Modeling of a pyrolysis batch reactor using COMSOL Multiphysics

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Abstract. Plastic Pyrolysis is a thermal degradation process; it offers an important alternative energy. The aim of this study is to model a batch reactor to be used for plastic pyrolysis. Consequently, four experiments with different heating and cooling cycles are done using an empty pyrolysis batch reactor and four temperatures are measured at different locations on the reactor. On the other hand, the empty reactor is modeled and several simulations are done, using COMSOL Multiphysics software, under the same experimental conditions. By comparing the temperatures obtained from simulation to those measured experimentally, it is noticed that the results are very close with a maximum error of 4%, hence the model is validated.

1 Introduction

Nowadays after the depletion of fossil energy reserves, which are the essential source of energy worldwide, seeking for alternative renewable energy became a crucial issue and subject for many researchers and academic institutions. On the other hand, there is a serious problem facing humanity, which is the enormous growth of the accumulated plastic waste every year. A statistic shows that 25 million tons of plastic waste were generated in Europe in 2012 and about 38% of the plastic waste are still treated in the landfill, while only 36% were utilized for energy recovery [1]. A solution of plastic waste accumulation and an alternative source of energy is plastic pyrolysis which converts waste plastic into a wide range of fuels and chemicals. Plastic pyrolysis is a thermal decomposition of large chain polymers into shorter ones by heating plastic to a given temperature, where an endothermic reaction occurs in the absence of oxygen [1].

In order to study the pyrolysis process, a batch reactor used at IMT Atlantique laboratories will be modeled using COMSOL Multiphysics software. The model will be validated by comparing the simulation of heating and cooling cycles of the empty reactor to the experimental results.

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2 Experimental study

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This batch reactor (Figure 1), is a hollow cylinder made of stainless steel of 0.3 cm of thickness and a volume of 954 cm$^3$. It is surrounded by two heating coils of 1500 W as maximum power and insulated by ceramic fiber. Four temperatures are measured for several positions on the reactor as shown in Figure 1(a). Heating rate and final temperature are controlled by the thermocouple $T_2$. Four experiments with different heating rates are done and the measured temperatures will be compared to the simulated results.

![Batch Reactor Sketch](image1.png)  
*Fig. 1. (a) 2D sketch of batch reactor with dimensions in cm. (b) Real image of the reactor.*

### 3 Boundary conditions and implemented equations

COMSOL is a flexible platform computer simulation environment; it allows users to model all relevant physical aspects as a translation of real-world physical laws into their virtual form designs. Heat Transfer is an important module in COMSOL Multiphysics that helps the user in investigating the heat transfer mechanism, such as conduction, convection and thermal radiation, and a combination of them with other physics [2]. The heat transfer mechanism in solid is governed by the following partial differential equations:

**Energy equation:**

$$\rho C_p \frac{\partial T}{\partial t} + \nabla . \dot{q} = Q$$

(1)

**Fourier law:**

$$\dot{q} = -k \nabla T$$

(2)

In order to determine the temperature distribution in a medium, the heat equations must be appropriately solved; the solution depends on the physical phenomena existing at the boundaries: Temperature, convection and radiation using equations (3), (4) and (5) respectively. Where $T_2$ is taken as the temperature of the heat source along the circumference of the heating coils (d$\Omega$). The free convection heat transfer coefficient $h$ is determined by the correlation of free convection built in COMSOL at the outer boundary of the reactor (insulator) and the surface emissivity $\varepsilon$ is taken constant of value 0.75.

$$T = T_2 \quad \text{on} \ d\Omega$$

(3)

$$\dot{q}_{conv} = hA\Delta T$$

(4)

$$\dot{q}_{rad} = \varepsilon\sigma A(T_{sur}^4 - T_{amb}^4)$$

(5)

Many parameters affect directly the heating process like the thermal conductivity and heat capacity for stainless steel and ceramic fiber. The thermophysical properties of the
stainless steel and ceramic fiber are respectively: for the thermal conductivity 22 and 0.2 (W/K.m), for the heat capacity 440 and 1200 (J/K.kg) and for the density 8000 and 190 (kg/m3) [3].

4 results

Figure 2 presents the results of one of these experiments where heating of the reactor is done, with full load (1500 W), during 7 minutes proceeded by a cooling for 157 minutes. As it is obvious in this figure, the simulated and experimental curves are approximately coincided for the four temperatures with an error varying between 1 and 4%. The simulation is also compared to other experiments; this validate the modeling of the batch reactor for different heating process.

Fig. 2. Comparison between experimental and simulation results for three temperatures along the reactor.

5 Conclusion

Using COMSOL, the batch reactor for plastic pyrolysis is modeled and validated by comparing experimental and simulated results with a maximum error of 4%. After the validation of the model, the future work is to study and simulate different phenomena occurring during pyrolysis process, i.e. heating of feedstock, phase change and cracking, before proceeding to the full study of plastic wastes pyrolysis in the batch reactor.

References