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Modeling of heat transfer and pyrolysis reactions in ethylene cracking furnace based on 3-D combustion monitoring

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ABSTRACT

In this paper, a distributed parameter model for tubular reactor in the ethylene cracking furnace based on 3-D temperature reconstruction is developed. The mathematical model was formulated to predict the distributions of the heat flux and the tube temperature while considering a non-uniform distribution of the surface heat transfer and the ethylene pyrolysis process. The results show that the heat flux distribution on the tubular reactor has four high heat flux zones, and the tube temperature reaches a maximum of 1088 °C. The value of the maximum tube temperature decreases compared with the value of the maximum heat flux due to the heat exchange coefficient of pyrolysis gas increasing slowly in the bend region. The tube temperature distribution was validated by using a spectrometer system and the errors between three major product yields at the tube outlet obtained by the proposed model and in-situ measured values were within 5%. This distributed parameter model can be used as a guide for ethylene cracking furnace operators and as a tool for design.

1. Introduction

Ethylene is one of the fundamental constituents of the petrochemical industry used as a main feed stock for the production of plastics, particularly polyethylene [1]. In the tubular reactor inside a cracking furnace, heat transfer and thermal cracking reactions closely interact with each other. It is important to understand the process and optimize its operation. A precise mechanistic model is fundamental in simulation, control and optimization of the ethylene pyrolysis process.

Considering the complexity of combustion and the heat transfer process in the cracking furnace, many researchers have used a lumped parameter to establish the model for the tubular reactor. Shahrokhi and Nejati [2] developed a 1-D steady state model of the thermal cracking of propane. Their aim was to determine the optimal process gas temperature profile based on the molecular reaction scheme of Sundaram and Froment [3]. They considered both ethylene and propylene production using an objective function that calculates operating profit. Masoumi et al. [4] and Gao et al. [5] also proposed a 1-D steady-state model for the tubular reactor for the thermal cracking of naphtha. However, all the models in these references are based on a reduced one-dimensional heat flux distribution model and cannot precisely calculate the heat transfer characteristics in the cracking furnace.

In recent years, many researchers have used a CFD method to simulate the 3-D combustion and heat transfer of the ethylene cracking furnace. Detemmerman and Froment [6] and Heynderickx et al. [7] combined the zone method and CFD method to carry out the coupled simulation for the radiative heat transfer in the firebox and the thermal cracking reaction in the reactor tubes, and obtained flow patterns of the flue gas inside the furnace, detailed information of species concentration and the temperature distribution. Afterwards, Stefanidis et al. [8,9] used the CFD method to carry out the detailed simulation for the combustion and radiation mechanism in the cracking furnace. The Discrete Ordinates model was applied to the simulation of radiative heat transfer of an 100kt/a SL-II ethylene cracking furnace [10]. Of course, some researchers have used the CFD method to simulate the combustion and heat transfer of other fossil fuel pyrolysis processes. Recently, Jamal Naser et al. [11–13] carried out comprehensive modeling for the combustion of pulverized dry lignite in lab scale [13] and large scale [11] furnaces under different combustion environments. The CFD technique can be used in off-line prediction, but it cannot be used in on-line measurement. The model for the tubular reactor will

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Nomenclature

A	frequency factor [s^{-1}] (for the first order reaction) and [$cm^3mol^{-1}s^{-1}$] (for the second order reaction)
C_p	specific heat capacity [J $kg^{-1}K^{-1}$]
D_{in}	inner diameter of furnace tube [m]
D_{out}	outer diameter of furnace tube [m]
E	activation energy [kJ mol^{-1}]
f	Fanning friction coefficient
G	mass velocity [kg $m^{-2}s^{-1}$]
k_i	reaction rate constant of the ith ($1 \le i \le 22$) reaction [s^{-1}] (for the first order reaction) and [$cm^3mol^{-1}s^{-1}$] (for the second order reaction)
L_s	length of straight tube [m]
L_d	length of bend tube [m]
N	total molecular Moore flow rate [mol s^{-1}]
N_l	molecular Moore flow rate of the lth ($1 \le l \le 18$) product [mol s^{-1}]
N_m,N_n	molecular Moore flow rate of component m or n in the ith ($1 \le i \le 22$) reaction [mol s^{-1}]
P	pressure [Pa]
Pr	Prandtl number
q	heat flux [W m^{-2}]
R	ideal gas constant 8.315 [J $mol^{-1}K^{-1}$]
r_i	reaction rate of ith reaction [mol s^{-2}]
Rd	READ number
Re	Reynolds number
S	the surface area [m^2]
T	absolute temperature [K]
V	volumetric flow rate of gas [cm^3s^{-1}]
V_g	gas volume [m^3]
Y	equivalent conversion factor

Greek symbols

α	total heat transfer coefficient [W $m^{-2}K^{-1}$]
β	heat transfer coefficient of pyrolysis gas [W $m^{-2}K^{-1}$]
$\gamma(i,l)$	stoichiometric coefficient of the lth ($1 \le l \le 18$) component in the ith ($1 \le i \le 22$) reaction
Δ	difference in any quantity
δ	tube thickness [m]
ε	emissivity
ζ	bending pipe radian
κ	absorption coefficient [m^{-1}]
Λ	angle of the bend
λ	thermal conductivity [W $m^{-1}K^{-1}$]
μ	dynamic viscosity [N $m^{-1}s^{-1}$]
ρ	density of pyrolysis gas [kg m^{-3}]
σ	Stefan–Boltzmann constant 5.67 × 10^{-8} [W $m^{-2}K^{-4}$]

Subscripts

f	pyrolysis gas
g	flue gas
i	number of element
p	the tube surface area
t	reactor tube
w	the wall surface area

Abbreviations

CCD	charge-coupled device
CFD	computational fluid dynamics

become more accurate and valuable by considering a 2-D, non-uniform distribution of the radiation heat flux. Due to the lack of on-line, 3-D combustion monitoring systems, this kind of model has seldom been reported for a cracking furnace.

Flame image processing techniques have been successfully applied to consider temperature reconstruction in pc-fired boilers [14–17]. We have resolved the 3-D temperature distribution in a W-shaped boiler [15] and revealed a distributed parameter model in a subcritical tangential once-through boiler [16], but this model is unsuitable for a cracking boiler due to the large difference in the furnace structure and the heat transfer characteristics. Also, the ethylene pyrolysis process in reactor tube is more complicated than no reaction process in a water-wall tube. Kumar and Kunzru [18] proposed a molecular reaction kinetics model which gained a worldwide concern in practical applications of ethylene plants and many chemical engineering institutions because of its the relatively simple reaction network. The Kumar reaction model represents the pyrolysis of naphtha with one primary reaction equation and 21 secondary equations, and marks the detailed reaction structures and parameters.

In this paper, a distributed parameter model is proposed for the tubular reactor in an ethylene cracking furnace. The mathematical model was formulated while considering the non-uniform distributions of the surface heat transfer and the ethylene pyrolysis process. Then, the heat flux and the temperature distribution on the reactor tubes were obtained by directly solving non-linear equations. The tube temperature (referring to the tube's outer surface temperature) distributions are validated by a spectrometer system at four observation ports, also the in-situ measured data of three major product yields are compared with the calculated values. Finally, some concluding remarks are given.

2. Distributed mathematical model

2.1. Physical model

Thermal cracking of light hydrocarbons is the main route for the production of important raw materials for the chemical industry, such as ethylene and propylene. The current and most used technology for ethylene production involves injecting naphtha into a long tubular coil located in a furnace with multiple burners that provide the required energy for the highly endothermic cracking reactions. As shown in Fig. 1 (a), steam is added to the naphtha at an appropriate ratio in order to control the reactive flow temperature and decrease the secondary reactions production. The furnace consists of three main zones: a convective zone where the reactive mixture is heated to a temperature close to 500 °C, a radiant zone where the pyrolysis reaction takes place and, finally a cooling zone where with a fast cooling of the products, the occurrence of secondary reactions is minimized. Fig. 1 (b) is the plot of two groups of tubes. This furnace adopts a “U” style and changing-diameter reactor tube design. There are 4 groups of tubes in the radiation section, each group with 12 tubes.

The configuration of the ethylene furnace and 3-D combustion visualizing system is shown in Fig. 2. The furnace is equipped with 16 bottom burners in two rows. Each burner includes five nozzles, where the primary nozzles are arranged in the air inlets, and other auxiliary nozzles are arranged around the air inlets. The combustion of the fuels belongs to the non-premixed combustion, that is, the fuels and the air spray out of different inlets and mix in the chamber, outside the burners, to combust. The dimension of the furnace is 3.47 m in depth × 14 m in width × 10.688 m in height.

16 flame image detectors were mounted in two layers at different heights, 8 CCD cameras are in one layer of each furnace. By