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The Impact of Electrified Process Heating on Process Design, Control and Operations

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ABSTRACT

We study the impact of switching from combustion heating to electric heating in processes comprising high temperature reaction/separation sequences, where the heat supporting the reaction(s) is substantially provided by combusting a reaction byproduct (fuel gas). A canonical process structure is defined. It is shown that the conventional combustion- based process presents significant interactions. An asymptotic analysis is utilized to investigate and compare the dynamic responses of the conventional and electric process configurations. It is demonstrated that the dynamic behavior of the two processes exhibits two timescales, with the faster corresponding to the evolution of the temperatures of the units with high heat duty, and the slow time scale capturing the variables involved in the material balance. A simplified ethylene cracking process example is used to demonstrate these findings.

Keywords: Energy Systems, Process Design, Process Electrification

INTRODUCTION

Process electrification using electricity generated by renewable sources has emerged as one of the routes for decarbonizing manufacturing processes [1,2]. Electrification may involve a complete change of processing technology (e.g., utilizing electrochemical reactions) [3] or upgrades and modifications of existing technology. Of particular interest in the latter area is the electrification of process heating, whereby existing combustion heaters are replaced with electric heating technologies [1,2].

Electrification can in principle eliminate combustion-heating-related CO_2 emissions and has the potential co-benefits of affording more precise/localized heating and providing additional degrees of freedom for operation and control [4]. Nevertheless, it presents several challenges. From a design perspective, electric heating may disrupt existing process integration structures, which rely on, e.g., combusting process-generated waste streams ("tail gas" or "fuel gas") to generate heat [5]. From an operation and control perspective, electric heating must account for the availability of renewable electricity, which may fluctuate during the day [6]. Motivated by the above, in this work, we provide a rigorous analysis of the design and process dynamics implications of electrified process heating in the context of integrated process systems. We note that there are other sources of CO_2 emissions in chemical/petrochemical processing (including scope 2) emissions, that are not accounted for in this work.

A prototype process structure with reaction, separation, and recycle is defined. It is shown that the conventional combustion-based process presents significant interactions due to the impact of the downstream units (via the heating value of the fuel gas) on the upstream units. An asymptotic analysis is utilized to investigate and compare the dynamic responses of the two process configurations. It is demonstrated that the dynamic behavior of the two processes exhibits two time scales, with the faster corresponding to the evolution of the temperatures of the units with high heat duty, and the slow time scale capturing the variables involved in the material balance. A simplified ethylene cracking process example is used to demonstrate these findings.

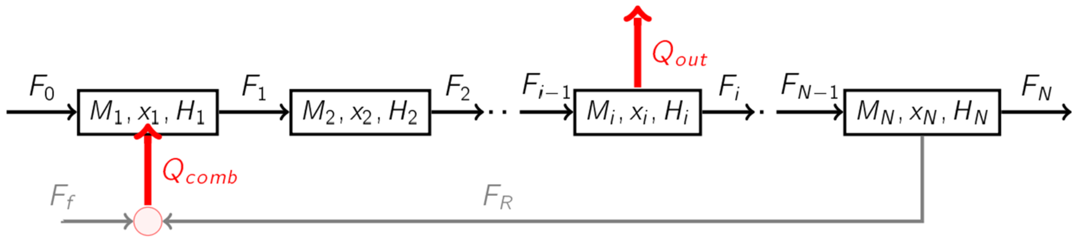


Figure 1: Structure of integrated process using combustion of fuel gas as the heat source. Black lines denote material streams connecting process units, grey lines denote streams of material used as fuel, red lines denote energy flow.

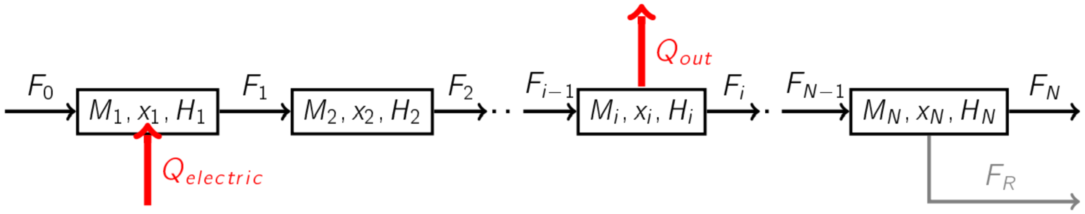


Figure 2: Structure of process with electric heating.

PROTOTYPE PROCESS

A system of N process units, each with mass holdup M, mass fraction x, and mass specific enthalpy H, connected in series is considered. The feed stream, of mass flow rate F_0 has mass specific enthalpy H_0 and contains a reactant with mass fraction x_0. The reactant undergoes a high-temperature, endothermic transformation in the first unit. Processing units 2, ... , *i - 1* follow, and heat is eventually removed/recovered from the resulting process stream in unit *i*. Finally, the product stream is obtained in unit N, along with a waste stream of flow rate F_R. The waste ("off gas", "tail gas" or "fuel gas") stream can be used as a fuel but does not have any economic value. Two process configurations are considered:

- A conventional, integrated design (Figure 1), whereby the majority of the heat required for the endothermic transformation occurring in Unit 1 is provided by combusting the fuel stream (possibly combined with a fresh fuel stream of mass flow rate F_f). The rate of heat generation by combustion is given by

  $$Q_{comb} = \lambda_f F_f + \lambda_R F_R \quad (1)$$

  where λ_f and λ_R refer to the heating values of the fresh fuel and the fuel gas, respectively. Combustion of fuel gas occurs in air, and a flue gas stream is generated (not shown in the figure).
- An electrified process configuration (Figure 2), whereby the heat required for the endothermic transformation in Unit 1 is provided by electric heating. In this case, other means to process the waste gas stream must be identified.

The structure of the two process configurations shown in Figures 1 and 2 is the same as far as material processing is concerned. From a steady state design point of view, it is important to ensure that the product streams resulting from the two configurations are the same (in terms of composition x and enthalpy H), and that the amount of heat recovered Q_{out} is the same. To this end, the rates of energy input to both processes must be the same, and the following condition must be met:

$$\bar{Q}_{comb} = \bar{Q}_{elec} \quad (2)$$

where the overbar denotes steady-state values. Note that the above condition assumes that heating is 100% efficient, that is, all the heat generated by combustion (as defined in equation (1)) or by electricity is transferred to the process. Heat transfer efficiency is lower in practice.

DYNAMIC ANALYSIS AND TIME SCALE DECOMPOSITION

The dynamic model of the process is based on the following assumptions: each unit is well-mixed, has constant holdups, constant physical properties, and has no heat loss. With these assumptions, the model of the conventional process shown in Figure 1 can be written as:

Unit 1 :

$$\frac{dx_1}{dt} = \frac{1}{M_1}[F_0x_0 - F_1x_1 + f_1(x_1, H_1)]$$

$$\frac{dH_1}{dt} = \frac{1}{M_1}[F_0H_0 - F_1H_1 + \lambda_f F_f + \lambda_R F_R + g_1(x_1, H_1)]$$

Unit 2 :

$$\frac{dx_2}{dt} = \frac{1}{M_2}[F_1x_1 - F_2x_2 + f_2(x_2, H_2)]$$

$$\frac{dH_2}{dt} = \frac{1}{M_2}[F_1H_1 - F_2H_2 + g_2(x_2, H_2)]$$

$$\vdots \qquad (3)$$

Unit i :

$$\frac{dx_i}{dt} = \frac{1}{M_i}[F_{i-1}x_{i-1} - F_ix_i + f_i(x_i, H_i)]$$

$$\frac{dH_i}{dt} = \frac{1}{M_i}[F_{i-1}H_{i-1} - F_iH_i - Q_{out} + g_i(x_i, H_i)]$$

Unit N :

$$\frac{dx_N}{dt} = \frac{1}{M_N}[F_{N-1}x_{N-1} - F_Nx_N - F_Rx_R + f_N(x_N, H_N)]$$
$$\frac{dH_N}{dt} = \frac{1}{M_N}[F_{N-1}H_{N-1} - F_NH_N - F_RH_R + g_N(x_N, H_N)]$$

The model of the electrified process in Figure 2 can be written in a similar fashion, replacing the sum $\lambda_f F_f + \lambda_R F_R$ (which represents Q_{comb}) in the energy balance of Unit 1 in equation (3) with Q_{elec}.

In order to proceed with the analysis, the following scaled entities are defined: $u_j = \frac{F_jH_j}{\bar{F}_j\bar{H}_j}$, $j = 1, \dots, N$, $u_r = \frac{F_RH_R}{\bar{F}_R\bar{\lambda}_R}$, $u_q = \frac{Q_{out}}{\bar{Q}_{out}}$.

Then, the following assumptions are made, that pertain to steady state operation (the overbar denotes again steady state values):

- Let $k_1 = \frac{\bar{F}_1\bar{H}_1}{\bar{F}_R\bar{\lambda}_R}$, and assume that $k_1 = \mathcal{O}(1)$, meaning that the amount of energy leaving unit 1 via flow is of comparable magnitude to the energy provided by combusting the waste gas.

- Let $k_0 = \frac{\bar{F}_f\bar{\lambda}_f}{\bar{F}_0\bar{H}_0}$, and assume that $k_0 = \mathcal{O}(1)$, meaning that the amount of heat provided by combusting fresh fuel is small and comparable with the amount of heat provided by convection by the feed stream.

- Let $\varepsilon = \frac{\bar{F}_0\bar{H}_0}{\bar{F}_R\bar{\lambda}_R} \ll 1$, meaning that the energy input from the feed stream is small compared with the amount of energy provided by combusting the fuel gas.

- Let $k_j = \frac{\bar{F}_j\bar{H}_j}{\bar{F}_R\bar{\lambda}_R}, j = 1, \dots, i-1$, and assume that $k_j = \mathcal{O}(1)$, meaning that the amount energy leaving unit $j = 1, \dots, i-1$ via flow is of comparable magnitude to the energy provided by combusting the waste gas stream.

- Let $I_j = \frac{\bar{F}_j\bar{H}_j}{\bar{F}_f\bar{\lambda}_f}, j = i, \dots, N$, and assume that $I_j = \mathcal{O}(1)$, meaning that the amount energy leaving unit $j = i, \dots, N$ via flow is of comparable magnitude to the energy provided by combusting fresh fuel feed.

- Let $I_\rho = \frac{\bar{F}_R\bar{H}_N}{\bar{F}_f\bar{\lambda}_f}$, and assume that $I_\rho = \mathcal{O}(1)$, meaning that the amount of energy contained in the waste stream is of comparable magnitude to the amount of heat provided by combusting fresh fuel feed.

With these definitions and assumptions, the model becomes:

Unit 1 :

$$\frac{dx_1}{dt} = \frac{1}{M_1}[F_0x_0 - F_1x_1 + f_1(x_1, H_1)]$$

$$\frac{M_1}{\bar{F}_0\bar{H}_0}\frac{dH_1}{dt} = u_0 + u_\mathrm{f}k_0 + \frac{g_1(x_1,H_1)}{\bar{F}_0\bar{H}_0} + \frac{1}{\varepsilon}(u_\mathrm{r} - k_1u_1)$$

Unit 2 :

$$\frac{dx_2}{dt} = \frac{1}{M_2}[F_1x_1 - F_2x_2 + f_2(x_2, H_2)]$$

$$\frac{M_2}{\bar{F}_0\bar{H}_0}\frac{dH_2}{dt} = \frac{g_2(x_2,H_2)}{\bar{F}_0\bar{H}_0} + \frac{1}{\varepsilon}(k_1u_1 - k_2u_2)$$

$$\vdots \qquad (4)$$

Unit i :

$$\frac{dx_i}{dt} = \frac{1}{M_i}[F_{i-1}x_{i-1} - F_ix_i + f_i(x_i, H_i)]$$

$$\frac{M_i}{\bar{F}_0\bar{H}_0}\frac{dH_i}{dt} = -I_ik_0u_i + \frac{g_i(x_i,H_i)}{\bar{F}_0\bar{H}_0} + \frac{1}{\varepsilon}(k_{i-1}u_{i-1} - k_qu_q)$$

Unit N :

$$\frac{dx_N}{dt} = \frac{1}{M_N}[F_{N-1}x_{N-1} - F_Nx_N - F_Rx_R + f_N(x_N, H_N)]$$
$$\frac{M_N}{\bar{F}_0\bar{H}_0}\frac{dH_N}{dt} = I_{N-1}k_0u_{N-1} - I_Nk_0u_N - I_\rho k_0u_\rho + \frac{g_N(x_N,H_N)}{\bar{F}_0\bar{H}_0}$$

This model is a singularly perturbed system of ordinary differential equations in standard form, and it is expected to have a dynamic behavior featuring two timescales[7]. The framework presented by Baldea and Daoutidis [7] is employed to study the dynamic behavior via an asymptotic analysis using singular perturbation arguments.

Its dynamic behavior is analyzed below, starting from the fast timescale. To this end, a new “stretched” time variable is defined as:

$$\tau = \frac{1}{\varepsilon} \qquad (5)$$

With this, the model (4) becomes:

Unit 1 :

$$\frac{dx_1}{d\tau} = \varepsilon\frac{1}{M_1}[F_0x_0 - F_1x_1 + f_1(x_1, H_1)]$$

$$\frac{M_1}{\bar{F}_0\bar{H}_0}\frac{dH_1}{d\tau} = \varepsilon\,[u_0 + u_\mathrm{f}k_0 + \frac{g_1(x_1,H_1)}{\bar{F}_0\bar{H}_0}] + u_\mathrm{r} - k_1u_1$$

Unit 2 :

$$\frac{dx_2}{d\tau} = \varepsilon\frac{1}{M_2}[F_1x_1 - F_2x_2 + f_2(x_2, H_2)]$$

$$\frac{M_2}{\bar{F}_0\bar{H}_0}\frac{dH_2}{d\tau} = \varepsilon\, \frac{g_2(x_2,H_2)}{\bar{F}_0\bar{H}_0} + k_1u_1 - k_2u_2$$

$$\vdots \tag{6}$$

Unit i :

$$\frac{dx_i}{d\tau} = \varepsilon \frac{1}{M_i}[F_{i-1}x_{i-1} - F_ix_i + f_i(x_i, H_i)]$$

$$\frac{M_i}{\bar{F}_0\bar{H}_0}\frac{dH_i}{d\tau} = \varepsilon\, [-I_ik_0u_i + \frac{g_i(x_i,H_i)}{\bar{F}_0\bar{H}_0}] + k_{i-1}u_{i-1} - k_qu_q$$

Unit N :

$$\frac{dx_N}{dt} = \varepsilon \frac{1}{M_N}[F_{N-1}x_{N-1} - F_Nx_N - F_Rx_R + f_N(x_N, H_N)]$$

$$\frac{M_N}{\bar{F}_0\bar{H}_0}\frac{dH_N}{dt} = \varepsilon\, [I_{N-1}k_0u_{N-1} - I_Nk_0u_N - I_\rho k_0u_\rho + \frac{g_N(x_N,H_N)}{\bar{F}_0\bar{H}_0}]$$

An expression of the dynamics in the fast time scale can be obtained by considering the limit case $\varepsilon \to 0$, which corresponds to the limit where the amount of heat obtained from combusting the tail gas is infinitely higher than the amount of heat derived from the combustion of fresh fuel. The fast dynamics thus take the form:

Unit 1 :

$$\frac{dx_1}{d\tau} = 0$$

$$\frac{M_1}{\bar{F}_0\bar{H}_0}\frac{dH_1}{d\tau} = u_\mathrm{r} - k_1u_1$$

Unit 2 :

$$\frac{dx_2}{d\tau} = 0$$

$$\frac{M_2}{\bar{F}_0\bar{H}_0}\frac{dH_2}{d\tau} = k_1u_1 - k_2u_2$$

$$\vdots \tag{7}$$

Unit i :

$$\frac{dx_i}{d\tau} = 0$$

$$\frac{M_i}{\bar{F}_0\bar{H}_0}\frac{dH_i}{d\tau} = k_{i-1}u_{i-1} - k_qu_q$$

Unit N :

$$\frac{dx_N}{d\tau} = 0$$

$$\frac{M_N}{\bar{F}_0\bar{H}_0}\frac{dH_N}{d\tau} = 0$$

The system of equations in (7) suggests that the variables whose dynamic response exhibits a fast component are the mass specific enthalpies (equivalently, temperatures) H_1,..., H_i of units $1, \dots, i$. Based on the assumptions made above, Unit 1 has a significant rate of heat input (via either combustion or electric heating). Heat is then conveyed to units $2, \dots, i$ until it is removed from Unit i at a rate Q_{out}. Thus, units $1, \dots, i$ represent a high energy throughput path through the process (Figure 3) [8].

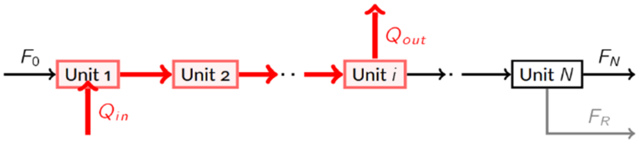


Figure 3 The fast component of the dynamics captures the energy balance of the units located in the high energy throughput pathway of the process. Q_{in} represents either Q_{comb} or Q_{elec}

The above arguments suggest that $\bar{Q}_{out}$ is of comparable magnitude to $\bar{Q}_{in}$; in the case where endothermic reactions occur in units $1, \dots, i$, the overall energy balance of the process suggests that the two quantities would differ by the heat consumed by the reactions (as reflected in the terms $g_i(x_i, H_i)$).

The dynamics in the fast time scale are influenced by the rate of energy input to the process (as reflected by the term u_r in equation (7)), the rate of energy removal (term k_qu_q in equation (7)), and are not influenced by the rate of raw material input, the production rate and the rate at which fuel is provided from external sources.

It is of note that, even though the dynamics of the variables in the energy balance of units $1, \dots, i$ are fast, the dynamic response of the individual units may be different; in other words, the time constants $\frac{M_j}{\bar{F}_0\bar{H}_0}$, $j = 1, \dots, i$ in equations (7) may be quite different.

The slow component of the dynamics evolves in time scale t. Considering the same limit $\varepsilon \to 0$ in the original (slow) time scale t gives rise to the following constraints:

$$0 = u_\mathrm{r} - k_1u_1 \tag{8a}$$

$$0 = k_1u_1 - k_2u_2 \tag{8b}$$

$$\vdots$$

$$0 = k_{i-1}u_{i-1} - k_qu_q \tag{8c}$$

These constraints correspond to a quasi-steady state of the fast dynamics and describe a manifold/subspace where the slow dynamics of the process evolve. By considering these constraints and substituting (8) in equation (6), the slow component of the dynamics can be described as:

Unit 1 :

$$\frac{dx_1}{dt} = \frac{1}{M_1}[F_0x_0 - F_1x_1 + f_1(x_1, H_1)]$$

$$\frac{M_1}{\bar{F}_0\bar{H}_0}\frac{dH_1}{dt} = u_0 + u_\mathrm{f}k_0 + \frac{g_1(x_1,H_1)}{\bar{F}_0\bar{H}_0}$$

Unit 2 :

$$\frac{dx_2}{dt} = \frac{1}{M_2}[F_1x_1 - F_2x_2 + f_2(x_2, H_2)]$$

$$\frac{M_2}{\bar{F}_0\bar{H}_0}\frac{dH_2}{dt} = \frac{g_2(x_2,H_2)}{\bar{F}_0\bar{H}_0}$$

$$\vdots \tag{9}$$

Unit i :

$$\frac{dx_i}{dt} = \frac{1}{M_i}[F_{i-1}x_{i-1} - F_ix_i + f_i(x_i, H_i)]$$

$$\frac{M_i}{\bar{F}_0\bar{H}_0}\frac{dH_i}{dt} = -I_ik_0u_i + \frac{g_i(x_i,H_i)}{\bar{F}_0\bar{H}_0}$$

Unit N :

$$\frac{dx_N}{dt} = \frac{1}{M_N}[F_{N-1}x_{N-1} - F_N x_N - F_R x_N + f_N(x_N, H_N)]$$

$$\frac{M_N}{\bar{F}_0\bar{H}_0}\frac{dH_N}{dt} = I_{N-1}k_0u_{N-1} - I_N k_0 u_N - I_\rho k_0 u_\rho + \frac{g_N(x_N,H_N)}{\bar{F}_0\bar{H}_0}$$

The model of the slow dynamics describes the evolution of the variables in the material balance (notably the product composition x_N, influenced by the product flow rate F_0), as well as the evolution of the slow component of the energy balance of the process.

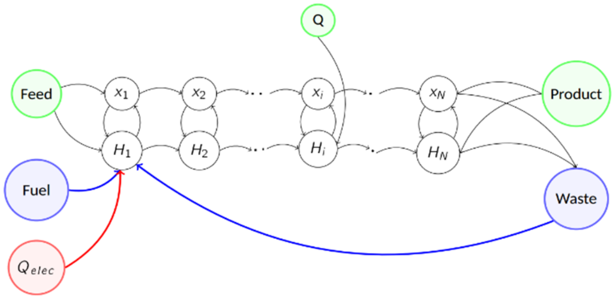


Figure 4 Directed graph of the dynamic model of the prototype process. Nodes and edges specific to the integrated process using combustion of fuel gas as the heat source are shown in blue. Nodes and edges specific to electric heating are shown in red. The green and black nodes/edges are common to the two digraphs.

OPERATIONAL IMPLICATIONS OF ELECTRIFICATION

The implications of the analysis presented earlier are discussed in this section. The presence of a two time scale behavior suggests that these processes lend themselves quite naturally to a two-tiered control and operational decision-making structure.[7] The management of energy use (including temperature control of Units $1, \dots, i$) should be pursued in the fast time scale, while the control and management of production (in terms of production rate, product purity) should be pursued in the slow time scale [7]. The latter can also involve production scheduling.

The fast dynamics (7) of Units $1, \dots, i$ means that changes in the rate of heat input to Unit 1 will be quickly reflected in the temperatures and compositions of units $2, \dots, i$. The impact on units $i+1, \dots, N$ will be apparent more slowly. In addition to deliberate operator (or control intervention), changes in the heat rate to Unit 1 can be caused by disturbances and constraints. The origin of these may be exogenous (from outside the process) or endogenous (from within).

To further investigate the impact of these disturbances and constraints on the heat rate, the structure of the two prototype processes is considered. Figure 4 shows the directed graph (digraph) of the system model (3). The fundamental difference between the conventional and electrified processes lies in the presence of a cycle in the graph of the conventional process, reflecting the fact that the heat rate provided to the Unit 1 depends on the composition x_N of the waste stream. Consider equation (7), and specifically the term u_r, that reflects the energy input due to combustion of the tail gas. The definition of u_r, i.e., $u_r = \frac{F_R H_R}{\bar{F}_R \bar{\lambda}_R}$, indicates that rate of energy input is a function of λ_R, the lower heating value of the waste gas. The lower heating value is a function of the composition of the waste gas, and hence of the variable x_R. x_R is, in turn, affected by (effectively any and all) disturbances affecting the process, from Unit 1 to Unit N. Thus, a feedback effect is present, whereby variables in the *downstream* sections of the process impact the *upstream* units. Additionally, the dynamics of x_R evolve exclusively in the slow time scale, meaning that this feedback effect will occur over a long-time horizon.

In the process with electric heating, the heat rate to Unit 1 is completely independent of the downstream units of the process and constitutes an additional degree of freedom for controlling/optimizing the process operation. On the other hand, given the goal of using *renewable* electricity for process heating implies that the rate of heat input may be subject to upper bounds that are lower than the nominal steady state value.

CASE STUDY: ETHYLENE CRACKER

Thermal cracking of hydrocarbon feedstock to obtain ethylene is one of the most energy-intensive chemical processes and one of the largest carbon emitters in the chemical industry. Its decarbonization potential lies in replacing the conventional combustion-based furnace with an electric furnace [9]. Relevant research efforts are underway in both industry and academia [10,11].

Ethylene crackers are highly integrated, and the byproducts of the cracking reactions (methane, hydrogen) constitute an important fraction of the fuel used to heat the cracking reactor (which operates at high temperatures, of around 900°C) [5,12], and the heating value of the fuel gas stream depends on its composition (and ultimately on the operation of the reactor, as argued above).

Ethylene plants are complex and comprise extensive separation sections. We use a simplified representation for the purpose of investigating the dynamic implications of electrified process heating. The model consists of three units: reactor, intermediate unit, and separator, with the latter two serving as a proxy for the separation section. The dynamics of each unit are represented by the material and energy balances, under similar assumptions as listed in developing the model (3), with the exception that holdups are not constant.

The reactor unit is fed with pure ethane. The complex reactions occurring in industrial furnaces are approximated using a simplified two reaction scheme, a reversible reaction emulating the cracking transformation, and the degradation of product ethylene; we utilize methane as a proxy of the hydrocarbon degradation products:

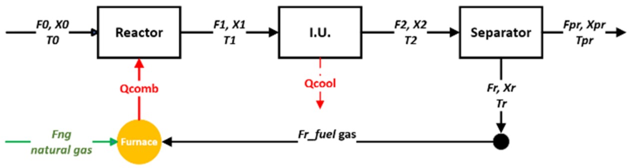
$$C_2H_6 \leftrightarrow C_2H_4 + H_2$$

$$r_1 = k_{0,1} C_{C_2H_6} \exp\left(\frac{-Ea_1}{RT}\right), r_{-1} = k_{0,-1} C_{C_2H_4} C_{H_2} \exp\left(\frac{-Ea_{-1}}{RT}\right)$$

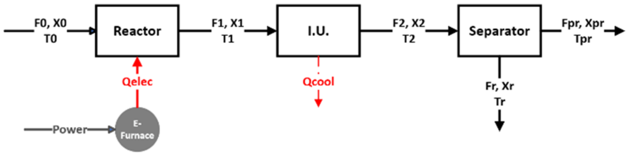
$$C_2H_4 \rightarrow C_xH_y$$

$$r_2 = k_{0,2} C_{C_2H_4} \exp\left(\frac{-Ea_2}{RT}\right) \qquad (10)$$

with r_m referring to reaction m = 1,2 and -1.



(a) Conventional Plant Configuration



(b) Electrified plant configuration

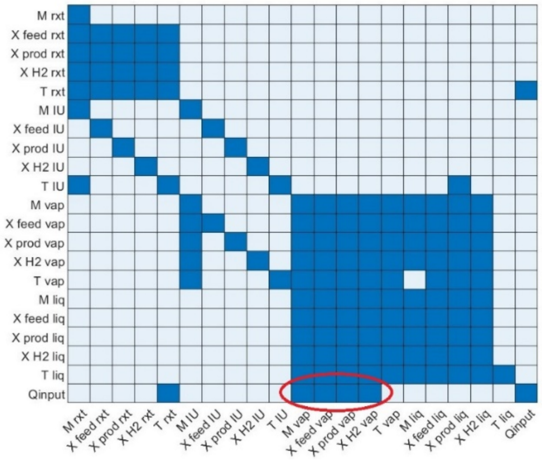
Figure 5. Structure of the ethylene cracker prototype model

The product stream consists of unreacted ethane, product ethylene, and by-products methane and hydrogen. The reactor is modeled as a CSTR with the appropriate material and energy balances.

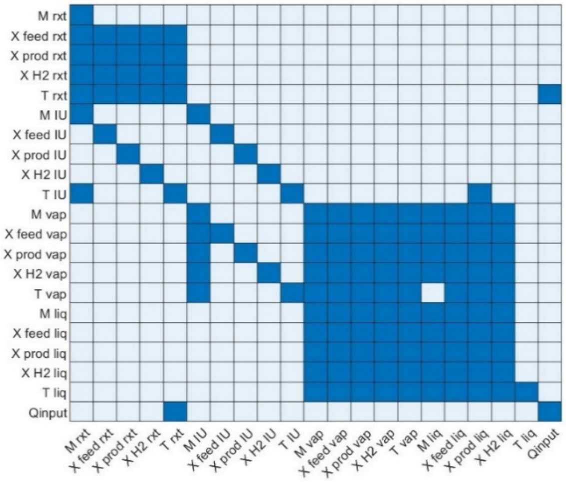
The intermediate units (I.U.) are intended to capture the (largely physical) transformations occurring post cracking, including the product quench step (represented as heat exiting the block Q_{cool}). The material and energy balances follow first order dynamics. A significantly larger holdup is used in the unit compared to that of the reactor, to reflect the large time constant of the separation section of an ethylene plant.

In the separation block, by-products hydrogen and methane are separated from the product (in this case, ethane and ethylene) and recovered to use as fuel. The unit is modeled as a rate-based separation with vapor and liquid holdups, with by-product fuel gas exiting as the vapor stream and ethylene and unreacted ethane exiting as the liquid product stream.

In the conventional system, the fuel gas is recycled to be combusted in the furnace, providing heat for the cracking reaction. The fuel gas composition, which determines the lower heating value (computed as a linear combination of individual heat values multiplied by their compositions in the fuel gas, $LHV = \sum_j X_{vap,j} LHV_j$), and the corresponding energy input to the reactor, depends on the performance of the reactor and separator. On the other hand, in the electrified system case, the energy is supplied to the reactor from a source outside the process and thus independent of the performance of the process itself.



Structure of matrix A for the integrated process



Structure of matrix A for the electrified process

Figure 6. Structure of system matrix A of the linearized process model

Holdup and temperature controllers were implemented in each unit to stabilize holdups and temperatures. Simple P controllers that manipulate outlet flowrates were implemented for holdup control. For temperature control, PI controllers were implemented to manipulate the heat supply to the units. An additional purity controller is implemented in the liquid phase of the separator to control the mass fraction of the product ethylene in the product stream by manipulating the temperature setpoint in the intermediate units.

An initial analysis focused on model structure; the two models (for the conventional and electrified processes) were linearized around their nominal steady states. The structure of the system matrices A in both cases is shown in Figures 6. As shown in Figure 6a, the matrix for the linearized model of the integrated process features additional non-zero entries that correspond to the impact of the states related to the composition of the fuel gas on the heat input rate to the reactor, as discussed above and confirming the findings of the graph-theoretical analysis and the structure of the graph in Figure 4.

Subsequent simulations focused on process dynamics. As an example, a 5°C increase in the reactor temperature setpoint, imposed at t = 1 h is shown and discussed.

Figure 7 shows the behavior of reactor temperature in the two systems. In both systems, the controller settings and the tuning parameters are identical, and the difference in the behaviors would arise solely due to the process structure. The reactor corresponds to Unit 1 in the theoretical analysis and is therefore a unit in the high energy-throughput path. Two-time scale behavior is expected in the integrated model with high energy recycle throughput via combustion of by-product fuel gas. In the electrified case, the setpoint is tracked accurately and quickly, corresponding to the fast dynamics of the temperature variable. On the other hand, in the conventional case, the dynamic behavior is more complex, with the fast dynamics being followed by a slower evolution of the temperature towards the set-point, which, as explained earlier, is due to the (slow) feedback effect linking the composition changes in the reactor and separator to the heating value of the fuel gas.

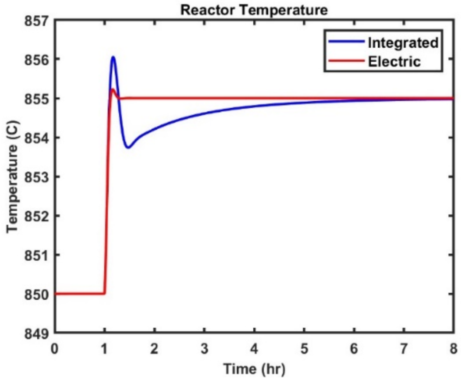


Figure 7. Reactor temperature profile subject to reactor temperature setpoint increase of 5 °C.

CONCLUSIONS

In conclusion, the effects of electric heating on process structures and dynamics were studied theoretically and were demonstrated using simulation results. Through singular perturbation analysis, the multiple time-scale behavior was predicted in conventional systems with mass- energy recycling via combustion of waste products, whereas such behavior was expected to disappear in new electrified heating systems. The theoretical results were proven via simulations depicting a conventional ethylene cracker model with tail gas recycle and an electric cracker model.

DIGITAL SUPPLEMENTARY MATERIAL

The Matlab implementation of the model is freely available on GitHub at https://github.com/Baldea-Group/EthylenePlant/ .

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NOMENCLATURE

Acronym

LHV	Lower heating value [kJ/kg]

Uppercase

A	Linearized system matrix
C	Concentration [mol/m^3]
E_a	Activation Energy [kJ/mol]
F	Mass flowrate [kg/s]
H	Mass enthalpies [kJ/kg]
I	Scaled variable
M	Mass holdup [kg]
N	Total number of units in the prototype process model
Q	Heating / cooling rate [kW]
T	Temperature [^{o}C]

Lowercase

f	Transformation in mass fraction in each unit
g	Transformation in mass enthalpy in each unit
i	Unit at which cooling occurs
u	Scaled input
k	Scaled energy flow
k_0	Rate constant
x	Mass fraction

Greek Letter

ε	Singular perturbation parameter
λ	Heating value [kJ/kg]
τ	Stretched time variable for the fast dynamics [s]

Subscript

$comb$	Combustion
$elec$	Electric heating
f	Fresh fuel stream
j	Units, streams [1,2,... i,... N]
m	Reactions [1,2,-1]
q	Heating / cooling flow
R	Recycle fuel gas flow

Superscript

⬚	Steady state

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