

## MODELING OF TUBE REACTOR FOR PYROLYSIS OF POLYETHYLENE

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### Abstract

A Mathematical model of a tubular reactor is used to describe the pyrolysis process of polyethylene with which it is possible to investigate the effects of tube reactor geometrical dimensions on pyrolysis behaviors of polyethylene, which is beneficial to scaling up the reaction system. The temperature and PE concentration profiles in the tube reactor are obtained using this model. By adjusting variants such as PE flow velocity, reactor diameter and length, the optimal parameters to realize the optimal process design for pyrolysis can be obtained.

**Keywords:** Modeling; Tube reactor; Pyrolysis; Waste polymers; Recycling

### 1. Introduction

Dutch government is planning to increase the plastic recycling by 42% by 2012. Pyrolysis of polymers is often regarded as the most promising technology for resource recovery from waste polymer materials. Quite a lot of research work on the pyrolysis of individual and mixed plastics into liquid products has been reported [1]. Especially, developing pyrolysis reactors is of special interest to realize industrial application. Among the various reactors, tube reactor possesses the advantages of simplicity and ability to conduct continuous process [2]. In this paper, mathematical model of the tubular reactor is developed to investigate the effects of tube reactor geometrical dimensions on pyrolysis behaviors of polyethylene.

### 2. Materials and Methods

Scheme of the tube reactor were shown in Fig.1.

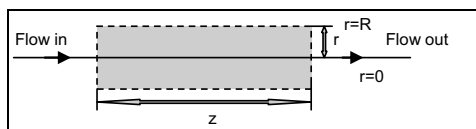


Fig.1 Scheme of the tube reactor

Assumptions were made to describe the heat transfer model in the tube reactor:

- Steady state;
- Heat transfer is in radial and axial directions;
- No velocity in r and  $\theta$  directions;
- Velocity profile is parabolic (laminar flow);
- Viscosity is constant;
- No shear stress;
- Feed is 1000 kg/h (~5000 t/y);
- $T_0 = 195^\circ\text{C}$ ,  $T_{\text{wall}} = 450^\circ\text{C}$ ;

- Heat conduction through the wall is neglected;
- Heat conduction in axial direction is neglected.

Assumptions were made for pyrolysis reaction of polyethylene:

- Reactions are first order;
- Reactions are irreversible;
- No mass transfer resistances;
- The temperature dependence of the rate constants is described by the Arrhenius equation.

The model was calculated with Borland Delphi 7 by adjusting the programming code Adinra.pas, which solves concentration and temperature profiles in the tube reactor based on an alternating direction implicit method.

### 3. Results and Discussion

Equations of continuity and energy based on the assumptions for the mathematical model are as follows:

**Equation of continuity (equation 1):**

$$v_z r \frac{\partial C_{PE}}{\partial z} = \frac{D_{PE}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C_{PE}}{\partial r} \right) - k C_{PE} \quad (1)$$

**Equation of energy (equation 2):**

$$v_z r \frac{\partial T}{\partial z} = \frac{\alpha}{r} \left( \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \right) + \frac{k C_{PE}}{\rho C_p} - \Delta H_r \quad (2)$$

Polyethylene pyrolysis is a well known process [3]. Table 1 listed related data for the model.

The pyrolysis reaction rate constants are summed up in Table 2. Where

- k1 describes the reaction Polyethylene  $\rightarrow$  heavy oils;
- k2: Polyethylene  $\rightarrow$  light oils;
- k3: Polyethylene  $\rightarrow$  gas;

k4: Polyethylene → polymer of lower molecular weight.

Table 1. The constants used for the modeling

Parameter	Constant
$T_{r=R}$ (Temperature of the reactor wall, °C)	450
Molecular weight of the polyethylene (Da)	200000
$C_p$ (Heat capacity, J/(kg·K))	49
Thermal conductivity (W/(m·K))	0.25
Density, kg/m <sup>3</sup>	920
Viscosity, Pa·s	2478
$C_{PE,z=0}$ (Initial concentration of PE, mol/m <sup>3</sup> )	5
$\Delta H_r$ (Enthalpy of the reaction, KJ/kg)	-1300

Table 2 The reaction rate constants for pyrolysis of polyethylene depending on temperature [3]

K[s <sup>-1</sup> ]	T [°C]			
	400	420	450	470
k1	0.0275	0.1006	0.0293	0.0332
k2	0.0021	0.0604	0.2315	0.4488
k3	0.0000	0.0003	0.0000	0.0000
k4	0.0777	0.1199	0.0693	0.1678

According to the mathematical model, a 3 D temperature profile along the tube reactor depending on the diameter and length were obtained (Fig.2)

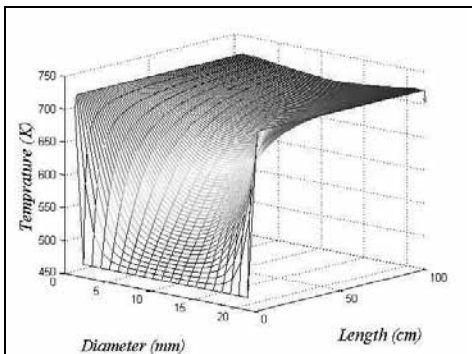


Fig. 2 3D temperature profile for the tube reactor (Diameter: 0.03m; Length: 1m)

#### 4. Conclusions

In summary, mathematical model of a tubular reactor is used to describe the pyrolysis system of PE. The temperature and PE concentration profiles during pyrolysis in the tube reactor were obtained.

By adjusting the variants such as PE flow velocity, reactor diameter and length, optimal parameters for pyrolysis can be obtained.

#### References

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