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Simulation of an innovative reactor for waste plastics pyrolysis

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HIGHLIGHTS

- An innovative pyrolysis reactor was proposed for waste plastics.
- Molten plastic pyrolysis proceeds in form of vertical falling film evaporation.
- The liquid film interface features wavier at higher heating temperature.
- The fluid temperature rises with the increase of the heating temperature.
- The molar concentration of volatile is higher in the lower region of the reactor.

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ABSTRACT

In this work, an innovative pyrolysis reactor for waste plastics pyrolysis was proposed based on phase change characteristics of waste plastics during their pyrolysis, which consisted of vertical tubes in parallel and molten polymer would fall down along the inner wall at the same time it "evaporates" to finish pyrolysis. In order to know the pyrolysis behaviors in this innovative reactor, the flow and "evaporation" processes of the molten polymer were simulated as the primary step. The pyrolysis process of molten polypropylene (PP) polymer when falling down along the inner tube wall was chosen as an example for the simulation. The effective conductivity of PP polymer was obtained through specially designed experiment. It has been found that the reactor can be modeled as a vertical falling film evaporator based on the volume of fluid (VOF) method, and the molten polymer film features a wavy structure, which is affected by the heating surface temperature. The fluid temperature rises during the pyrolysis process. Those calculation results provide guide for the reactor design.

1. Introduction

Pyrolysis of waste plastic is considered one of the most feasible large-scale methods of energy regeneration, since waste plastic is a valuable source of liquid and gas fuels, as well as chemicals [1,2]. According to the previously researches [3], the pyrolysis of plastic is obviously divided into several stages including: melting (from solid to liquid), pyrolysis characterized with volatile evaporating (from liquid to gas) and coke formation at the end. During melting and pyrolysis stages heat is needed and the ratio of heat required in melting stage to that of volatile evaporating stage is about 1:4 [4]. So stagewise reactors are reasonable to be applied for the plastic pyrolysis, and in the volatile evaporating stage considerable amount of heat should be supplied. Coke formation is an important issue and should be avoided during the volatile evaporation process. The molten plastic is a kind of non-Newtonian fluid [5], and it is usually characterized with high viscosity and low thermal conductivity, which made it hard to flow and difficult to heat up, so how to improve the heat transfer efficiency is a main problem of molten plastic pyrolysis. Liquid film heat transfer is one of the common methods for heat transfer enhancement [6], which is widely used for various industrial purposes, for example liquid evaporation process [7], micro-structured falling film reactor [8], seawater desalination [9], and so on. Falling film reactor is fit to deal with high viscosity material for its unique heat and mass transfer characteristics [10]. When studied the flow and heat transfer process of molten polymer, Zdanski et al. [11] found out that the heat transfer performance of molten polymer is similar to Newtonian fluid, both of which are the function of Reynolds number and Prandtl number, so the research methods of Newtonian fluid can be adopted as reference for non-Newtonian fluid. Although a few researches have reported their experiences on applying vertical falling film to study non-Newtonian fluid [12], however the viscosity of the fluid they used was much less than molten plastic. There has no report on applying vertical falling film reactor to molten plastic pyrolysis yet.

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In this work, a vertical falling film reactor was designed for the pyrolysis of molten plastic with high viscosity. As a preliminary attempt, the main purse is to verify the feasibility of this innovative pyrolysis reactor for waste plastics pyrolysis by predicting reaction behaviors in it.

As mentioned above, the chemical reaction process of molten plastic pyrolysis is indeed a volatile evaporation process coupled with heat and mass transfer. To find out the gas–liquid flow behaviors in evaporation process, heat transfer performance in detail, and avoid heat transfer deterioration, the gas–liquid-two-phase flow with heat transfer and chemical reaction during plastic pyrolysis process was investigated by applying numerical simulation method. Velocity profile and temperature distribution of the gas–liquid in the reactor and some other parameters that cannot be measured by experiments were obtained simultaneously. Moreover, simulation can help to design the proper tube length under certain conditions; for example, deterioration caused by coke formation can be totally avoided.

One of the key problems of gas–liquid-two-phase numerical simulation is the tracking of the gas–liquid interface, and presently the volume of fluid (VOF) method is widely used [13]. The VOF method can model two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of the fluids throughout the domain. Based on the VOF model, Ho et al. [14] calculated the gas–liquid-two-phase flow in a falling film micro-reactor, obtained the velocity profiles in the liquid film and found that the near-liquid gas zone are complex. Liu and Hao [15] simulated the free surface between the gas and liquid, and analyzed of velocity vector in the front of falling films and the varieties of pressure in the tube. Coke-like material deposition will naturally happen if pyrolysis process completes [1] and it will cause resistance to heat transfer. The expected length of tube in the reactor should ensure no appearance of coke deposition and another special section of reactor can be arranged for final pyrolysis stage where decoke measures are available. In this work, VOF model was adopted to track the gas–liquid interface of molten polymer in the vertical falling film reactor.

2. An innovative pyrolysis reactor for waste plastics

During numerous experiments of waste plastics pyrolysis, it has been found that their volatile evaporation stage is similar to water evaporation that characterized with bubble formation (see Fig. 1a) evaporation on a well-heated surface. Based on these characteristics, an innovative vertical falling film pyrolysis reactor was proposed, as shown in Fig. 1b.

The vertical falling film reactor for waste plastics' pyrolysis consists of vertical tubes in parallel with round or rectangular outer frame. The molten plastic falls down along the inside of tube surfaces, and the hot gas flows outside the tubes. There is no movable parts inside the reactor therefore the reactor is safe and suitable for large scale. Applying this vertical falling film reactor to molten plastic pyrolysis cannot only improve the heat transfer efficiency, but also can solve the flow problem easily. For the final pyrolysis stage with coke deposition, a conventional reactor like kiln can be adopted [16]. To design the reactor reasonable, we should know the pyrolysis "evaporation" law of molten plastics in it exactly, so a tentative numerical simulation is done before experiment firstly, and then the simulation result will be compared with the experiment data.

3. Mathematical model

During calculating, PP is used as typical plastics to set up the model. The molten plastic and coke-induced nuclear are considered as the same phase, namely liquid phase when no coke deposition appears, and the pyrolysis gas and oil (together volatile) are considered as the gas phase because they originally evaporate from molten polymer in form of gas. The content of each species is determined by the mass fraction. The chemical reaction equation is:

$$\text{PP} \rightarrow \text{Coke} + \text{Gas} + \text{Oil} \tag{1}$$

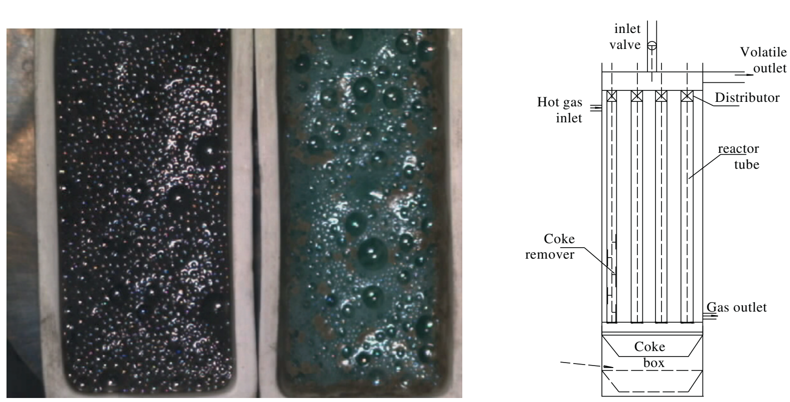
As both gas and oil evaporate in form of volatile and in the beginning coke-like material is only small coke-induced nuclear in the molten phase, the above reaction can be revised to:

$$\text{PP} \rightarrow \text{coke-induced-nuclear} + \text{volatile} \tag{2}$$

Continuity equation:

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial \rho_f u_i}{\partial x_i} = 0 \tag{3}$$

where ρ_f is the density of fluid, determined by the presence of the component phases in each control volume:



(i) PE (ii) PP

(a) Volatile bubbling and evaporating from molten polymer (b) Vertical falling film reactor

Fig. 1. Pyrolysis process of waste plastics and the proposed vertical falling film reactor.