Interactions between process design and process control: Passive cooling in a micro refinery process

Authors:

Mahdi Sharifian, Nicolas Hudon, Gregory S. Patience

Date Submitted: 2022-10-31

Keywords: process control, micro refinery, passive cooling

Abstract:

A micro refinery unit at Polytechnique Montreal converts natural gas to diesel range fuel as the main product in two high pressure and high temperature reacting units. First, it transforms methane to syngas by catalytic partial oxidation (CPOX) at 20 bar and 800?C. Then, it produces the medium-chain hydro-carbons from syngas by Fischer-Tropsch (FT) reaction at 20 bar and 300?C.
The aim of this study is to evaluate the impact of passive intercooling on the performance and robustness of a pre-set control configuration for this sequence of interconnected chemical reactors. We simulate the whole process in Aspen Plus v8.4 and first design a PI temperature controller for the Fischer-Tropsch re-actor in Aspen Plus Dynamics. As the FT process is highly exothermic, the controller is essential to properly remove the heat generated in the reactor. Despite being feasible in simulations, the closed-loop results suffer from many shortcomings, notably with respect to process constraints.
The impact of intercooling on the closed-loop dynamics is studied by decoupling thermally the reactors using a passive intercooler to remove the excess heat from the syngas at the exit of the CPOX reactor.
Simulation results show that intercooling improves the performance of the FT operation and reduces the control cost as it keeps the control system far from the cooling flow constraints in the FT reactor. In this case, the controller has an acceptable performance against the step changes in temperature and has a built-in robustness against underestimated heat exchange within the FT process.

Record Type: Published Article

Submitted To: LAPSE (Living Archive for Process Systems Engineering)

Citation (overall record, always the latest version):	LAPSE:2022.0088
Citation (this specific file, latest version):	LAPSE:2022.0088-1
Citation (this specific file, this version):	LAPSE:2022.0088-1v2

CSChE Systems & Control Transactions
Open Access | Original Research

Conference Proceedings
Canadian Chemical Engineering Conference 2022
October 23-26, Vancouver, BC, Canada

PSEcommunity.org/LAPSE:2022.0088

PSE PRESS

Interactions Between Process Design and Process Control: Passive Cooling in a Micro Refinery Process

Mahdi Sharifian[a], Nicolas Hudon[b], Gregory S. Patience[a]*

[a] Polytechnique Montreal, Department of chemical engineering, Montreal, Quebec, Canada
[b] Department of chemical engineering, Queens University, Kingston, ON
* Corresponding Author: Gregory-s.patience@polymtl.ca

ABSTRACT

A micro refinery unit at Polytechnique Montreal converts natural gas to diesel range fuel as the main product in two high pressure and high temperature reacting units. First, it transforms methane to syngas by catalytic partial oxidation (CPOX) at 20 bar and 800°C. Then, it produces the medium-chain hydrocarbons from syngas by Fischer-Tropsch (FT) reaction at 20 bar and 300°C.
The aim of this study is to evaluate the impact of passive intercooling on the performance and robustness of a pre-set control configuration for this sequence of interconnected chemical reactors. We simulate the whole process in Aspen Plus v8.4 and first design a PI temperature controller for the Fischer-Tropsch reactor in Aspen Plus Dynamics. As the FT process is highly exothermic, the controller is essential to properly remove the heat generated in the reactor. Despite being feasible in simulations, the closed-loop results suffer from many shortcomings, notably with respect to process constraints.
The impact of intercooling on the closed-loop dynamics is studied by decoupling thermally the reactors using a passive intercooler to remove the excess heat from the syngas at the exit of the CPOX reactor.
Simulation results show that intercooling improves the performance of the FT operation and reduces the control cost as it keeps the control system far from the cooling flow constraints in the FT reactor. In this case, the controller has an acceptable performance against the step changes in temperature and has a built-in robustness against underestimated heat exchange within the FT process.

Keywords: process control, micro refinery, passive cooling

Date Record: Original manuscript received October 14, 2022. Published October 19, 2022.

INTRODUCTION

The energy demand is growing dramatically as the world's population keeps on increasing and economies proceed [1]. Since the capacity of the exploitable oil is decreasing, other virgin resources such as associated and stranded gas reservoirs are notably marked [2]. Among these options, Gas-to-Liquid (GtL) processes have the potential to transform the natural gas or associated gas into the higher-value hydrocarbons as synthetic fuel. In particular, the liquid synthetic fuels are promising alternatives of oil-related transportation sector since the price of crude oil gradually rises while its reservoirs are going to finish [3]. However, large scale industrial GTL plants are not always economical as in most cases, building a commercial plant needs a huge investment resulting in the plant to be infeasible. Moreover, in some areas, providing the industrial utilities such as water resource and electricity is limited or sometimes impossible.

In such cases, to exploit the gas reservoir and convert it to the added value fuels, micro-scale GTL process which is called Micro Refinery Unit (MRU) is feasible as it needs a lesser investment and consume much lower utility as well. The FT reaction is highly exothermic [4, 5] and one of the main challenges of such reactions is having a safe and accurate start up and to provide a stable operation [6]. Among research on the reactor design and configuration to improve the heat removal from FT process, a few studies focused on the design of temperature controller [7]. An appropriate feedback control throughout the process is essential to prevent runaway reaction which causes catalyst deactivation, loss of selectivity and conversion and/or loss of operability that can induce the reactor explosion [8, 9].
In this paper, we first describe the overall CPOX/FT process. We first consider PI control for the temperature of the FT reactor. We then consider the combination of passive cooling and PI control to regulate the temperature of the FT reactor. Finally, we study via simulations the impact of heat exchange uncertainty on the closed-loop dynamics.

PROCESS OVERVIEW AND CHALLENGE

The process consists of thermal-sustained catalytic partial oxidation (CPOX) at 800°C and 20 bar to convert the natural gas into syngas (H_2 and CO) and Fischer-Tropsch reaction (FT) at 300°C to produce diesel from syngas on Iron-based catalyst. The FT reactor is a coiled fluidized bed. To remove the generated heat and adjust the temperature of FT reactor, a control system is considered to manipulate the cooling water flow through the coil. Two challenges in the design of FT section are:

- To decrease the temperature of the syngas from CPOX to FT reactor.
- To improve the performance of the temperature controller against the disturbances in the syngas feed to the FT reactor.

Hence, we develop a simulation-based controller design by Aspen Plus Dynamic v8.4 in two scenarios; with a passive intercooler between the reactors and without it and then compare the results of FT temperature to complete the design based on the efficient method.

PROCESS CONTROL

Modeling and simulation

We first solve the gas to liquid (GtL) process in steady state. A Gibbs reactor resembles the CPOX by considering all the possible components in the product. To simulate the fluidized bed FT reactor, we applied a CSTR and attached a Longmuir-Hishelwood-Hougen-Watson (LHHW) kinetics [10] which is adopted to the experimental data of RIPI for the commercialized iron-based catalyst [11, 12]. Thus, the governing stoichiometry and kinetics for the Fischer-Tropsch and water gas shift (WGS) reactions are:

$$\mathrm{FT:}\ \ 9\mathrm{CO} + 19\mathrm{H_2} \rightarrow \mathrm{C_9H_{20}}\ (\mathrm{C^*}) + 9\mathrm{H_2O} \tag{1}$$

$$\mathrm{WGS:}\ \mathrm{CO} + \mathrm{H_2O} \rightarrow \mathrm{CO_2} + \mathrm{H_2} \tag{2}$$

$$r_{FT} = K_{FT}\frac{P_{H_2}P_{CO}}{P_{CO} + a_{FT}P_{H_2O} + b_{FT}P_{CO}} \tag{3}$$

$$r_W = K_W\frac{P_{CO}P_{H2O} - \frac{P_{H_2}P_{CO_2}}{K_P}}{P_{CO} + a_w P_{H_2O} + b_w P_{CO_2}} \tag{4}$$

$$K_i = k_i^{\circ}\, exp\left(-\frac{E_i}{RT}\right) \tag{5}$$

$$ln(K_P) = \frac{4578}{T} - 4.33 \tag{6}$$

C^* is the mixture of hydrocarbons in the product stream based on [12]. Table (1) shows the parameters of the equations (3) to (6).

Table 1. Kinetic parameters of FTs

Parameter	Value	Unit
k_{FT}°	2.1×10^{-3}	kmol/(kg. s. Pa)
E_{FT}	86	$kJmol^{-1}$
a_{FT}	1.25×10^{-7}	Pa^{-1}
b_{FT}	7×10^{-6}	Pa^{-1}
k_W°	1079.4	kmol/(kg. s. Pa)
E_W	132	$kJmol^{-1}$
a_W	2.78×10^{-6}	Pa^{-1}
b_W	1.23×10^{-5}	Pa^{-1}

The intercooler cools down the syngas stream from 800ºC to 300ºC which is the operating temperature of fluidized bed FT reactor. Table 2 summarizes the characteristics of the MRU.

Table 2. Specifications of the FT reactor

Spec	Value
FT reactor dimensions (mm)	200×1600
Coil diameter (in.)	3/4
Coil length (m)	12
Density of the Iron catalyst (kg/m^3)	1290
Bed porosity	0.6
Catalyst diameter (m)	2×10^{-4}
Air flow (mole/h)	1190
Natural gas flow (mole/h)	500

Equations (7, 8) determine the heat transfer coefficient as well as inlet and outlet temperature of cooling water through the internal coil of FT reactor.

$$Q = UA\Delta T_{LM} = \dot{m}_c\left(T_{c,o} - T_{c,i}\right) \tag{7}$$

$$\Delta T_{LM} = \frac{\left(T_b - T_{c,i}\right) - \left(T_b - T_{c,o}\right)}{\ln\left(\frac{T_b - T_{c,i}}{T_b - T_{c,o}}\right)} \tag{8}$$

The resulted values for $T_{c,i}$ and $T_{c,O}$ as well as liquid holdup of the coil required for the dynamic simulation are filled in the dynamic sheet of the CSTR in Aspen Plus.

Next, we switch to the pressure driven mode and export the simulation to the dynamic module.

Control strategy

A temperature control module is attached to the reactor based on the “heating medium flow” as the process variable. Then, we applied the internal model control technique to tune the parameters of a PI controller [13]. Figure (1) represents the process flow diagram in the dynamic mode.

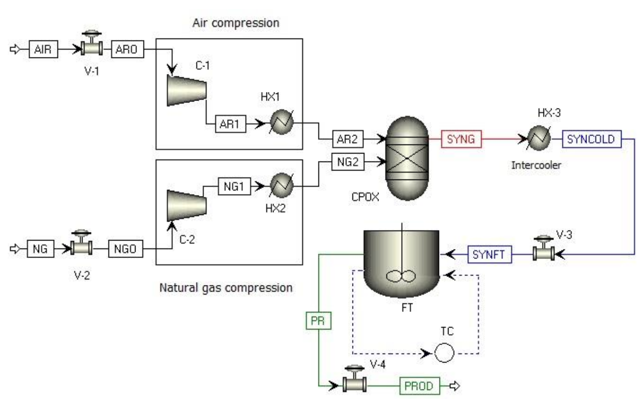

Figure 1. Process flow of MRU in Aspen Plus Dynamics V8.4

RESULTS AND DISCUSSION

Steady-state simulation and heat transfer functions determine the characterizations of the cooling coil (Table 3).

Table 3. Computed parameters of FT for the dynamic simulation

Spec	Value
Q_{FT} , kW	12.3
$\dot{m}_c, kgh^{-1}$	540
UA, WK^{-1}	167
$T_{c,i}$, °C	208
$T_{c,o}$, °C	226
T_{app}, °C	74

In the dynamic mode, a step change in the output variable (cooling flow rate) in the open loop determines the parameters of the PI controller (Figure 2).

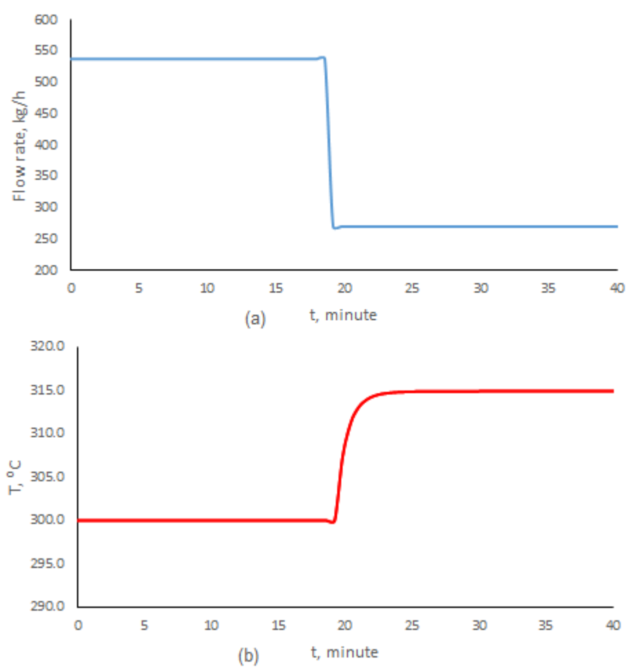

Figure 2. Open-loop response of the FT temperature, (a) step change in coolant flow rate, (b) temperature response.

Thus, the transfer function of the FT process is:

$$G(s) = \frac{0.06e^{-0.005s}}{0.92s + 1} \tag{9}$$

And the parameters of the PI controller are $K_c = 18.1$ and $\tau_I = 0.92\ minute$.

Control without passive cooling

To investigate the impact of passive cooling system, first we removed the intercooler by putting the duty of HX3 equal to 0 in the dynamic simulation meaning no change in the temperature of syngas to FT reactor (800°C). In this case, the simulation shows that the control system of FT fails to recover the desirable temperature of FT process (Figure 3).

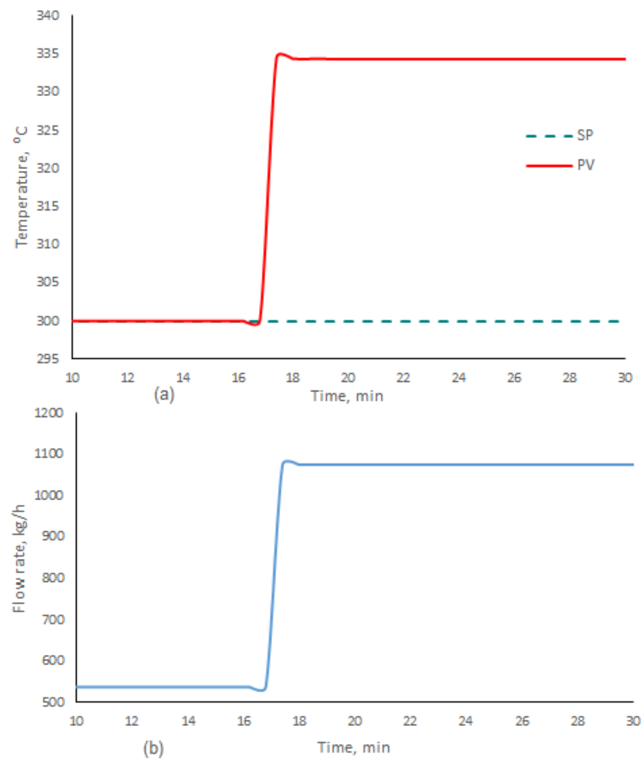

Figure 3. Response of the temperature controller in case of no passive cooling, (a) FT temperature and set point, (b) coolant flow rate. SP is setpoint and PV is the process variable.

Therefore, designing the process without passive cooling not only damage the catalyst, also cause a control failure and reaction run away.

Control with passive cooling

In this case, we keep the intercooler, HX3 (Figure 1) between the reactors to decrease the syngas temperature and make it close to the operating temperature of the FT reactor (300°C). However, HX3 has no automatic temperature control and the coolant flow rate is adjusted in the start-up by a manual valve.

Step change in the set point

The response of the FT temperature against ±5°C in the set point confirms that the controller has an appropriate performance in case of involving the passive cooling (Figure 4).

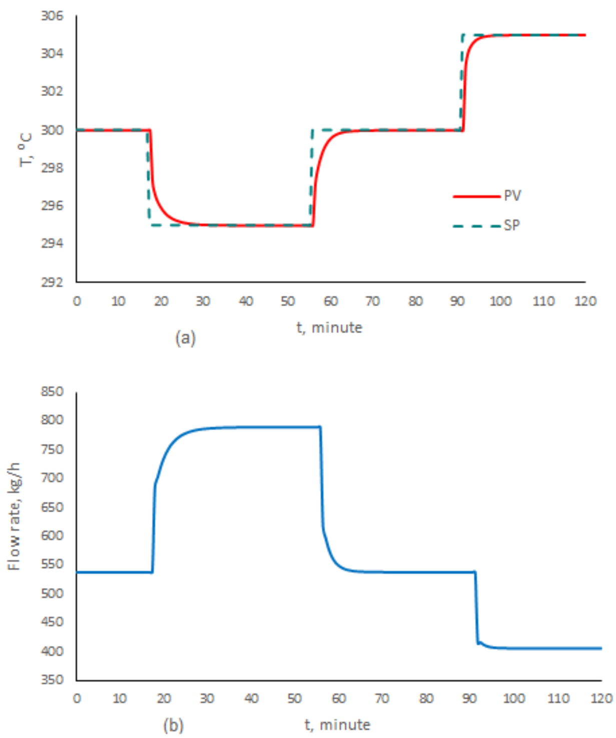

Figure 4. Closed loop response of the FT temperature by ±5°C in set point, (a) temperature variation, (b) coolant flow rate as the control output

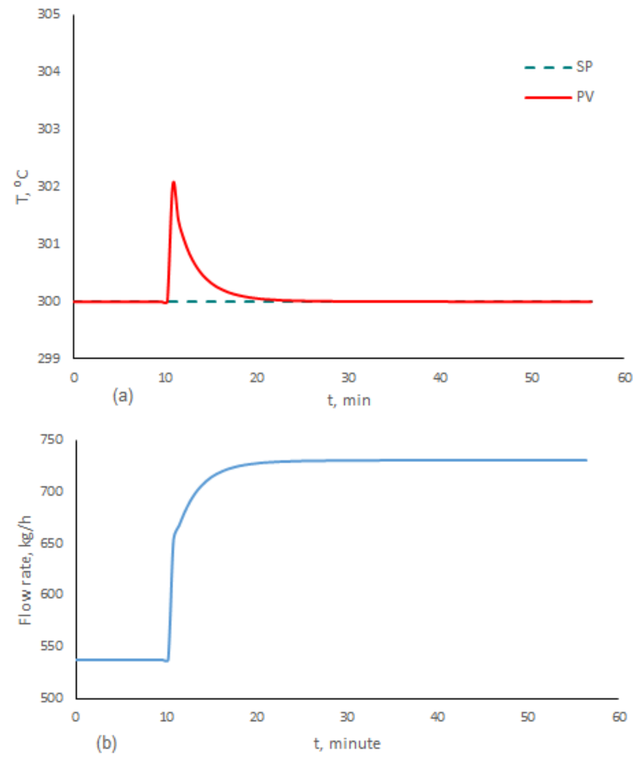

Figure 5. Closed loop response of the FT temperature in case of 10% thermal inefficiency of the intercooler, (a) temperature and set point in FT, (b) coolant flow rate as the control output.

Disturbance in the syngas temperature

The temperature of the syngas entering the FT reactor may changes due to an upstream variation or insufficient heat transfer across the intercooler. We simulate this case by decreasing the heat duty of HX3 by 10% which rises the temperature of SYNFT from 300°C to 350°C (Figure 1). The results show that the controller properly recovers the set temperature inside the FT reactor (Figure 5).

It also reconfirms the positive impact of the passive cooling in the design of MRU. Although the intercooler may not perfectly cool down the syngas stream up to the operating temperature of the FT, it assists the temperature controller to adjust the temperature and concentrations in FT reactor.

Robustness of the controller

One challenge in the modeling and simulation of the FT synthesis as an exothermic process is the uncertainty of the overall heat transfer coefficient (U) since the real value is higher than what is obtained from the correlations [14].

We increased the UA as the manipulated variable in Aspen dynamics by 10%. According to the results, the controller is capable to adjust the temperature on its set point if U is underestimated (Figure 6).

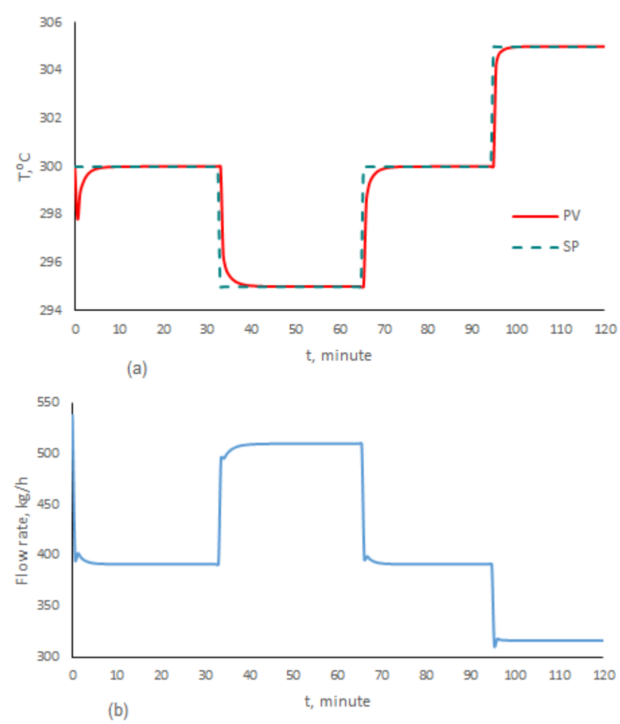

Figure 6. Robustness of the temperature controller against 10% increase in overall heat transfer coefficient between the cooling coil and the reactor, (a) FT temperature, (b) coolant flow rate

CONCLUSION

A micro refinery process was simulated by Aspen plus dynamics v8.4. This process consists of CPOX and FT both of which are exothermic reactions. Thus, the designing a proper cooling system improves the operability and efficiency of the process. In the conceptual design, we considered a passive intercooler between the two reactors to cool down the syngas stream into the operating temperature of the iron catalyzed FT reaction. The CPOX is simulated by a Gibbs reactor and the FT reactor is simulated by a CSTR. For the FT process, we combine a practical LHHW kinetic model with heat transfer between the internal cooling coil and the fluidized bed of FT reactor. Then we design a PI temperature controller based on the dynamic behavior of FT to remove the generated heat inside the reactor. The results show that involving a passive intercooler improves operability of the FT reactor, prevent reaction runaway, and gently decreases the thermal shocks through the reactor. In addition, the control system is robust in case of underestimation of overall heat transfer coefficient and is capable to recover the temperature of FT reactor against the step change in the set point and disturbances in the temperature of the feeding syngas to FT reactor. It is notable that the controller needs to change the cooling water flow rate so much just to change a few on the temperature which mainly refers to the strong exothermic nature of the FT reaction. Hence, other cooling alternative such as evaporative cooling might be more appropriate.

ACKNOWLEDGEMENTS

This project is supported by Canada research chair in high temperature, high pressure heterogeneous catalysis.

REFERENCES

1. Wood DA, Nwaoha C, Towler BF. Gas-to-liquids (GTL): A review of an industry offering several routes for monetizing natural gas. *J. Nat. Gas Eng.* 9:196–208 (2012).
2. Ostadi M, Dalane K, Rytter E, Hillestad M. Conceptual design of an autonomous once-through gas-to-liquid process—Comparison between fixed bed and microchannel reactors. *Fuel process. technol.* 139: 186–195 (2015).
3. Sudiro M, Bertucco A. Production of synthetic gasoline and diesel fuel by alternative processes using natural gas and coal: Process simulation an optimization. *Energy*. 34(12):2206–2214 (2009).
4. Zhang X, Qian W, Zhang H, Sun Q, Ying W. Effect of the operation parameters on the Fischer–Tropsch synthesis in fluidized bed reactors. *Chin. J. Chem. Eng.* 26(2):245–251 (2018).
5. Rafiq MH, Jakobsen HA, Schmi R, Hustad JE. Experimental studies and modeling of a fixed bed reactor for Fischer–Tropsch synthesis using biosyngas. *Fuel process. technol.* 92(5):893–907 (2011).
6. Haugwitz S, Hagander P. Challenges in start-up control of a heat exchange reactor with exothermic reactions; a hybrid Approach. *IFAC Proc. Volumes*. 39(5):185–190 (2006).
7. Méndez CI, Ancheyta J. Modeling and control of a Fischer-Tropsch synthesis fixed-bed reactor with a novel mechanistic kinetic approach. *J. Chem. Eng.* 390:124489 (2020).
8. Caetano R, Lemos MA, Lemos F, Freire F. Modeling and control of an exothermal reaction. *J. Chem. Eng.* 238:93-99 (2014).
9. Schweitzer JM, López-García C, Ferré D. Thermal runaway analysis of a three-phase reactor for LCO hydrotreatment. *Chem. Eng. Sci.* 65(1):313–321 (2010).
10. Zimmerman WH, Bukur DB. Reaction kinetics over iron catalysts used for the fischer-tropsch synthesis. *Can. J. Chem. Eng.* 68(2):292–301 (1990).
11. Marvast MA, Sohrabi M, Zarrinpashne S, Baghmisheh G. Fischer-Tropsch Synthesis: Modeling and performance study for Fe-HZSM5 bifunctional catalyst. *Chem. Eng. Technol.: Industrial Chemistry-Plant Equipment-Process Engineering-Biotechnology.* 28(1):78–86 (2005).
12. Rahmati M, Mehdi M, Bargah Soleimani M. Rate equations for the Fischer-Tropsch reaction on a promoted iron catalyst. *Can. J. Chem. Eng.* 79(5):800–804 (2001).
13. Seborg DE, Edgar TF, Mellichamp DA, Doyle III FJ. Process dynamics and control. John Wiley & Sons, 2016.
14. Zhang Y, Wei Q. CPFD simulation of bed-to wall heat transfer in a gas-solids bubbling fluidized bed with an immersed vertical tube. *Chem. Eng. Process.: Process Intensification.* 116:17–28 (2017).

This conference proceeding has not been peer reviewed.