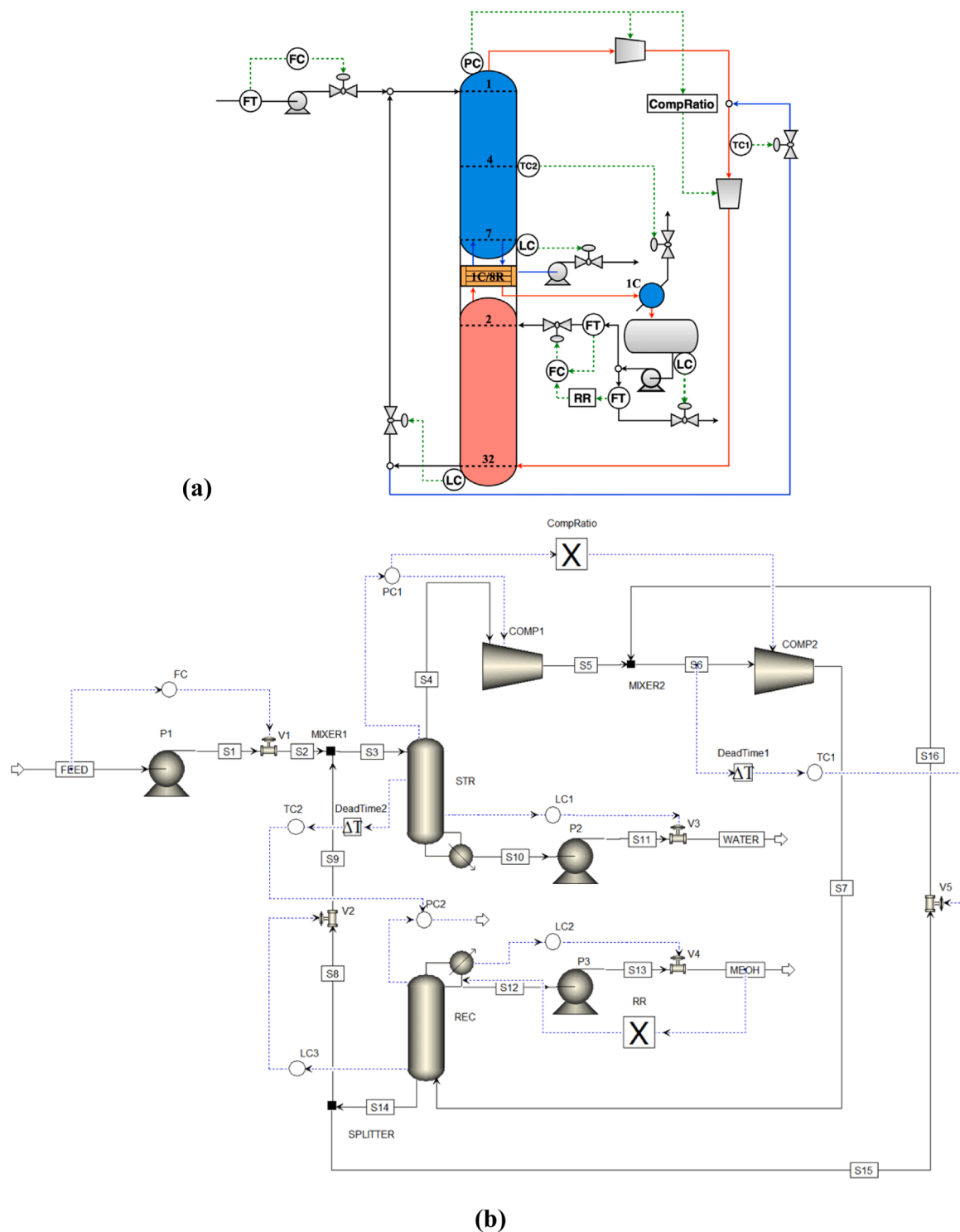


Fig. 8. (a) Control structure of Design #2; (b) Aspen Dynamics layout of Design #2.

to control the compressor inter-stage temperature by manipulating the liquid injection flow rate. Figs. 9 and 10 give results for $\pm 20\%$ throughput and composition disturbances, respectively. It can be observed that the control performance is generally good. This proves the robustness of the proposed control structure.

4. Conclusions

This study provided a comprehensive analysis of the dynamics and control of D-HIDiCs, focusing on two innovative configurations designed

to enhance energy efficiency and operational flexibility. The first configuration **Design #1** employs a liquid pumparound loop to recover inter-stage cooling duty, while the second **Design #2** utilizes a liquid injection method for the same purpose. Both designs eliminate the need for vapor splitters, simplifying operation and improving control stability. Through dynamic simulations, the proposed control structures demonstrated robust performance under $\pm 20\%$ disturbances in throughput and feed composition. The results show that inferential temperature-based control strategies can effectively manage the complex interactions within D-HIDiC systems, maintaining product

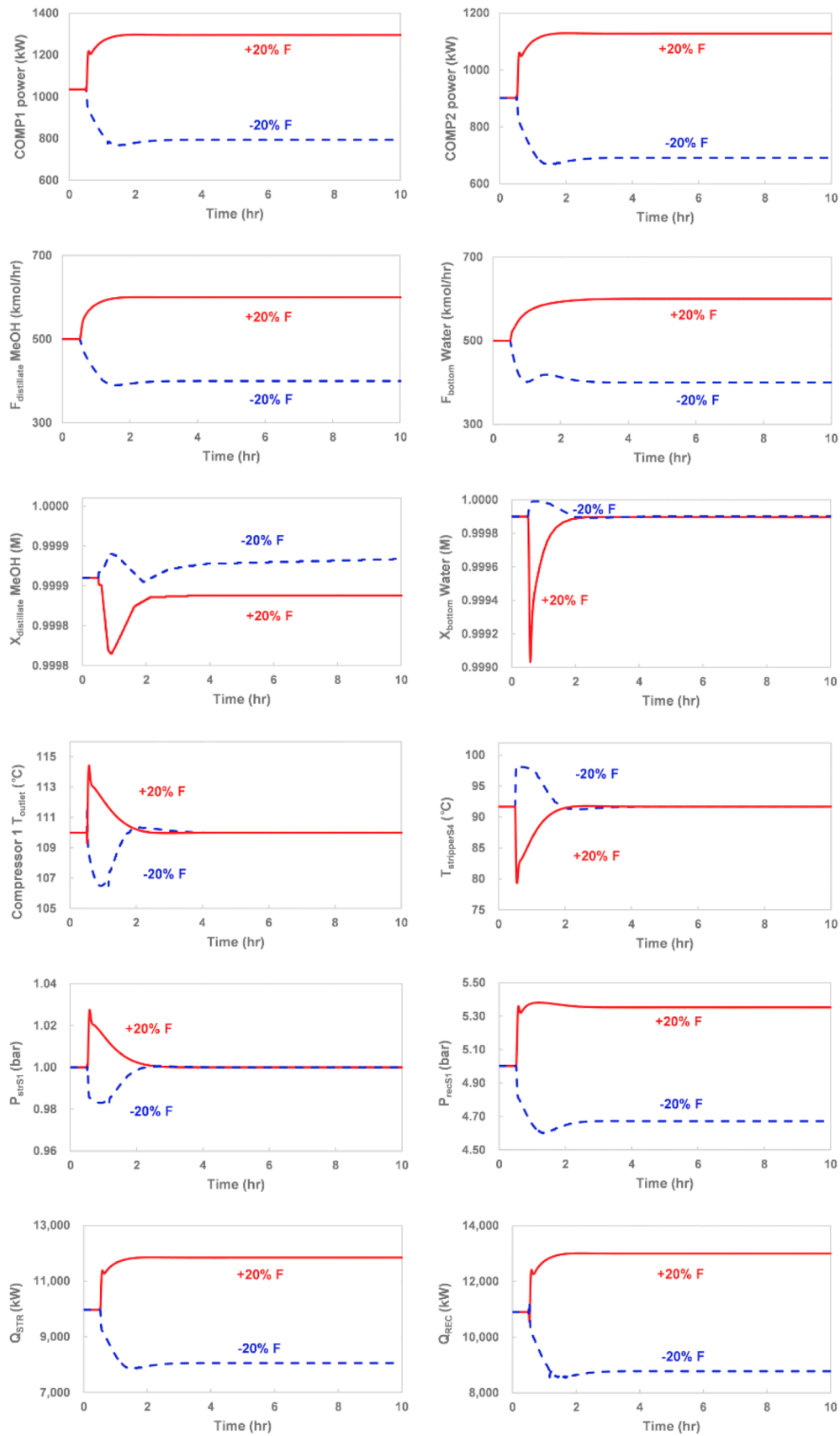


Fig. 9. Dynamic responses of control structure for Design #2 under $\pm 20\%$ throughput disturbance.

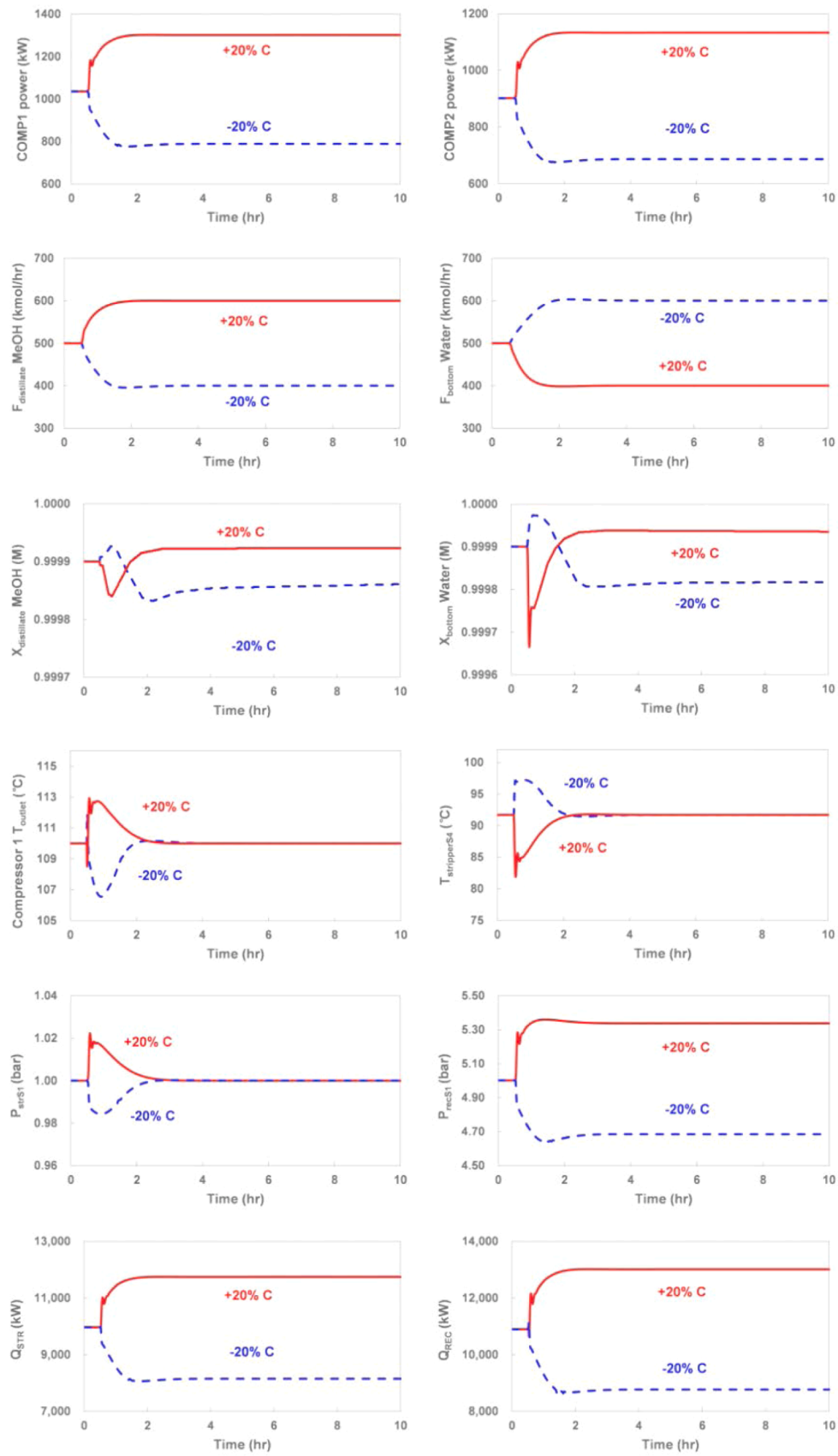


Fig. 10. Dynamic responses of control structure for Design #2 under $\pm 20\%$ methanol composition disturbance.

specifications and ensuring stable operation.

These findings highlight the potential of D-HIDiC technology as a practical and energy-efficient solution for electrifying distillation processes. For greater turndown/up flexibility, such electrified processes may need to accommodate variations in power availability (in case of significant renewables component). While this aspect is not the primary focus of this study, the modular nature of compressor-driven heat integration in D-HIDiC could provide more flexible operation as compared to steam-based systems.

CRedit authorship contribution statement

Chengtian Cui: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Qing Li:** Writing – review & editing, Visualization, Validation, Software, Formal analysis, Data curation. **William L. Luyben:** Writing – review & editing, Validation, Methodology, Formal analysis. **Anton A. Kiss:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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