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Control of fully electrified heat pump assisted distillation process by flash vapor circulation

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ABSTRACT

This study investigates the dynamics and control of a fully electrified heat pump assisted distillation system based on the flash vapor circulation (FVC) concept. The proposed configuration enables complete electrification without auxiliary steam. Two control structures are developed and evaluated in Aspen Dynamics under $\pm 20\%$ disturbances in throughput and composition. The first structure CS1 employs single-end temperature control with fixed reflux ratio and demonstrates satisfactory performance in most cases. However, it shows minor deviations in product purity under large composition changes. To address this, a second structure CS2 incorporates an additional composition controller to adjust the reflux ratio, achieving improved purity regulation and energy flexibility. The results confirm the dynamic feasibility and controllability of FVC-based distillation, supporting its integration in future sustainable and flexible separation systems.

1. Introduction

Distillation is one of the most energy- and carbon-intensive separation processes in the chemical industry, responsible for up to 95 % of the energy consumption in liquid phase separations and around 2.5 % of the total energy used in the United States (Mathew et al., 2022). In recent years, electrification of distillation has emerged as a promising strategy for process decarbonization and integration of renewable energy sources (Adami et al., 2025a; Cui et al., 2024a, 2025b; Mekidiche et al., 2024). Among various electrification pathways, mature technologies with a technology readiness level (TRL) of 9, such as electric heaters, electrode boilers, and heat pumps, have already been widely used in industrial applications (Element Energy & Jacobs, 2018).

Heat pump assisted distillation (HPAD) offers a particularly effective route to improve energy efficiency by upgrading low-grade heat within the process (Jana, 2014, 2010; Kiss, 2013; Kiss and Smith, 2020). Among the available HPAD configuration, mechanical vapor recompression (MVR) is widely applied due to its simplicity and effectiveness (Kiss et al., 2012). However, in many cases, the heat supplied by the compressed vapor is insufficient to fully drive the reboiler, necessitating an auxiliary reboiler. If this auxiliary reboiler relies on steam derived from fossil fuels, the environmental benefits of electrification are

diminished. Alternatively, the use of electric heaters or electrode boilers, while cleaner, delivers a low coefficient of performance (COP ≈ 1), leading to suboptimal energy usage compared to heat pumps.

To address this limitation, we recently proposed a novel configuration based on flash vapor circulation (FVC) concept (Cui et al., 2024b), and applied it in an industrial methanol distillation case study (Zhang et al., 2025). Some recent extensions of the FVC concept can be found in related studies (Adami et al., 2025b; Nogaja et al., 2024). In this approach, part of the flash vapor generated after throttling is recycled back to the compressor inlet, effectively increasing the vapor throughput and the reboiler heat duty. This configuration enables full electrification without auxiliary heating and offers improved load adaptability and flexible operation, which is particularly relevant under fluctuating electricity prices and renewable supply variability (Qi et al., 2025).

While the steady-state advantages of FVC-based configurations have been demonstrated, their dynamic behavior and control strategies remain unexplored. Prior research in this field has primarily focused on dynamics and control of MVR-based systems (Cui et al., 2022; Jogwar and Daoutidis, 2009; Patraşcu et al., 2019, 2017; Yang et al., 2025, 2023). However, the FVC concept introduces internal vapor circulation and induces significant nonlinear interactions and couplings, which substantially alter the dynamic response and pose non-trivial control

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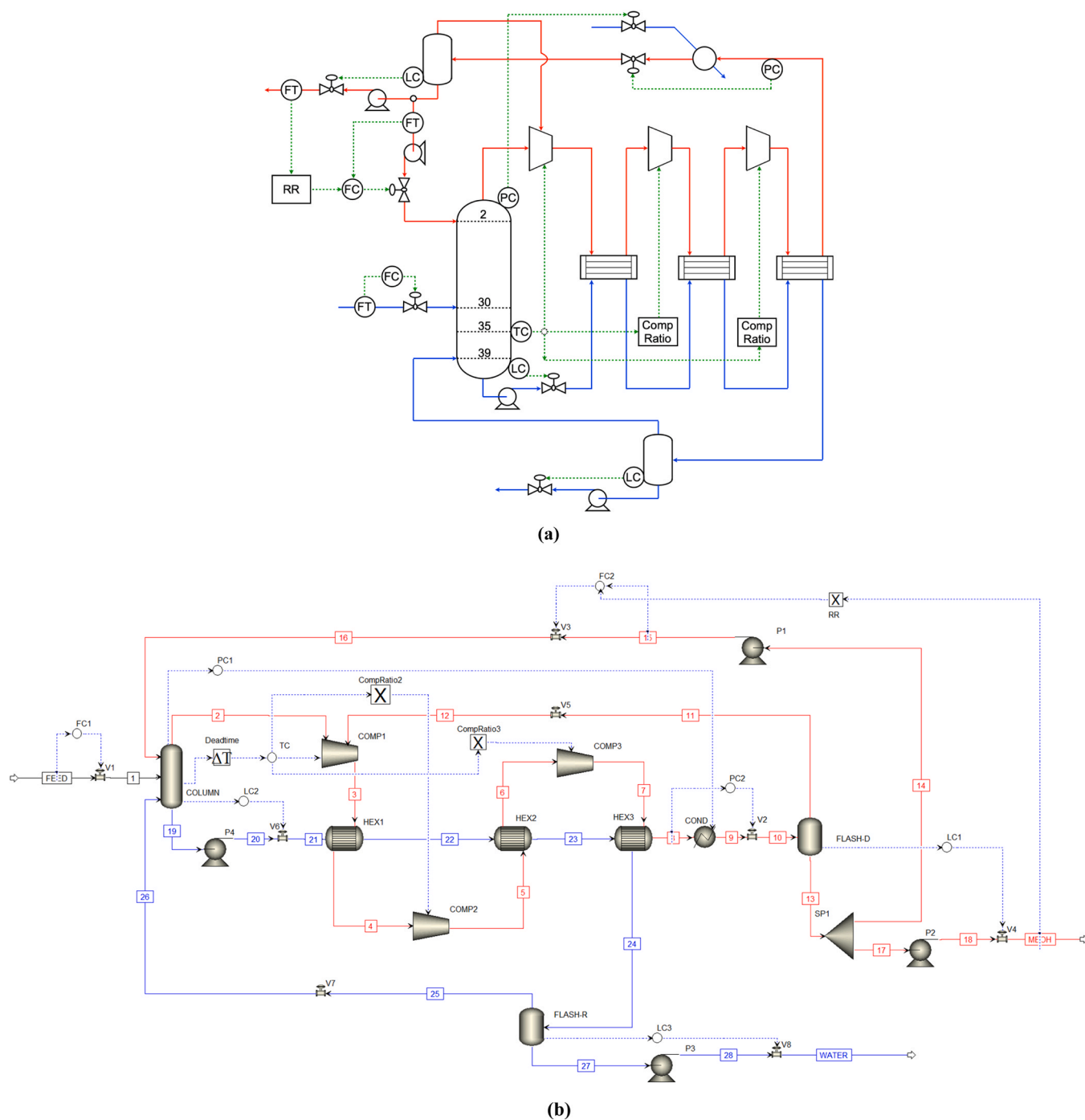


Fig. 3. (a) Control structure CS1; (b) Aspen Dynamics layout of CS1.

challenges. In this work, we address this research gap by investigating the control challenges of the FVC-assisted distillation system. We propose and evaluate robust control structures designed to maintain product quality and process stability under $\pm 20\%$ feed flow rate (throughput) and feed composition disturbances. To the best of our knowledge, this is the first study to assess the dynamic controllability of a fully electrified distillation system based on the FVC concept. The results highlight the feasibility of integrating FVC into electrified and flexible distillation systems while ensuring dynamic operability. This work contributes new insights into the control design of emerging electrified distillation technologies.

2. Process studied

The process studied is based on the FVC-2 configuration proposed in our previous work, aimed at fully electrified distillation of a methanol/water mixture (Cui et al., 2024b). The steady-state process flowsheet and its corresponding Aspen Plus layout are illustrated in Fig. 1. Due to the added hydraulic connections in the simulation, slight variations are observed in stream properties and heat loads compared to the simplified schematic. Two valves (V5 and V7) are inserted between the vessels to ensure proper flow initialization, as mandated by Aspen Dynamics. These valves introduce negligible pressure drops and are not utilized as manipulated variables. Full stream information, column specifications, and control performances are provided in the [Supporting Information](#)

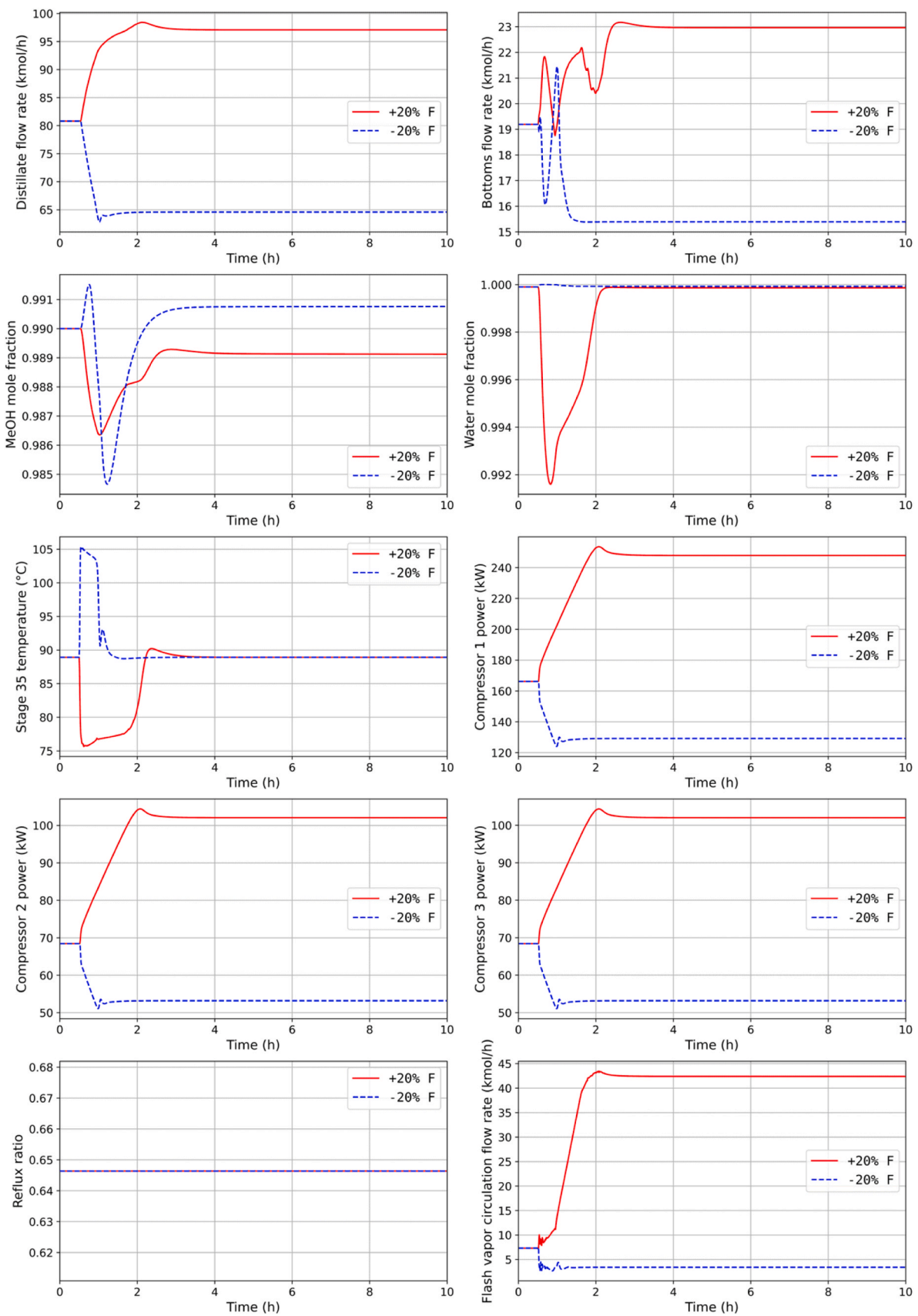


Fig. 4. Dynamic responses of CS1 under ± 20 % throughput disturbance.

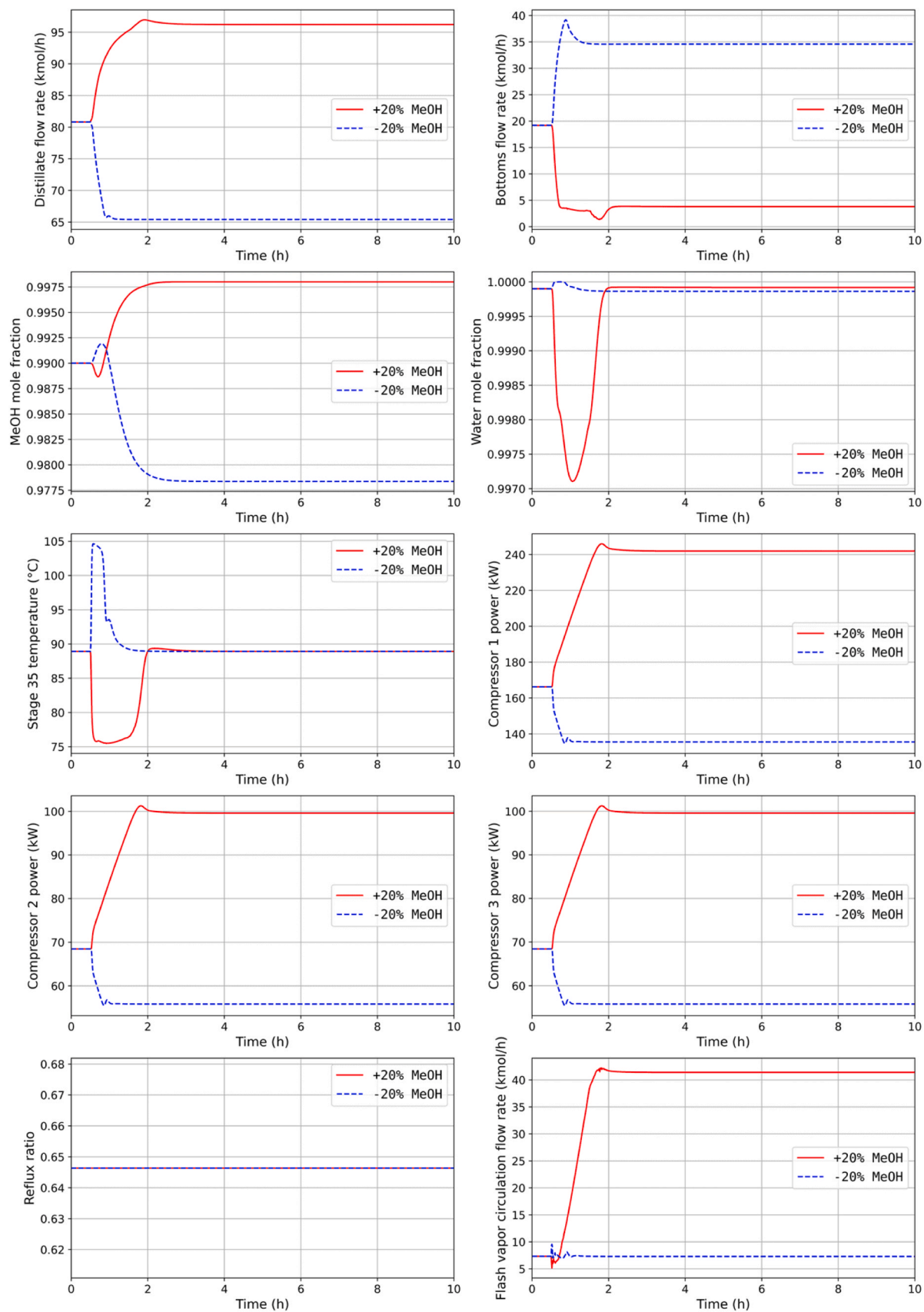


Fig. 5. Dynamic responses of CS1 under $\pm 20\%$ methanol composition disturbance.

file.

The feed stream is a saturated liquid at 30 °C and 5 bar, consisting of 80 mol% methanol and 20 mol% water, with a total flow rate of 100 kmol/h. The target purities are 99 mol% methanol in the distillate and 99.99 mol% water in the bottoms. The column consists of 40 theoretical stages (including condenser and reboiler), with the feed entering at stage 30. The column overhead at 1.007 bar (stage 2), while a stage pressure drop of 0.7 kPa is assumed throughout the column. The steady-state temperature and composition profiles are demonstrated in Fig. 2. These profiles are critical for identifying temperature sensitive stages.

Simulation of the conventional column without heat pump yields condenser and reboiler duties of 1307 kW and 1426 kW, respectively. In the FVC configuration, the reboiler duty is fully supplied by heat pump, with no external steam input required. Three stages of isentropic compression (efficiency = 0.75) are employed to upgrade the overhead vapor from 1.007 bar and 64.76 °C to 6.258 bar and 150 °C. Intermediate cooling is applied to limit the compressor discharge temperature below safety thresholds. The total compression power is 302 kW, and the resulting COP reaches 4.72.

3. Dynamics and control

This section presents the development and evaluation of control structure for the FVC configurations. The dynamic performance is assessed under $\pm 20\%$ step changes in throughput and composition, which represent typical process disturbances in industrial operation. Two alternative control strategies are investigated. Control structure 1 (CS1) utilizes temperature-only control loops, relying on inferential temperature signals for product quality regulation. Simulation results show that CS1 performs satisfactorily in most disturbance scenarios with small deviation in product purity. To further correct the methanol purity deviation, control structure 2 (CS2) incorporates an additional composition controller. The integral of absolute error (IAE) is employed as a standard metric to evaluate the overall control performance by quantifying the accumulated deviation between the controlled variable and its setpoint.

3.1. Control basis

Dynamic simulations and control structure development are conducted using Aspen Dynamics V14. Reflux drum and column sump are sized to provide 5 min of holdup when 50 % full at steady-state conditions. Pump heads and valve pressure drops are specified to ensure sufficient rangeability, enabling the system to accommodate up to $\pm 20\%$ throughput variations without valve saturation. Control valves are initially designed with a typical pressure drop of 3 bar at nominal flow conditions, corresponding to the valve being approximately 50 % open. However, it is later observed that the pressure drop across the bottoms product valve (V8) is insufficient to accommodate an approximately 80 % increase in flow rate during -20% methanol composition disturbance scenario. To ensure adequate controllability and rangeability, the valve pressure drop is increased to 12 bar in the final design. Standard control strategies are employed across the flowsheet. Level control loops utilized proportional-only (P-only) controllers with a gain of $K_c = 2$ and a large integral time of $\tau_I = 9999$ min to avoid integral action. For flow, pressure, temperature, and composition regulation, proportional-integral (PI) controllers are used. Flow controllers are tuned with parameters $K_c = 0.5$ and $\tau_I = 0.3$ min. Pressure controllers are set with parameters $K_c = 20$ and $\tau_I = 12$ min. Temperature and composition loops are tuned using the Tyreus-Luyben tuning method. Loop deadtimes are set to be 1 min for temperature controllers and 3 min for composition controllers (Luyben, 2013).

3.2. Control structure CS1

CS1 employs temperature control to regulate product purities. As

observed from the temperature profile in Fig. 2, the rectifying section exhibits relatively flat temperature gradients, indicating limited sensitivity in those stages. Consequently, temperature control in the upper stages of the column was found to be ineffective. Preliminary investigations using dual-end temperature control configurations confirmed that these strategies did not provide adequate regulatory performance due to low temperature sensitivity and increased control interactions. To improve controllability and reduce complexity, a single-end temperature control strategy is adopted by fixing the reflux ratio. Temperature-sensitive stages are identified based on the slope criterion (Luyben, 2013). As shown in Fig. 2, stage 35 exhibits the steepest temperature slope and therefore selected as the controlled variable in the temperature control loop. Controlling the temperature at this location effectively prevents methanol leakage into the bottoms. Fig. 3 shows the control structure CS1 and its corresponding Aspen Dynamics layout.

The basic control loops are the following:

1. Fresh feed is flow controlled (FC1).
2. Reflux drum level is controlled by the distillate flow rate (LC1).
3. Column sump level is controlled by manipulating the withdrawal stream (LC2).
4. Base level of distillation column is controlled by the bottoms flow rate (LC3)
5. Reflux ratio (RR) is maintained constant to implement single-end temperature control. This is achieved by using a multiplier, where the first input is linked to the distillate mass flow rate via a *ControlSignal* stream, and the second input is a fixed RR value. The output defines the reflux flow rate.
6. Overhead pressure of the distillation column is controlled by manipulating the condenser duty (PC1).
7. Compressor discharge pressure is regulated via a valve located downstream of the condenser and upstream of the reflux drum (PC2), as proposed by Luyben (2016).
8. Stage 35 temperature (TC) is controlled by manipulating the total compressor power. To distribute power among the three compressors, two multipliers (CompRatio2 and CompRatio3) are added. Their inputs receive the power signal from compressor 1, while their outputs determine the power of compressors 2 and 3, following the predefined ratios (Cui et al., 2025a).

The closed-loop system is subjected to $\pm 20\%$ step disturbances in throughput and composition, introduced at 0.5 h and completed after 10 h.

Fig. 4 presents the system responses to throughput disturbances. The temperature controller regulates stage 35 within 2 h, maintaining the product purities close to their target values. The distillate flow rate and composition stabilize smoothly, while the bottoms stream exhibits moderate oscillations and overshoot in flow rate and composition, respectively. Under the $+20\%$ throughput disturbance, the FVC flow rate increases from 7.3 kmol/h to 42.4 kmol/h, approximately 6 times higher. This is driven by the increased reboiler duty requirement, which rises to 1713 kW [HEX1 (83) + HEX2 (95) + HEX3 (1535)], representing a $+20.13\%$ from the nominal 1426 kW. Consequently, the total compression duty rises from 302 kW to 452 kW ($+49.67\%$), and the COP drops to 3.79, compared to 4.72 at nominal flow. In contrast, when a -20% throughput disturbance is introduced, the FVC flow rate decreases from 7.3 kmol/h to 3.4 kmol/h. The corresponding reboiler heat drops to 1138 kW (61 + 54 + 1023), equivalent to -20.75% . The total compression duty reduces to 235 kW (-22.19%), and the COP increases to 4.84.

Fig. 5 shows the system responses to $\pm 20\%$ step changes in feed composition (from 80 mol% to 96 mol% and 64 mol% MeOH). Under the -20% composition disturbance case, the bottoms flow rate increases significantly from approximately 20 kmol/h to 36 kmol/h ($+80\%$), causing the level controller LC3 to encounter valve saturation. This issue is resolved by increasing the pump head in the dynamic mode

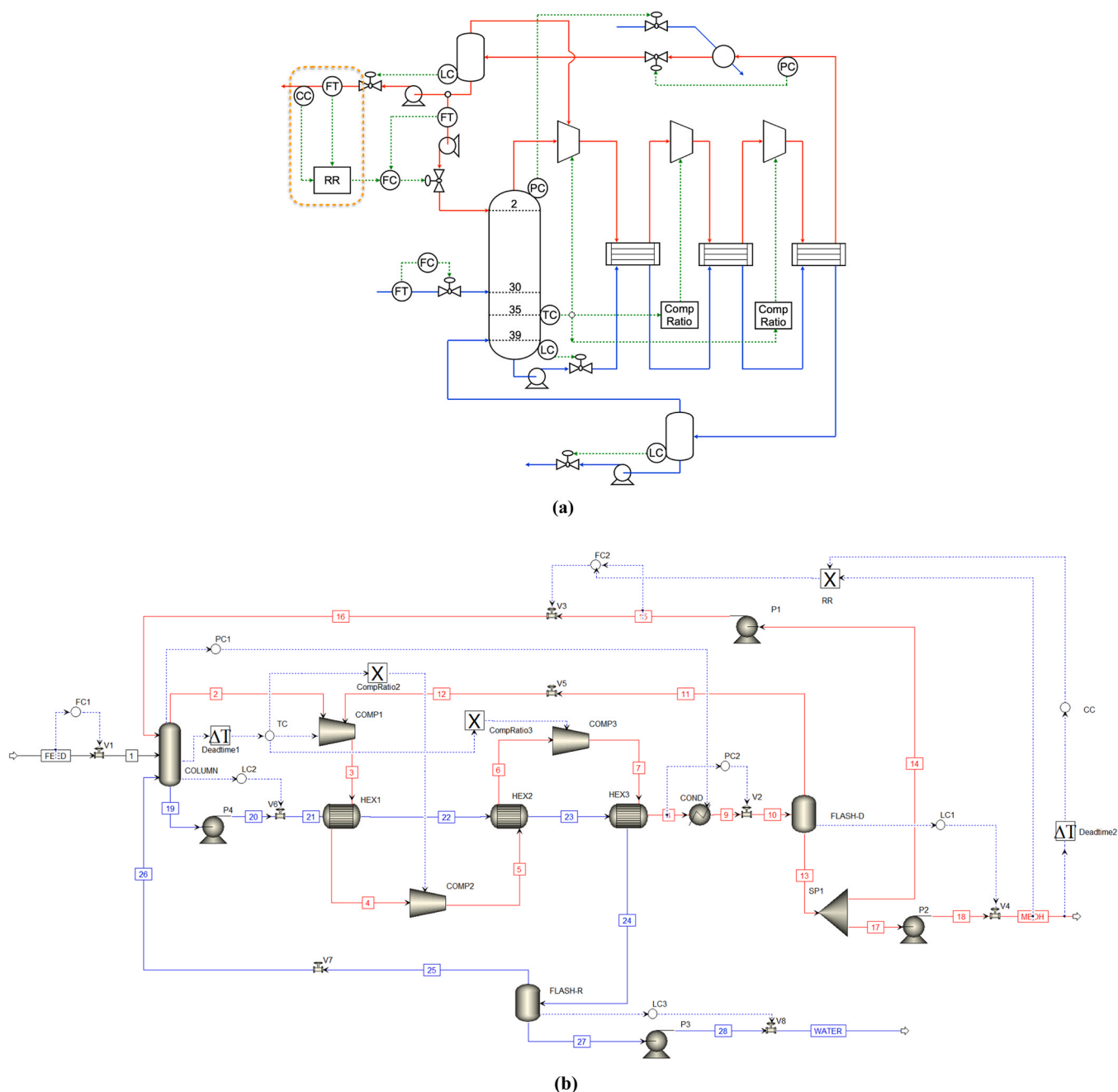


Fig. 6. (a) Control structure CS2; (b) Aspen Dynamics layout of CS2.

(Luyben, 2002). With a fixed reflux ratio, the +20% composition disturbance results in an over-purified methanol product (99.76 mol%), while the -20% case leads to a reduction in methanol purity to 97.75 mol%. This behavior reveals a limitation of temperature-only control under large feed composition variations. When feed methanol concentration increases to 96 mol%, the required reboiler duty rises to 1654 kW (80 + 93 + 1481), which is +15.99% compared to the original 1426 kW. As a result, total compression power increases from 302 kW to 442 kW (+46.36%), and the COP drops to 3.74. In contrast, when methanol concentration drops to 64 mol%, the FVC flow rate remains nearly unchanged. The reboiler duty decreases to 1194 kW (64 + 57 + 1073), equivalent to -16.27%. Compression power is reduced to 247 kW (-18.21%), and COP increases to 4.83.

These results indicate that the FVC configuration is more energy-efficient when handling negative disturbances. The floating FVC flow

rate plays a central role in regulating total power consumption. To address the purity deviation and better coordinate power usage under varying feed conditions, control structure CS2 incorporates a composition controller. This controller directly corrects methanol purity by adjusting the reflux ratio, which also indirectly influences the FVC flow rate. The performance of CS2 is discussed in the following section.

3.3. Control structure CS2

Compared to CS1, the only modification in CS2 is the addition of a composition controller to regulate methanol product purity by adjusting reflux ratio, as marked in Fig. 6. In practice, controlling the water impurity in the distillate is more effective (Ling and Luyben, 2009).

Fig. 7 gives results for $\pm 20\%$ throughput disturbances. The FVC flow rate increases to provide more compressed vapor to meet the

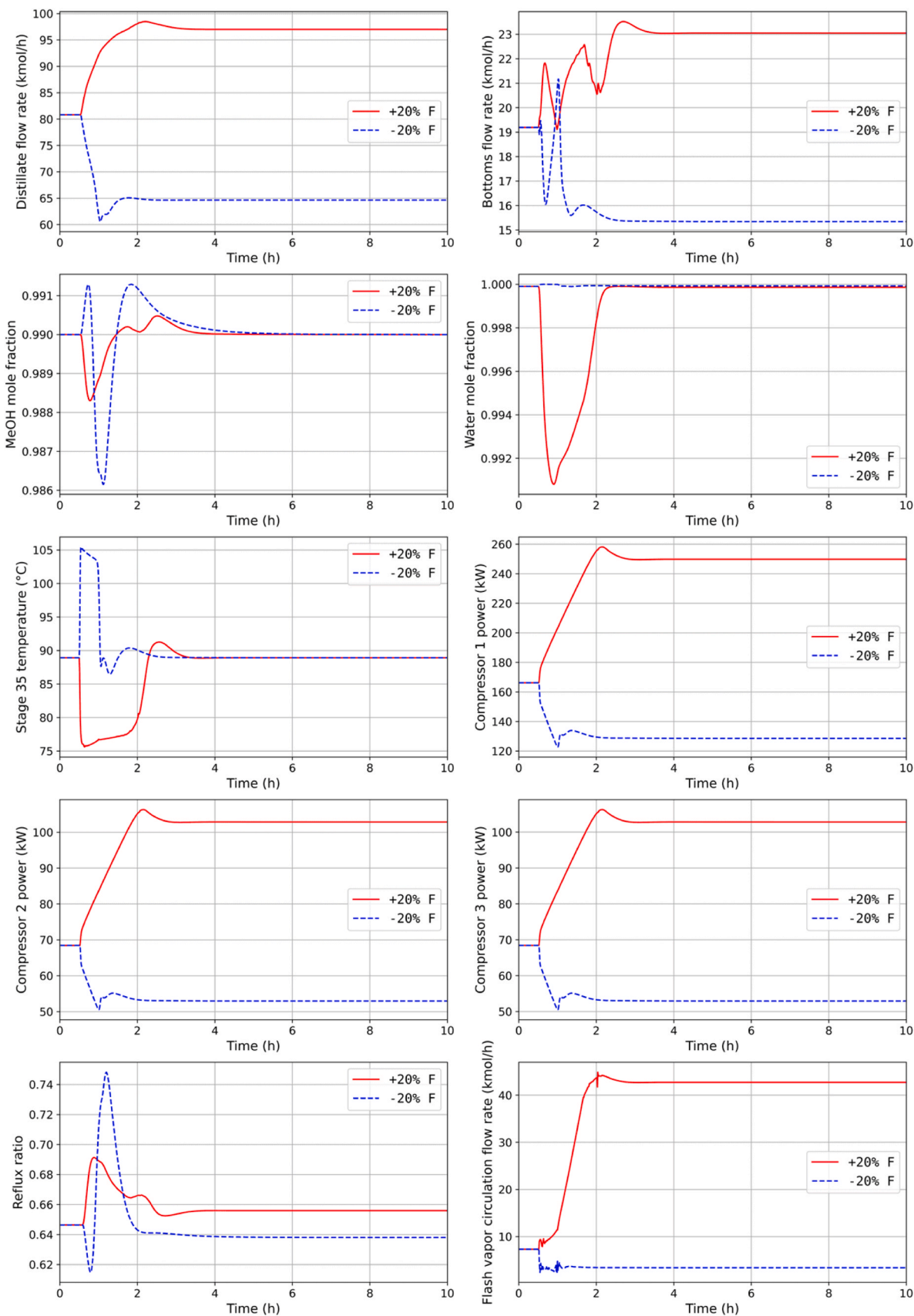


Fig. 7. Dynamic responses of CS2 under $\pm 20\%$ throughput disturbance.

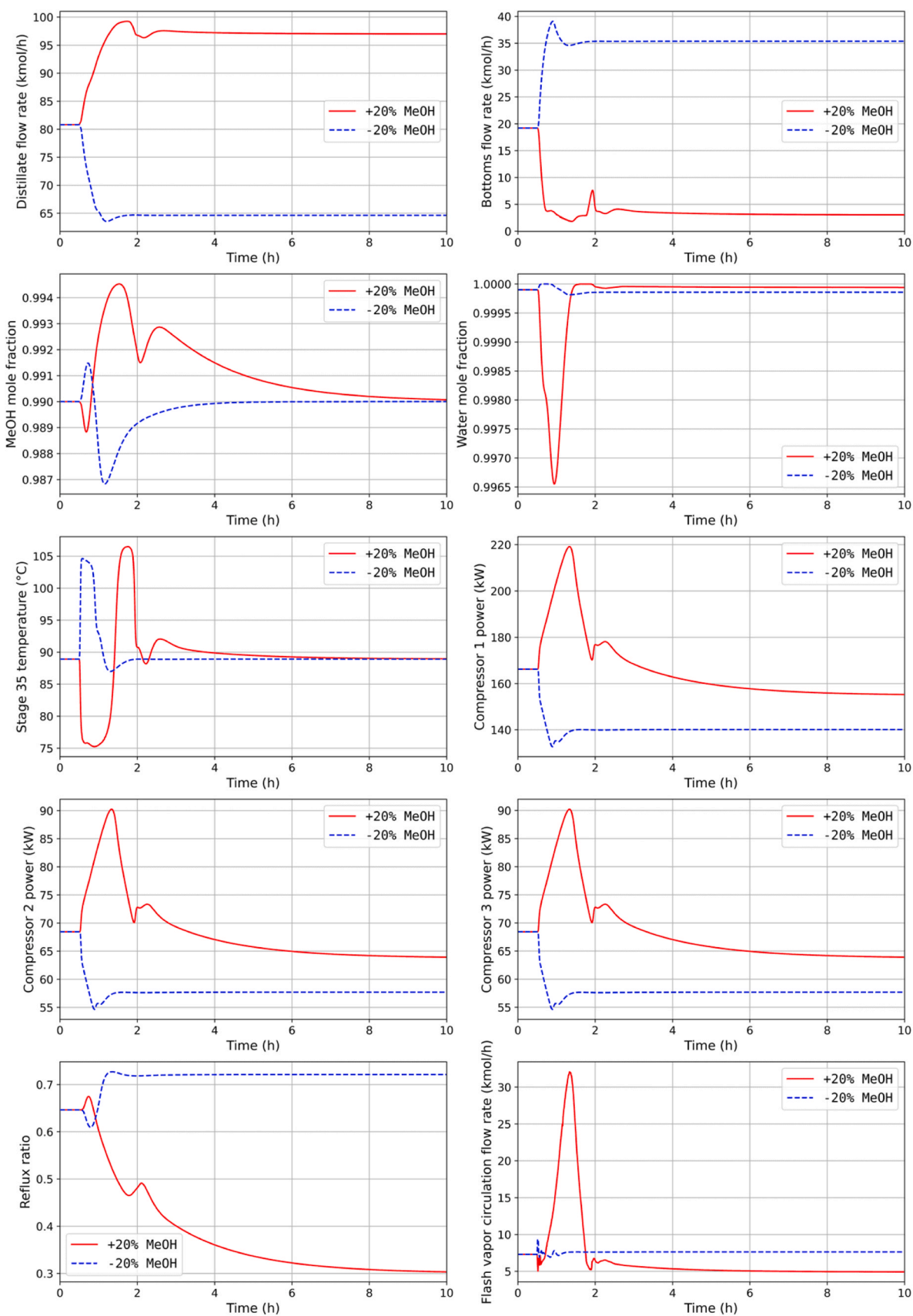


Fig. 8. Dynamic responses of CS2 under ± 20 % methanol composition disturbance.

Table 1
Settling time comparison for CS1 and CS2.

Disturbance	CS1 (MeOH)	CS2 (MeOH)	CS1 (Water)	CS2 (Water)
+ 20 % throughput	2.5 h	3.5 h	1.6 h	2.5 h
– 20 % throughput	2.5 h	4.0 h	0.5 h	1.5 h
+ 20 % MeOH	1.8 h	9.5 h	1.6 h	2.5 h
– 20 % MeOH	1.8 h	3.5 h	1.0 h	1.5 h

Table 2
IAE comparison for CS1 and CS2.

IAE	+ 20 % throughput	– 20 % throughput	+ 20 % methanol	– 20 % methanol
CS1				
IAE _{MeOH}	0.010580	0.009107	0.070604	0.100947
IAE _{Water}	0.007575	0.000274	0.002605	0.000367
IAE _{Total}	0.018154	0.009381	0.073209	0.101314
CS2				
IAE _{MeOH}	0.001212	0.003157	0.011353	0.003038
IAE _{Water}	0.009474	0.000275	0.001962	0.000435
IAE _{Total}	0.010687	0.003432	0.013315	0.003473

reboiler duty, similar to CS1. However, methanol purity is more precisely controlled in CS2 by allowing slight adjustments to the reflux ratio. The steady-state reflux ratios shift from the nominal value of 0.646–0.656 and 0.638 for + 20 % and – 20 % throughput disturbances, respectively.

Fig. 8 illustrates the process response to $\pm 20\%$ feed composition disturbances. In both scenarios, the composition controller successfully maintains methanol purity by manipulating the reflux ratio. For the – 20 % case, the required reflux ratio increases to 0.721, which is close to the nominal value, resulting in dynamic behavior similar to CS1. In contrast, the + 20 % case requires the reflux ratio to drop to 0.303, significantly lower than nominal, which leads to slow dynamics.

These results highlight that CS2 not only enhances purity regulation, but also provides improved energy flexibility. The manipulation of the reflux ratio directly corrects composition deviation and simultaneously alters the FVC flow rate, which in turn affects the reboiler duty, compression power, and overall COP. For example, under the + 20 % methanol disturbance, the FVC flow rate drops from 7.3 kmol/h to 4.9 kmol/h. The lower reflux ratio reduces the reboiler duty to 1341 kW (66 + 64 + 1211) and a compressor power to 283 kW, resulting in a COP of 4.74, which matches the nominal condition. In comparison, CS1 maintains a fixed reflux ratio and exhibits a lower COP of 3.74 under the same disturbance.

3.4. Control performance

To comprehensively evaluate the control performance of the proposed strategies, both settling time and IAE are used as performance metrics. While CS2 clearly improves product purity control and reduces energy consumption compared to CS1, it also suffers from slower dynamics, attributed to two main sources of time delay: (1) the inherent measurement lag from the online composition analyzer (assumed as 3 min in this work), and (2) transport delay induced by the variable FVC flow rate. These delays postpone the corrective action for reflux adjustment, leading to longer settling times. As shown in Table 1, under the + 20 % methanol disturbance, the settling time for methanol purity increases from 1.8 h in CS1 to 9.5 h in CS2. Despite this, the enhanced regulatory performance provided by the composition controller justifies the dynamic slowdown in applications where product quality is critical.

The impact of these control strategies is further quantified using IAE values for methanol and water mole fractions in the distillate and bottoms. As summarized in Table 2, CS2 consistently achieves lower IAE across all scenarios. For example, in the + 20 % throughput case, the total IAE for CS1 is 0.0182, while CS2 achieves a reduced value of

0.0107 (a 41.2 % improvement). Similar trends are observed in the – 20 % case, where CS2 achieves more than a 60 % reduction in total IAE compared to CS1. The performance gap is more pronounced under feed composition disturbances. For the + 20 % methanol case, CS1 exhibits a significant deviation in methanol purity (IAE = 0.0706), while CS2 maintains control with a much smaller error (IAE = 0.0114). The total IAE drops from 0.0732 in CS1 to 0.0133 in CS2 (an 81.8 % reduction). In the – 20 % methanol case, the total IAE is reduced by approximately 96.6 % (from 0.1013 to 0.0035) when switching from CS1 to CS2. These results confirm the superior performance of CS2 in disturbance rejection and product quality maintenance, especially under challenging composition variations.

Despite the promising results, some limitations of this study should be acknowledged. The case study is based on a binary methanol/water system. In industrial application involving multicomponent mixtures, the presence of additional components may introduce significant control challenges not captured in this simplified model. In addition, from an implementation perspective, CS2 requires the use of real-time composition analyzers, which introduces practical considerations related to reliability, calibration, and maintenance. In future work, the integration of soft sensors or model predictive control could help mitigate analyzer lag and further improve dynamic response.

4. Conclusions

This work presents the dynamics and control of a fully electrified distillation process using FVC configuration. The FVC eliminates the need for auxiliary heating by recycling flash vapor to boost reboiler duty. Control structures are developed and tested under $\pm 20\%$ disturbances in throughput and composition. CS1, which uses single-end temperature control with a fixed reflux ratio, achieves stable dynamic behavior and acceptable product purity in most cases. However, it exhibits slight methanol purity deviations under decreased methanol composition conditions. CS2 addresses this issue by introducing a composition controller that adjusts the reflux ratio in response to purity changes. CS2 delivers more accurate control of product specifications and improved energy flexibility, although at the cost of slower dynamics. Overall, the study confirms the feasibility of implementing robust control in FVC-based electrified distillation processes, providing a promising solution for future low-carbon chemical separation systems.

CRedit authorship contribution statement

Chengtian Cui: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Data curation, Conceptualization. **Xiaodong Zhang:** Writing – original draft, Validation, Methodology, Investigation, Formal analysis. **Meng Qi:** Writing – original draft, Validation, Methodology, Investigation, Formal analysis. **Anton A. Kiss:** Writing – review & editing, Validation, Supervision, Methodology, 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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Appendix A. Supporting information

Supplementary data associated with this article can be found in the

online version at [doi:10.1016/j.cherd.2025.07.023](https://doi.org/10.1016/j.cherd.2025.07.023).

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