Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Modeling and Simulation of a Novel Process that Converts Low Density Polyethylene to Ethylene

Xiaoyan Wang[a], Omar Almaraz[a], Jianli Hu[a] and Srinivas Palanki[a*]

[a]Department of Chemical and Biomedical Engineering, West Virginia University,
Morgantown, WV 26506, USA
* Corresponding Author: srinivas.palanki@mail.wvu.edu

ABSTRACT

In this research, a novel process is developed that utilizes low density polyethylene from plastic waste to produce ethylene. In this process, waste polyethylene is reacted in a microwave reactor to produce ethylene. A conceptual flowsheet based on this reactor is developed in the ASPEN Plus environment. Heat integration tools are utilized to reduce the hot and cold utilities used in this process. This novel design is compared with the conventional process of making ethylene from ethane via cracking. A technoeconomic analysis is conducted to demonstrate the economic feasibility of this process.

Keywords: Ethylene, Process Design, Process Development

INTRODUCTION

Plastics are used in a wide variety of products and have displaced other materials – such as wood, metal, and glass – that were previously used for applications that plastics are currently used. The worldwide annual production of plastics has increased nearly 200-fold to 400.3 million metric tons in 2022 from 2 million metric tons in 1950 [1]. While plastic products have a service-life of around 10 years, plastics can take up to 500 years to decompose, depending on their composition and disposal. Most of the plastic waste generated is either landfilled or incinerated. It takes a long time for landfilled plastic waste to degrade, and incinerated plastic waste generates harmful air pollutants. Mismanaged plastic waste is mainly disposed of at illegal dumpsites or burned in open pits, while a considerable amount also leaks into rivers and oceans. From 1970 to 2019, an estimated 30 million metric tons of plastics have accumulated in the ocean, while more than 100 million tons have accumulated in rivers and lakes [1]. Such large amounts of plastic waste pollution in waterways can have a devastating impact on marine life and ecosystems.

In this research, a novel process is developed in which waste low-density polyethylene (LDPE) is converted into ethylene using a microwave reactor. A conceptual flowsheet for this reactor-based process is developed in the ASPEN Plus environment that is at industrial-scale. Heat integration tools are applied to optimize the use of hot and cold utilities in the process. This innovative design is compared with the current industrial production method of ethylene via ethane steam cracking to evaluate the cost constraints of the microwave reactor.

PRODUCTION OF ETHYLENE

While ethylene was traditionally produced via steam cracking of petroleum (naphtha) at 800–900°C (1,470–1,650°F), followed by separation to isolate ethylene from the resulting gas mixture, there is an increasing trend to use ethane, derived from natural gas, to produce ethylene via steam cracking [2]. Ethane forms a major component of natural gas liquids (NGL) that is obtained from shale gas while purifying methane. This NGL feed stream is pre-heated by a heat exchanger, mixed with steam, and then further heated to its incipient cracking temperature (500°C to 680°C). At this point, it enters a reactor (typically, a fired tubular reactor) where it is heated to cracking temperatures, 750°C to 875°C. After cracking reaction, cracked gas mixture leave the furnace at 750°C to 875°C. The gases must be cooled immediately in the quench tower to preserve the current composition of the gas and prevent undesirable side reactions. After the

cracked gas mixture has been cooled in the quench tower and compressed, it is sent to the fraction section at a pressure of 464 to 551 psi (32-38 bar) for further separation into different products and fractions at specified qualities. This is done through a series of distillation columns and results in the separation of ethylene from the unreacted ethane, as well as the side products propylene, hydrogen and methane. Steam cracking of ethane is an energy intensive process due to the high reaction temperature (> 800°C). Furthermore, this process generates a significant amount of greenhouse gas (GHG) emissions and utilizes a non-renewable hydrocarbon feed resource. The process generally results in approximately 1.2 to 1.6 tons of CO_2-equivalent (CO_2e) per ton of ethylene produced [2,3].

The availability of a large amount of plastic waste provides the motivation to develop technologies to convert this waste product to ethylene instead of using ethane from non-renewable sources to produce ethylene. Tertiary recycling uses chemical and thermochemical methods to recover various components of waste plastic into monomers or fuels. This type of recycling is called “upcycling” as the waste plastic is converted back to monomeric forms of molecules that can be further processed into useful forms (polymeric or otherwise). The depolymerization process involved in upcycling of plastics can be enhanced by the use of catalysts, which promote deep cracking of primary products and accelerate the breaking of C–C and C–H bonds, resulting in high yields of liquid products with enhanced combustion performance and high-quality fuel production in a shorter time and at lower temperatures (280–500°C) compared to pure pyrolysis [4]. The products from catalyzed depolymerization processes include a mix of gasoline hydrocarbons (C5-C12), aromatics, light olefins, and other chemical feedstocks. Suitable catalysts and process conditions can be chosen for commercial applications to target the recovery of specific desired products.

The depolymerization process requires energy and different forms of thermal energy can utilized. The efficiency of this thermal energy utilization can vary significantly depending upon the type of energy. There is current interest in the use of microwave heating as a source of energy for depolymerization reactions. Microwave is a form of electromagnetic wave with perpendicular oscillating electric field and magnetic field that result in heat generation via (1) dielectric heating, (2) Joule heating, and (3) inductive heating. Compared with traditional hydrocarbon-based jacketed reactors as well as more novel resistive-heating reactors, microwave heating provides advantages in utilization efficiency, rapid heating, and lower bulk temperatures during reaction. For instance, it has been shown in laboratory-scale experiments that microwave-enhanced ethane catalytic cracking can produce the same conversion of ethane as conventional thermally heated cracking at an average temperature that is 150-200°C lower [5,6].

This provides the motivation to develop a process that utilizes polyethylene as a feed source in a microwave reactor to produce polymer-grade ethylene.

PROCESS MODELING

Conventional Production of Ethylene via Ethane Steam Cracking

A process simulation model is developed for the conversion of ethane to ethylene based on current industry practice [7]. This model is used as a basis of comparison for studying the advantages and disadvantages of the novel microwave-enhanced process for producing ethylene from LDPE. Ethylene is produced via thermal steam cracking of ethane gas. A process flow diagram based on industrial practice is shown in Figure 1.

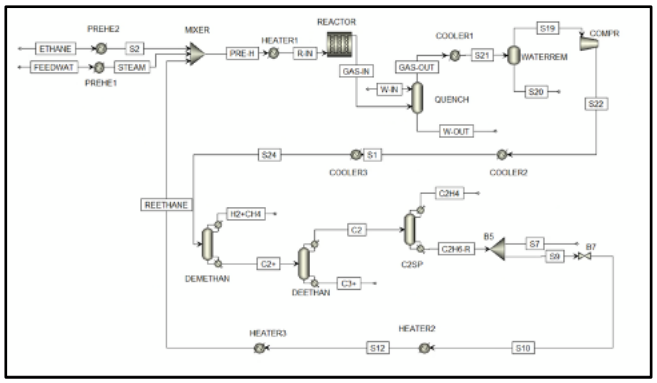

Figure 1: Process Flow Diagram for Ethane Cracking

The feed to the production process is ethane gas that comes from an ethane gas pipeline. Fresh ethane gas is fed into the process at a rate of 149 tons/h. The ethane gas is mixed with 50 tons/h of process steam to achieve a steam to hydrocarbon ration of 0.33 by mass and passed through the thermal stream cracking reactor at inlet conditions of 700 °C and 3.2 bar. The reaction conditions are 840 °C and 3.2 bar in the reactor. Under these conditions, the thermal steam cracking reaction occurs in the absence of a catalyst, converting the ethane feedstock into a gas mixture containing primarily ethylene, methane, hydrogen, and residual ethane. The exit gases from the reactor are cooled and sent through a flash unit to remove water. The organic vapors are compressed and sent through a series of three distillation columns. The top product of the last column is polymer-grade ethylene.

A simulation model is developed in ASPEN Plus v11 for this process. The feed specifications are listed in Table 1. The reaction kinetics [7] used in this model are shown in Table 2 and the reactor specifications are shown in Table 3. The Grayson thermodynamic property

model is used for this module. The flash unit and the three distillation columns utilize the Soave-Redlich-Kwong thermodynamic property model and rigorous modeling tools are used (e.g. RADFRAC) to model these separation units.

Table 1: Feed Specifications for Ethane Cracking

Component	Ethane	Steam	Initiator
Pressure (bar)	3.21	3.21	2,010.00
Temperature (°C)	700.00	700.00	0.00
Flow Rate (kmol/hr)	3,259.77	2,517.82	0.84
Flow Rate (tons/hr)	149	50.00	0.20

Table 2: Kinetics of Ethane Cracking

No	Reaction	Order	Forward Reaction	Reverse Reaction
			A [s^{-1}] or [L (mol s)$^{-1}$]	A [L (mol s)$^{-1}$]
			E [kJ mol^{-1}]	E [kJ mol^{-1}]
1	$C_2H_6 \leftrightarrow C_2H_4 + H_2$	1	A = 4.6 x 10^{13} E = 272.8	A = 8.49 x 10^{8} E = 136.5
2	$C_3H_6 \leftrightarrow C_2H_2 + CH_4$	1	A = 7.2 x 10^{12} E = 274.2	A = 3.81 x 10^{8} E = 147.2
3	$C_2H_2 + C_2H_4 \rightarrow C_4H_6$	2	A = 1.0 x 10^{15} E = 172.6	
4	$C_2H_4 + C_4H_6 \rightarrow C_6H_6 + 2H_2$	2	A = 8.3 x 10^{9} E = 144.6	
5	$C_3H_8 \leftrightarrow C_3H_6 + H_2$	1	A = 5.8 x 10^{10} E = 214.6	A = 9.03 x 10^{5} E = 93.5
6	$C_3H_8 + C_2H_4 \rightarrow C_2H_6 + C_3H_6$	2	A = 2.5 x 10^{13} E = 247.1	
7	$2C_3H_6 \rightarrow 3C_2H_4$	1	A = 7.3 x 10^{12} E = 268.5	
8	$2C_2H_6 \rightarrow C_3H_8 + CH_4$	1	A = 3.8 x 10^{11} E = 273.0	
9	$C_4H_{10} \leftrightarrow C_4H_8 + H_2$	1	A = 1.6 x 10^{12} E = 260.9	A = 1.78 x 10^{7} E = 135.1
10	$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$	2	A = 7.0 x 10^{13} E = 252.8	
11	$C_3H_6 + C_2H_6 \rightarrow C_4H_8 + CH_4$	2	A = 1.0 x 10^{14} E = 251.8	

Table 3: Ethane Cracking Reactor Specifications

Reactor Specifications	
Pressure (bar)	3.2
Temperature (°C)	840
Length (m)	10.5
Diameter (m)	0.085
No. of Tubes	240
Heat Duty MW	132.81

The product gas from the reactor unit is 40.35 mol% ethylene, 41.75mol% hydrogen, 3.97 mol% methane, 11.67 mol% unreacted ethane and with slight impurities of other products. The results closely align with the industrial data available in literature [8] as shown in Table 4. The outlet gas of the cracking reactor is cooled down to 10 °C with the help of a quench tower. The condensed water vapor is separated from the bottom in a flash separator. Vapor products from the flash separator are compressed to 8 bars and then cooled down to -100 °C. This stream is sent to the demethanizer column where methane and hydrogen are separated as top products.

Table 4: Comparison of Simulation with Industrial Data

Main Products	Product Yield [mol %]		
	Simulation	Industrial Data	% Diff.
H_2	37.47	36.49	2.69
CH_4	4.75	8.42	43.59
C_2H_4	34.41	33.07	4.05
C_2H_6	19.89	18.86	5.46

The bottom products are sent to the deethanizer column, where ethane and ethylene flow out of the top of the column while the remaining (undesired) products are separated from the bottom of the column. Finally, the top product stream is sent to the final column where ethylene is separated as the top product from ethane. The purified ethylene (99.97mol%) is recovered at 8 bar and -58.4 °C. The unreacted ethane is recovered from the bottom of the column and recycled back to the feed stream. The columns specification for ethylene separation are listed in Table 5.

Table 5: Column Specifications

	Columns		
	DEMETHAN	DEETHAN	C2SPLIT
Purpose	Distillation	Distillation	Distillation
No. of Stages	10	24	50
Feed Stage	5	10	27
Feed Temperature (°C)	-100	-50.8	-42.68
Pressure (bar)	8	8	8
Reflux Ratio	1.4	0.38	4.05
Condenser Duty (MW)	-18.17	-5.85	-28.73
Condenser Temperature (°C)	-156.89	-42.68	-58.4
Distillate Rate (kmol/h)	3068.65	4126.49	2492.85
Reboiler Duty (MW)	19.70	20.51	22.57
Reboiler Temperature (°C)	-50.80	82.87	-39.02
Bottom Rate (kmol/h)	4194.48	67.99	1631.33
Tray Spacing (m)	0.8 (2-4)	0.6 (2-9)	0.85 (2-26)
	1 (5-10)	0.8 (10-23)	0.85 (27-49)
Tray Type	Sieve	Sieve	Sieve
Column Diameter (m)	3.3 (2-4)	3.1 (2-9)	4.5 (2-26)
	3.5 (5-10)	3.5 (10-23)	3.6 (27-49)

Figure 2 shows the temperature and composition profiles of ethane and ethylene in the final distillation column. Since the reactor outlet matches industrial data closely and the final product results in polymer-grade ethylene, this simulation model is of high-fidelity and can be used in a technoeconomic analysis to compare with the economics of producing ethylene via a novel microwave process that utilizes LDPE.

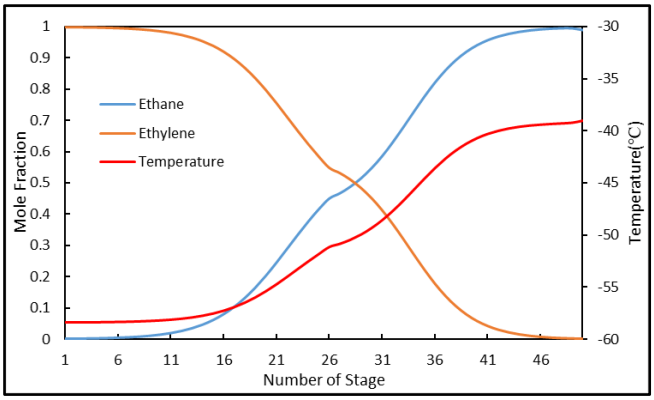

Figure 2: Temperature and Composition Profiles for Ethylene and Ethane in column C2SPLIT

Microwave Enhanced Catalytic Conversion of LDPE to Ethylene

The focus of this section is the development of an ASPEN Plus simulation for the microwave-enhanced process to convert LDPE to ethylene. The objective is to match the same ethylene production as the conventional ethane cracking process in terms of quantity as well as product purity. A process flow diagram of the microwave process under consideration is shown in Figure 3. The reactor in the conventional process is replaced by a microwave reactor and a suitable distillation train is designed to recover the ethylene.

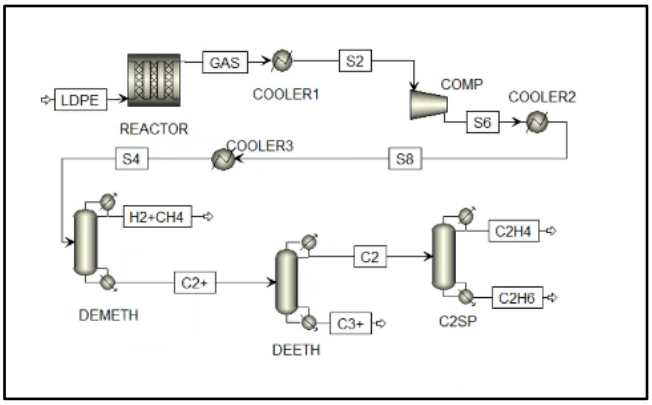

Figure 3: Flow Diagram of Microwave Enhanced Process for Converting LDPE to Ethylene

Preliminary data from laboratory-scale microwave reactor experiments [9] indicates that the product composition of the reactor under microwave heating with LDPE as feed is not the same as the product composition of conventional heating with ethane as feed as shown in Table 6. In particular, the microwave reactor produces a significant amount of propylene, which is also a valuable product, in addition to ethylene. This implies that the separation train specifications for the microwave process will be different from that of the conventional ethane-to-ethylene process. If propylene is included as a target product, additional costs for distillation to recover propylene, as well as the associated profits, will need to be considered. If the cost of recovering propylene is not competitive, it is necessary to redesign the microwave reactor to produce more ethylene and less propylene.

Table 6: Reactor Outlet Composition

Gas components (ton/h)	$LDPE/N_2$	Ethane
	MW	Conventional
	400°C	840°C
Hydrogen	2.06	6.05
Methane	16.58	6.10
Ethylene	77.29	77.29
Ethane	16.21	47.90
Acetylene	0.09	0.00
Propane	8.42	0.99
Propylene	54.37	7.87
C4 and higher	39.15	2.81

In the novel microwave process, it is necessary to determine the feed rate of LDPE as well as the separation train design that results in the same amount of polymer-grade ethylene as the conventional process (77 tons/h). This allows for a comparison of capital cost, operating cost and life-cycle cost for the two processes. It was determined that a feed of 214 tons/hour of LDPE was required to produce the required amount of ethylene (77 tons/h) in the microwave reactor. The reactor is modeled as a yield reactor that has the same outlet composition as shown in Table 6. The reactor is assumed to operate at a temperature of 400 °C and a pressure of 1 bar. The outlet of the reactor is cooled and sent to a demethanizer column, followed by a deethanizer column, and finally to an ethylene column, similar to the separation process used in conventional ethane steam reforming product separation. In addition, an extra column is designed to recover propylene. The columns specifications for this process are listed in Table 7. Figure 4 shows the temperature and composition profile of ethylene from the C2 splitter.

ECONOMIC EVALUATION

Aspen Energy Analyzer (AEA) V11 is used to develop and optimize a HEN for both the conventional as well as the novel process. The software employs a pinch analysis technique in the optimization algorithm to compute overall matches with heat load, surface area and cost target. The objective function of the HEN is to minimize utility cost, which is formulated as a mixed integer linear programming (MILP) problem. The solution consists of the

best set of matches rather than a single match.

Table 7: Column Specifications for Microwave Enhanced Process

	Columns		
	DEMETHAN	**DEETHAN**	**C2SPLIT**
Purpose	Distillation	Distillation	Distillation
No. of Stages	15	24	60
Feed Stage	6	10	31
Feed Temperature (°C)	-100	-40.85	-54.52
Pressure (bar)	8	8	8
Reflux Ratio	0.74	0.47	2.39
Condenser Duty (MW)	-3.14	-4.67	-19.09
Condenser Temperature (°C)	-142.54	-54.52	-58.4
Distillate Rate (kmol/h)	1864.76	2991.49	2501.02
Reboiler Duty (MW)	9.3	17.35	17.38
Reboiler Temperature (°C)	-40.85	22.85	-39.29
Bottom Rate (kmol/h)	4960.87	1969.38	490.47
Tray Spacing (m)	0.6 (2-5)	0.6 (2-9)	1 (2-30)
	1 (6-14)	0.9 (10-23)	1 (31-59)
Tray Type	Sieve	Sieve	Sieve
Column Diameter (m)	1.7 (2-4)	2.7 (2-9)	3.85 (2-30)
	2.6 (5-10)	3.2 (10-23)	3 (31-59)

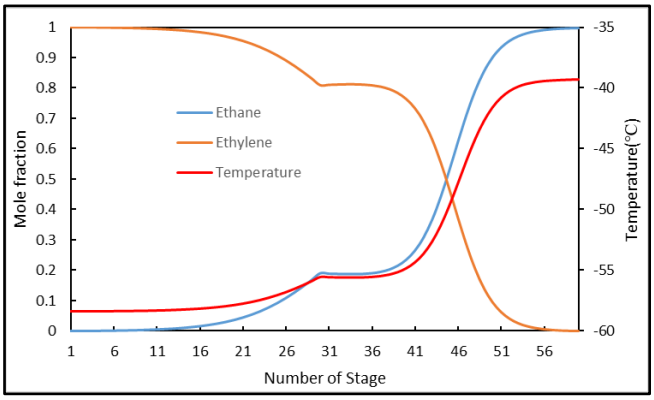

Figure 4: Temperature and Composition Profiles for Ethylene, Ethane in C2 splitter

Capital costs for standard equipment items were estimated by mapping the equipment items from the Aspen Plus plant-wide model to Aspen Process Economic Analyzer (APEA) V11. Costs for the microwave-assisted reactor (MW-reactor) was estimated separately as quoted equipment in APEA, broken down into the magnetron (including other electrical ancillaries) and pressure vessel. The magnetron cost, including electrical ancillaries, accounts for components such as the cavity, generator, controls, transformers, switches, installation, and setup, obtained from a vendor based on the power (kW) rating [10]. The pressure vessel cost was estimated using correlations from Turton et al [11]., considering the material of construction and operating pressure. Additional costs, such as assembly, commissioning, and markup, were accounted for with escalations, given the novel state of MW-assisted reactor technology. Utilities such as electricity, cooling water, steam, and flow rates of raw materials were obtained from the Aspen Plus process model.

A comparison of capital cost, operating cost, and utility cost between conventional steam reforming and microwave-enhanced LDPE upcycling (excluding the reactor component) is conducted as shown in Table 8. The objective of this comparison is to estimate the cost constraints of the microwave reactor necessary to ensure that the microwave-enhanced LDPE upcycling process is economically comparable to the conventional ethylene production process.

Table 8: Comparison of Capital and Operating Costs

Scenario	Capital Cost (USD/Year)	Operating Cost (USD/Year)	Utility Cost (USD/Year)	Product
Conventional Ethane Steam Reforming	36,557,700	48,770,700	42,463,100	Ethylene
LDPE Conversion (MW/ excluding reactor)	18,313,500	5,063,400	2,921,440	Ethylene

Currently a microwave reactor at industrial scale is not available for the proposed LDPE microwave enhanced conversion process and hence it is difficult to estimate its cost accurately. A rough estimate the microwave reactor cost based on magnetron price and reactor materials can be used as a first step. The LDPE feed rate of 214 ton/h is required to meet the ethylene production rate of 77 ton/h to match the ethylene production in the conventional ethane-to-ethylene process. The overall cost of the microwave reactor systems depends on the number of magnetron units needed to generate the necessary power requirement. As the batch time lowered down, the magnetron cost declines proportionally. When the batch time is 10 minutes, the magnetron cost is approximately $11 million as shown in Table 9. As this time is lowered, the cost of the microwave reactor systems falls further. Table 9 shows that if the batch time for the microwave-enhanced LDPE conversion process is reduced to less than 10 minutes, it has the potential to be competitive with conventional ethylene production.

Table 9: Cost Estimation of Microwave Reactor

(Magnetron Power: 100kW/module, Magnetron Price: 113872.82$/module, Power Needed: 66921420.69W)

Batch time(min)	0.5	1	2	5	10
Batch volume(m^3)	8.45	16.89	33.79	84.47	168.94
Microwave reactor power	557678.51	1115357.01	2230714.02	5576785.06	11153570.11
Magnetron needed(unit)	5.58	11.15	22.31	55.77	111.54
Total cost of Magnetron ($)	683,236.92	1,366,473.84	2,732,947.68	6,376,877.92	12,753,755.84

CONCLUSION

Simulation of industrial-scale production of ethylene via two distinct routes, ethane steam cracking and polyethylene upcycling, were considered. While the product compositions at the reactor outlet differ between the two processes, the feed rate of the reactants has been

adjusted to achieve the same ethylene production capacity. The novel microwave-enhanced process demonstrates the potential to produce both ethylene and propylene. The economic viability of using microwave reactors for LDPE conversion depends on the balance between the high efficiency and selectivity of the process against capital and operating costs. Technoeconomic analysis indicates that this integrated plant has the potential to be profitable.

ACKNOWLEDGEMENTS

This study was supported by the United States Department of Energy grant DE-EE0010838.

REFERENCES

1. Geyer, R., Jambeck, J.R., Law, K.L., Production, Use, and Fate of All Plastics Ever Made, Sci. Adv., 3 (7) (2017) e1700782
2. Ren, T., Patel, M.K., Blok, K. Olefins from Conventional and Heavy Feedstocks: Energy Use in Steam Cracking and Alternative Processes, Energy, 33(6), 817-833 (2008)
3. Yao, Y., Graziano, D.J., Riddle, M., Cresko, J., Masanet, E., Understanding Variability To Reduce the Energy and GHG Footprints of U.S. Ethylene Production, Environ. Sci. Technol., 49, 14704–14716 (2015)
4. Peng, Y., Wang, Y., Ke, L., Dai, L., Wu, Q., Cobb, K., Zeng, Y., Zou, R., Liu, Y., Ruan, R., A Review on Catalytic Pyrolysis of Plastic Wastes to High-Value Products, Energy Conversion and Management, 254, 115243 (2022)
5. Robinson, B., Caiola, A., Bai, X., Abdelsayed, V., Shekhawat, D., Hu, J., Catalytic Direct Conversion of Ethane to Value-Added Chemicals Under Microwave Irradiation, Catalysis Today, 356 3–10 (2020)
6. Wang, X., Wang, Y., Robinson, B., Caiola, A., Hu, J., Selectivity Modulated Oxidative Dehydrogenation of Ethane with CO2 under Microwave Catalytic Processing, Catal. Sci. Technol.,13, 3499-3504 (2023)
7. Sundaram, K. M., Froment, G. F., Modeling of Thermal Cracking Kinetics —I: Thermal Cracking of Ethane, Propane and their Mixtures, Chem. Eng. Sci., 32,601 (1977)
8. Ranjan, P., Kannan, P., Al-Shoaibi, A., Srinivasakannan, C., Modeling of Ethane Thermal Cracking Kinetics in a Pyrocracker. Chemical Engineering Technology, 1093-1097 (2012)
9. Wang, X., Modeling and Simulation of a Process for Upcycling Of Low-Density Polyethylene Plastic Waste To Ethylene, Doctoral Research Proposal, West Virginia University (2024)
10. Ogunniyan, O., Haque, M. E., Wang, Y., Bhattacharyya, D., Hu, J., Low-Pressure Microwave-Assisted Ammonia Synthesis: Evaluation of Novel Separation Technologies, Plant-Wide Process Design, and Techno-Economic Analysis." Applied Energy, 373, 123877 (2024)
11. Turton R., Shaeiwitz J.A., Bhattacharyya D., Whiting W.B., Analysis, Synthesis, and Design of Chemical Processes. fifth ed. Pearson Education, 2018