

Fast Startup Dynamics of Diabatic Distillation with Electric Heating

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Abstract: The electrification of process heating presents an opportunity to decarbonize distillation column operations and enhance operational strategies to save energy. Conventional column configurations are adiabatic and have low thermodynamic efficiencies due to heat degradation. Further, the startup process for conventional columns is slow and has significant energy requirements for re-establishing steady state hydraulic, composition, and flow profiles. In this paper, a speculative fully diabatic distillation column configuration with modular electric stage heating is introduced. A dynamic simulation model is built from first principles using a compartmentalization approach for equilibrium stages, as well as a hierarchical modeling framework for column control and auxiliary heating. We demonstrate that this structure has exceptionally small startup times compared to conventional columns through a simulation case study considering the binary separation of an equimolar mixture of acetic acid/propanol, as well as illustrate its significant energy savings over the startup period, which can translate into grid-integrated operating strategies for electrified distillation systems.

Keywords: Diabatic distillation, Process electrification, Startup

1. INTRODUCTION

Distillation is a widely used thermal separation operation that consumes a significant amount of energy for process heating. Most existing distillation columns use fuel-based process heating systems to generate steam, that is typically used in the column reboiler. Fuel- and steam-based heating systems cumulatively correspond with approximately 50 percent of all onsite energy use and 30 percent of industrial emissions (Cresko et al, 2022; Orr et al, 2015); therefore, distillation contributes significantly to the carbon footprint of the chemical sector. Efforts to decarbonize distillation have mainly focused on steady-state energy reduction strategies that decrease fuel requirements rather than replace the heat source (Lee et al, 2024), such as heat-pump assisted distillation or thermally coupled columns. With the significant growth in renewable electricity generation rates from wind and solar farms, electric heating devices have the potential to eliminate carbon emissions related to distillation process heating. Recent works on electrified column configurations (Kim, Kim and Son, 2022) have considered the techno-economic aspects of retrofitting existing columns, but operational advantages that an electrified system enables for energy saving as well as the associated process dynamics, specifically for column startup, have received little attention.

Renewable electricity generation is inherently variable and grid-integrated operation involves modulating the load of electrified processes. Changes in energy input propagate to distillation process variables (liquid and vapor flow rates, temperature, pressure, product purity, etc.), leading

to complex operational challenges. From a systems-level perspective, coupled scheduling and control approaches as well as capacity planning have been proposed to address shortages in electricity supply (Palys and Daoutidis, 2022). However, at the process-level, distillation columns are largely considered to be uninterruptible, core operations that are not amenable to production cycling, let alone frequent startup and shutdown cycles.

In a different vein, conventional columns are typically treated as adiabatic, which is not true in practice since their shells are not thermally insulated. The sole heat source is the boiler at the bottom of the column, with heat removal in a condenser at the top (Fig. 1a). The minimum operational energy requirements depend on the latent heat of vaporization for the mixture components within the column and the desired product purity. Heat propagates tray-to-tray and generates a transient temperature cascade. Consequently, thermal energy is degraded owing to significant temperature differences between trays, an energy efficiency problem that is maintained, albeit to a lesser degree, at steady state. Diabatic distillation was proposed (Fonyo, 1970) as a means to conserve internal heat within the column. There are multiple stage heating sources distributed spatially in this configuration that maximize heat recovery by minimizing stagewise temperature differentials. Previous designs have utilized sequential heat exchangers or vapor recompression systems to increase internal heat transfer between column sections (Lee et al, 2024), but these energy savings schemes are limited during startup as the liquid and vapor streams would introduce additional disturbances during semi-continuous column control (Skogestad and Morari, 1988; Jørgensen, Eden, Koggersbøl and Hallager, 2000).

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Motivated by the above, we introduce a speculative modular diabatic column configuration that features distributed electric heating on each stage (Fig. 1b), providing additional degrees of freedom for modulating material flow rates between stages and substantial energy savings during column startup. We show that the diabatic column has faster startup than an adiabatic column through dynamic simulations. The concept for modular stage heating is described in Section 2 and the hierarchical models for both the adiabatic and diabatic columns are presented in Section 3, as well as an integrated framework for the control and auxiliary heating systems. Section 4 presents a simulation case study that compares the startup of adiabatic and diabatic column configurations with identical feed and product specifications. Section 5 provides concluding remarks and discusses the role of a fast startup operating strategy for a column with fluctuations in power availability.

2. MODULAR STAGE HEATING CONCEPT

2.1 Rationale

The prospect of using clean electricity to power an electric process heating system is challenged by the issue of intermittency. Unlike fuel-based process heating sources, renewable energy generation is inherently fluctuating (Li, Fang, Zeng and Chen, 2016). Current manufacturing facilities also lack the resources to reliably produce carbon-free electricity on-site at the levels required by switching to electric heating (Kirkerud, Bolkesjø and Trømborg, 2017). In response to the possibility of energy supply constraints, we consider that an electric process heating system may need to frequently shutdown when at low power capacity and startup rapidly when renewable power generation levels increase. An operational strategy for fast startup is implemented with the newly proposed concept of modular stage heating.

2.2 Conventional Shutdown/Startup Procedure

The dynamic behavior of conventional distillation columns is defined by the response of a system of interacting stages that are highly sensitive to small disturbances in process variables: liquid and vapor flows and compositions, including the feed stream. It is these interactions that become fundamentally problematic during startup, as stage hydraulics and internal flow rates must be carefully controlled to prevent unstable operation.

There are three sequential periods that describe the dynamic operating policy for a distillation column: shutdown, cooldown, and startup. The shutdown period starts at the nominal operating conditions and is described by a rapid decrease in external mass and energy flow into and out of the column to zero, closing the column system for operation at total reflux. With zero heat input, the column enters the cooldown phase and gradually loses heat to the surroundings. The pressure on each tray drops as vapor condenses while the tray holdup drains, with liquid accumulating in the lower column sections. By the time the startup protocol is initiated, stages are likely cold and empty, and the three aforementioned periods commence sequentially to re-establish internal flow, temperature, and

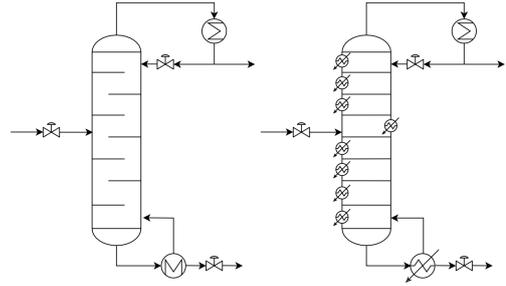


Fig. 1. Schematic representation for two distillation column configurations: (a) conventional column with a reboiler and condenser and (b) electrified column with stage-wise electric heating.

pressure profiles as well as re-start feed and output flow streams that meet desired product specifications.

The startup sequences for conventional columns are slow and energy-intensive, as individual stages operate far from their nominal conditions and internal liquid and vapor flow rates are constrained to prevent adverse hydrodynamic events that may cause mechanical or hydraulic issues. The widely accepted startup procedure is divided into three phases: discontinuous, semi-continuous, and continuous (Ruiz, Cameron and Gani, 1988). The discontinuous phase is described by cold, empty plates where heat is applied while the column operates at total reflux. Trays exhibit weeping until stage liquid-levels approach their nominal steady state values, which initiates the semi-continuous phase. This phase is defined by highly non-linear dynamics and a complex control procedure as the column transitions to the specified reflux rate (Luyben and Choi, 1987). Process variables, such as composition and internal flow rates, are highly coupled between stages and fluctuate until the column enters the continuous phase, where individual stages reach their nominal operating conditions. Adequately managing vapor-liquid flow traffic while re-establishing tray holdups is the source of the high energy requirements for column startup, but it is also an artifact of the low thermodynamic efficiency attributed to adiabatic configurations (Rivero, 2001).

During the startup of the column, heat duties in the reboiler and condenser; the reflux and boil-up stream flow rates; and the feed flow rate are the only degrees of freedom that can be manipulated to control liquid-vapor flow traffic and tray liquid level. In addition to the limited number of manipulated variables, significant hydraulic constraints translate to long startup times, high energy requirements, and loss of production. As a result, conventional columns are rarely shut down in practice.

Table 1. Fast Startup Operating Protocol

State	Step	Procedure
Shutdown	1	Switch operation to total reflux
	2	Set heat duty to zero
	3	Close valves
Cooldown	4	Column in "Stand-by"
Startup	5	Activate heaters and control T
	6	Open valves, start feed
	7	Reset reflux/boil-up ratios, control x_B, x_D
	8	Return to nominal steady-state

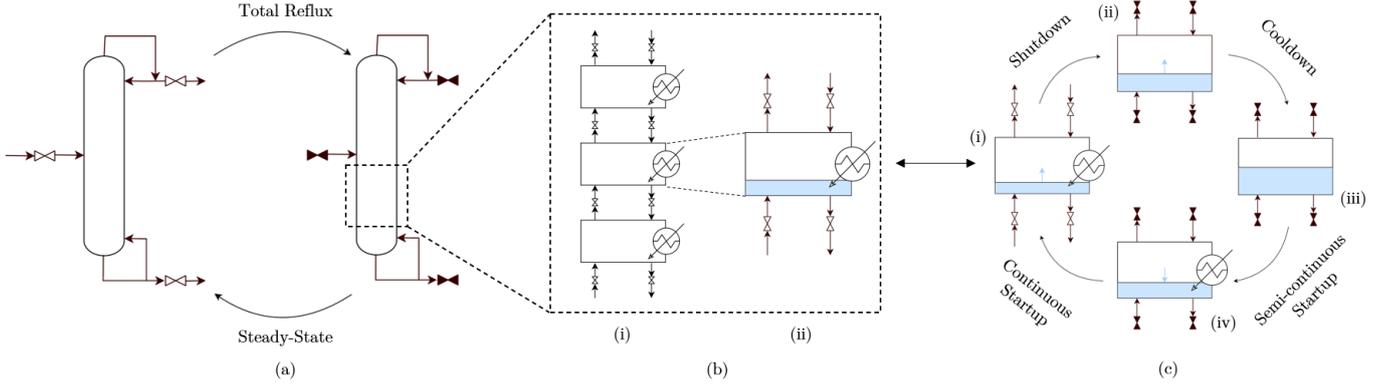


Fig. 2. Finite state machine representation for the principles of modular stage heating: (a) column operational states; (b): (i) diabolic column architecture, (ii) modular stage schematic; (c) dynamic stage operating cycle: (i) warm, open state, (ii) cool, closed state, (iii) cold, closed state, (iv) warm, closed state. "Open" valves are white and "Closed" valves are black.

2.3 Modular Column Architecture with Fast Startup

In place of interacting, adiabatic stages, we introduce a modular stage concept that is equipped with an electric heater and outfitted with control valves at the top and bottom of the stage to regulate vapor and liquid flow traffic (Fig. 2b-ii). The state of the valves is "Open" or "Closed" depending on the column state. "Open" is the default case for steady-state operation and is an interacting configuration within the column. The "Closed" case is relevant to the dynamic operating procedure as the valves quickly close and each stage becomes independent, retaining the totality of the material present at steady state. During the cooldown period, vapor condenses, and liquid level rises in each stage.

The presence of an electric heater on each stage leads to a diabatic distillation column (Fig. 2b-i). As described in Table 1 and illustrated in Figure 2c, during startup and steady-state operation, electric heaters on each individual stage are activated and their heat input is manipulated to control the stage temperature. Each stage returns to its nominal liquid levels and, by design, its nominal vapor/liquid holdups during the semi-continuous portion of startup. It is important to note that since the material holdup is retained at shutdown, the nominal composition of the material in each stage is constant for the duration of the shutdown-startup cycle. For steady-state operation, the valve setting is then switched to "open" and the stages return to interacting, with the external flow reintroduced to the column (Fig. 2a), while the control variable for the electric heaters is set to the nominal steady state temperature. The duties of the electric heaters are thus variable as internal flow is re-established until the column returns to steady-state.

The key feature for this column architecture and dynamic operating policy is that the stages skip the discontinuous phase and enter a pseudo-semi-continuous phase, having already established nominal liquid levels and compositions prior to returning to an interacting system. This simplifies the startup procedure too, as the only task becomes managing internal vapor and liquid traffic. The stage

electric heaters provide $N-2$ additional degrees of freedom for process control.

3. MODEL DEVELOPMENT

We extend the rigorous modeling framework for conventional and heat-integrated distillation columns proposed by Bisgaard et al. (2013) to simulate a diabatic distillation column with modular stage heating and fast startup policies. The model is formulated as a system of differential-algebraic equations, implements the multicomponent Wilson equation for pressure-volume (PV) flash calculations, and includes the mass, energy, equilibrium, and summation (MESH) equations.

The following assumptions are made:

- (1) ideal mixing and phase equilibrium on all stages
- (2) vapor on stages modeled as an ideal gas
- (3) total condensation of the overhead vapor (no reflux drum)

A compartmentalization approach is used to decompose the dynamic model into sub-models at three hierarchical levels: module-level (Fig. 2b-ii), column-level (Fig. 2b-i), control system-level. For brevity, only the conservation and hydraulic equations are presented for the module model while the complete set of equations for the column mixing relations and control structure are described.

3.1 Modular Stage Model

Let the set $j = 1, \dots, N_C$ denote the mixture components, and the set $i = 1, \dots, N_S$ denote the number of stages. The column model is a set of N_S modular stage sub-models. The condenser, the top-most stage, is indexed as 1 and the reboiler, the bottom-most stage, as N_S . The feed streams F_i and stage heat duties Q_i are specified. Temperature T_i and pressure P_i are calculated by stage, as well as enthalpy u_i . Constitutive relations involving the overall, liquid, vapor, and feed mole fractions, $z_{i,j}$, $x_{i,j}$, $y_{i,j}$, and $z_{i,j}^F$, respectively, describe the phase equilibrium between the vapor and liquid components of each stage. Within the energy balance, the heat loss term Q_i^{loss} accounts for heat transfer to the surroundings based on the overall

heat transfer coefficient of the wall U_{wall} and the ambient temperature T_{amb} .

Conservation Equations The conservation of mass and energy for all components considers an accumulation term to account for the overall molar holdup M_i and overall molar enthalpy u_i^{stage} on each stage:

$$\frac{dM_i}{dt} = L_{i-1} + V_{i+1} - L_i - V_i + F_i \quad (1)$$

$$\frac{dM_i z_{i,j}}{dt} = L_{i-1} x_{i-1,j} + V_{i+1} y_{i+1,j} - L_i x_{i,j} - V_i y_{i,j} + F_i z_{i,j}^F \quad (2)$$

$$\frac{dM_i u_i^{stage}}{dt} = L_{i-1} u_{i-1}^L + V_{i+1} u_{i+1}^V - L_i u_i^L - V_i u_i^V + Q_i - Q_i^{loss} \quad (3)$$

$$Q_i^{loss} = U_{wall} \cdot (T_i - T_{amb}) \quad (4)$$

Tray Hydraulics The holdup equations are necessary to describe the stage composition, temperature, pressure, and internal flow. Molar vapor flow V_i is proportional to the square root of the pressure gradient between trays i and $i - 1$. Molar liquid flow L_i is described by the Francis correlation for a segmental weir h_{weir} .

$$V_i = C^V \cdot \sqrt{|P_i - P_{i-1} + \Delta P_i|} \quad (5)$$

$$L_i = \begin{cases} f^h \cdot (h_i^L - h_{weir})^{\frac{3}{2}}, & h_i^L \geq h_{weir} \\ 0, & h_i^L < h_{weir} \end{cases} \quad (6)$$

$$h_i^L = \frac{M_T^L \cdot MW_i^L}{\rho_i^L \cdot A_t} \quad (7)$$

$$v_L = h_i^L A_t = v_T - v_V \quad (8)$$

The clear liquid height h_i^L is derived from the relation between the total liquid molar holdup M_T^L , molecular weight MW_i^L , and liquid density ρ_i^L . It is algebraically related to the stage liquid volume v_L , assuming the total stage volume v_T and plate area A_t are static and that the ideal vapor holdup is based on the difference between v_T and v_L .

3.2 Column Model

Control Valves The modular stage sub-models are connected by mixing relations to construct an interacting system.

$$V_i^{in} = g(t) \cdot V_{i+1}^{out} \quad (9)$$

$$L_i^{in} = g(t) \cdot L_{i-1}^{out} \quad (10)$$

The switching term $g(t)$ is implemented to model the valve arrangement proposed in Section 2.3.

$$g(t) = \begin{cases} 1 & \text{if "Open"} \\ 0 & \text{if "Closed"} \\ \frac{4e^{-\epsilon t}}{(1 + e^{-\epsilon t})^2} & \text{if "Switch"} \end{cases} \quad (11)$$

The "Open" state describes the general mixing relations for interacting stages while the "Closed" state describes a column with non-interacting stages. The "Switch" state uses a sigmoidal function as a smooth approximation for the dynamic transition between the "Open" and "Closed" states. The parameter ϵ characterizes the transition rate between "Open" and "Closed" states.

3.3 Control Structure

The control strategy for this column configuration involves dual-composition control and closed-loop temperature control on each stage.

External Flow Relations The distillate D and bottoms B compositions are controlled by manipulating the reflux and boil-up flow rates, which are characterized by the normalized reflux α_R and boil-up α_B ratios.

$$\alpha_R = 1 - \frac{D}{V_1} \quad (12)$$

$$\alpha_B = 1 - \frac{B}{L_{N_s}} \quad (13)$$

During shutdown, the feed is set to zero while α_R and α_B are set to 1, reducing distillate and bottoms flow to zero. The startup protocol then ramps the feed, α_R , and α_B back to nominal steady-state values through an exponential forcing function.

Modular Heating Control Electric heaters supply heat Q_i to stages $i = 2$ to N_s through a proportional-integral control scheme. Added heat is described by conductive heat transfer based on the temperature difference between the stage T_i and electric heater T_i^h .

$$Q_i = U_{wall} \cdot (T_i^h - T_i) \quad (14)$$

The heater temperature T_i^h is assumed to have a first-order dependence on the heat input signal Q_i^h to the electric heater and the resistance to heat transfer λ_h . The temperature controller calculates the error between T_i and the temperature setpoint T_i^{sp} , which is assigned as the nominal steady-state operating temperature, to manipulate the power input P_i^s . The stage disturbance variables are the vapor and liquid flows from the tray as well as heating losses.

$$\frac{dT_i^h}{dt} = \lambda_h \cdot (Q_i^h - Q_i) \quad (15)$$

$$P_i^s = K_P [T_{sp,i} - T_i + \frac{1}{T_I} \int (T_{sp,i} - T_i) dt] \quad (16)$$

Q_i^h is computed as a function of P_i^s as follows: (1) a maximum power setting $P_i^{s,max}$ is imposed and (2) the heat input must be greater or equal to zero. On/of switching

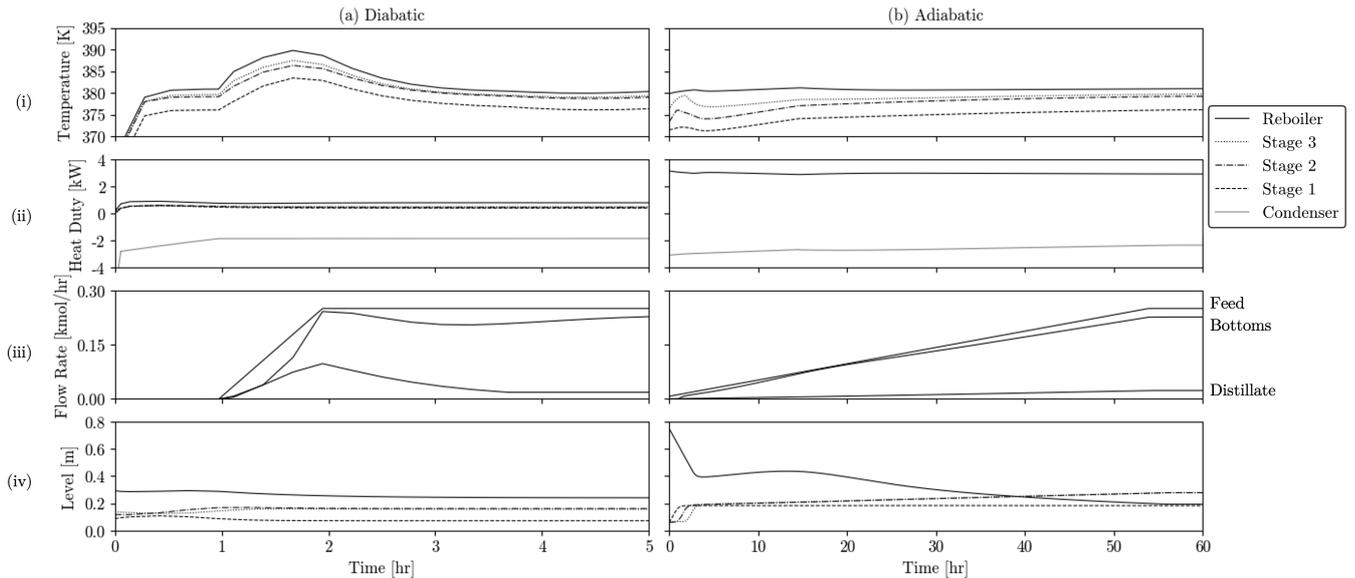


Fig. 3. Dynamic profiles of process variables during startup for (a) diabatic and (b) adiabatic columns: (i) temperature T_i , (ii) heat duty Q_i , (iii) feed F_2 , bottoms B , and distillate D molar flow rates, (iv) and liquid level h_i^L .

is also included; the "On" state enables heating, while the "Off" state sets Q_i^h to zero.

$$Q_i^h = \begin{cases} \min(\max(P_i^s, 0), P_i^{s,max}) & \text{if "On"} \\ 0 & \text{if "Off"} \end{cases} \quad (17)$$

4. CASE STUDY

In this section, we illustrate the concept of diabatic distillation column featuring modular stage heating through a dynamic simulation of the binary separation of an equimolar acetic acid/propanol mixture. To demonstrate the operational advantages of diabatic distillation, an ideal four stage column with a total condenser and one feed stream at $i = 2$ is developed for both adiabatic and diabatic configurations. The purpose of this simulation is to provide a proof-of-concept for fast startup compared to a conventional startup policy.

The models are implemented in gPROMS Process 2023.1.0, and share identical specifications for the distillate, bottoms, and feed streams, as described in Table 2. The model parameters presented in Table 3 are also equivalent between the two systems. The nominal steady-state specifications for internal flow rates, temperatures, pressures, holdups, and compositions are slightly different between the two configurations as the adiabatic column employs a sieve tray model with a $0.05 \text{ m } h_{weir}$ while the modular stage model h_{weir} is set to 0 m . It is assumed that the adiabatic trays can drain to a minimum of h_{weir} .

4.1 Fast Startup by Retaining Holdup

It is first shown that the startup time for the diabatic column is approximately 5 hours while the adiabatic column requires 57 hours. The long startup of the adiabatic column is largely attributed to re-establishing liquid holdup on each stage (Fig. 3b-iv). During adiabatic column shutdown, the upper tray holdups drain and accumulate in the reboiler. The nominal column composition

profile is also reset, as the lighter components condense and accumulate in the lower column section. The startup period then initiates when the reboiler evaporates off its holdup, coinciding with a slow return to steady-state while hydraulic conditions are carefully controlled. In contrast, the diabatic column shutdown traps the hold-up on each tray (Fig. 3a-iv), retaining its nominal composition while skipping the slow procedure to refill each stage.

Table 2. Nominal steady-state specifications

Description	Variable	Value	Unit
Feed flow	F_2	0.9	$\text{kmol} \cdot \text{hr}^{-1}$
Distillate flow	D	0.08	$\text{kmol} \cdot \text{hr}^{-1}$
Bottoms flow	B	0.82	$\text{kmol} \cdot \text{hr}^{-1}$
Distillate composition	x_{D1}	0.2	mol/mol
	x_{D2}	0.8	mol/mol
Bottoms composition	x_{B1}	0.53	mol/mol
	x_{B2}	0.47	mol/mol
Feed composition	z_i	0.5	mol/mol
Feed temperature	F_i	381.5	K
Differential pressure	ΔP_i	≤ 850	Pa
Reflux ratio	α_R	0.775	$\frac{\text{kmol}}{\text{hr}} / \frac{\text{kmol}}{\text{hr}}$
Boil-up ratio	α_B	0.215	$\frac{\text{kmol}}{\text{hr}} / \frac{\text{kmol}}{\text{hr}}$

Table 3. Model parameters

Description	Parameter	Value	Unit
V_i flow factor	C^V	$1.2 \cdot 10^{-5}$	$\text{kmol m}^{0.5} \text{kg}^{-0.5}$
L_i flow factor	f^h	43.2	$\text{kmol m}^{0.67} \text{hr}^{-1}$
Ambient temp.	T_{amb}	298	K
Switch parameter	ϵ	10^{-6}	hr^{-1}
Plate area	A	0.20	m^2
Stage height	h_L	0.55	m
Reboiler height	h_R	0.825	m
Wall coefficient	U_{wall}	0.001	$\text{W} \cdot \text{K}^{-1}$
Heater resistance	λ_h	0.056	$\text{K} \cdot \text{J}^{-1}$
Maximum power	P_i^{max}	1500	kW
Proportional gain	K_P	1000	$\text{kW} \cdot \text{K}^{-1}$
Integral time	τ_I	0.056	hr

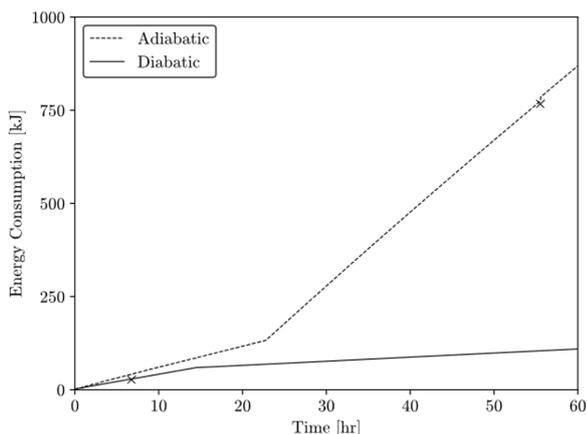


Fig. 4. Cumulative energy consumption during startup of adiabatic and diabatic columns. The \times denotes the transition from startup to steady-state.

4.2 Improved Startup Energy Efficiency

The temperature distribution of the diabatic column (Fig. 3a-i) is tighter than the adiabatic column (Fig. 3b-i), a result that is attributed to the distributed heat input to each stage (Fig. 3a-ii). The adiabatic column exhibits greater temperature fluctuations than the diabatic column when tray hydraulic conditions are being re-established. Further, control of stage-wise heat duties provides flexible reflux/boil-up rates (Fig. 3a-iii), a significant deviation from the slow ramp up of the adiabatic reflux/boil-up flow (Fig. 3b-iii).

Comparing Figures 3a-ii and 3b-ii, we observe that the diabatic setup has 30% lower power requirements at nominal steady-state operation than the adiabatic counterpart. Faster startup times also mean lower net energy requirements during transient operation. As shown in Figure 4, the startup energy consumption of the adiabatic column is eight times higher than that of the diabatic column.

5. CONCLUSION

We propose a novel speculative distillation column architecture comprising connected modular stages with individual heating. We show that this provides more precise energy delivery throughout the column while lowering overall energy consumption at steady-state. It is found reductions in startup time are significant, which will be exploited to define new grid-integrated operating strategies.

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