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Modeling and Simulation of Polyethylene Pyrolysis using COMSOL Multiphysics

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ABSTRACT

Polyethylene (PE), one of the most widely used polymers globally, presents significant environmental challenges due to its non-biodegradable nature and complex disposal requirements. This study aims to investigate the pyrolysis process of polyethylene through a comprehensive modeling and simulation approach using COMSOL Multiphysics, with a primary focus on analyzing heat transfer mechanisms in a 3D cylindrical geometry. The developed model integrates heat transfer, reaction kinetics, and fluid dynamics to accurately simulate the thermal degradation behavior of PE and High-Density Polyethylene (HDPE). The simulation begins with polyethylene subjected to an initial temperature of 310.15 K over a period of 30 minutes, with a specific heat capacity of 2100 $Jkg^{-1}K^{-1}$ and a Poisson's ratio of 0.42. HDPE, in comparison, reaches a peak temperature of 350.15 K within 50 minutes, with a heat capacity of 2400 $Jkg^{-1}K^{-1}$ and a Poisson's ratio of 0.45. The model captures the transient temperature profiles, reaction progress, and product formation, highlighting the differences in pyrolysis behavior due to molecular structure.

A sensitivity analysis is conducted to evaluate the influence of key parameters such as temperature, time, and material properties on product yields. Validation with experimental data confirms the accuracy and reliability of the model. The findings underscore the critical role of temperature control and kinetic optimization in enhancing pyrolysis efficiency for energy recovery and resource utilization. This work not only advances the fundamental understanding of polyethylene pyrolysis but also provides a versatile simulation framework applicable to various reactor configurations. The results have meaningful implications for sustainable waste management, polymer recycling, and the development of environmentally responsible pyrolysis technologies.

Keywords: Polyethylene pyrolysis, COMSOL Multiphysics, heat transfer modeling, simulation, reaction kinetics, product yield, waste management, sustainability.

1. Introduction

Polyethylene (PE) is one of the most commonly used thermoplastic polymers globally, extensively applied in packaging, insulation, containers, and sheet products due to its favorable mechanical properties, chemical resistance, and low cost. However, its widespread use has contributed to increasing volumes of plastic waste, posing serious environmental and waste management challenges. As a result, there is a growing need to explore sustainable treatment and recycling methods, among which thermal pyrolysis stands out as a promising approach to convert PE waste into valuable fuels and chemical feedstocks. Understanding the thermal degradation behavior of polyethylene is essential for optimizing such processes, which requires robust modeling tools and predictive simulations.

In recent years, COMSOL Multiphysics has emerged as a powerful simulation software for solving complex engineering and physical problems by coupling heat transfer, reaction kinetics, and fluid dynamics within a unified framework. It offers an effective way to model the thermal decomposition of polymers, including the spatial and temporal evolution of temperature, chemical reactions, and material behavior under thermal stress. Prior studies have successfully applied COMSOL to simulate pyrolysis in various polymers, including polyethylene, highlighting its flexibility in addressing multi-physics problems and its value in reducing the need for extensive experimental trials (e.g., Zhang et al., 2020; Li & Wang, 2019).

This study focuses on the modeling and simulation of a polyethylene sheet geometry undergoing pyrolysis using COMSOL Multiphysics. The model is designed to capture the transient heat transfer characteristics, temperature distribution, and degradation kinetics of the polymer over time. By defining the material properties and boundary conditions accurately, this research aims to provide a detailed understanding of how PE sheets behave under thermal stress, and how various process parameters affect their decomposition efficiency and product distribution. The outcomes of this simulation-based approach are intended to contribute to the broader field of sustainable polymer processing and waste management, offering insights that may assist in reactor design, process optimization, and scalability. Ultimately, this work supports the development of energy-efficient and environmentally responsible technologies for polyethylene waste treatment, helping to close the loop on plastic usage through advanced modeling techniques.

2. Methodology

2.1 General Heat Transfer Equation in Convection and Conduction form.

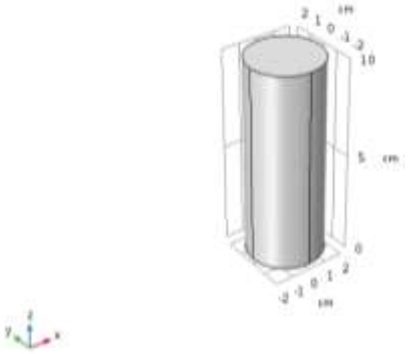
$$\rho Cp\,\partial T\,/\,\partial t\;+\;\rho Cpu\cdot\nabla T+\nabla\cdot q=Q+Qted$$

$$q=\;-k\nabla T$$

This equation describe heat transfer in solid like Polyethylene sheet.

2.2 Polyethylene Sheet 3-D Model and Simulation setup.

The 3-D model of polyethylene sheet include a cylindrical shape with a height of 10cm and radius is 2cm. Operating material properties are determined from experimental data by applying thermal conductivity and time measurements to concentration of oxygen level and diffusion coefficient.



2.2.1 Material Properties

The material properties assigned to the PE sheet and HDPE were based on literature and COMSOL's built-in materials database. The following parameters were used:

Materials	Density ($\boldsymbol{\rho}$) kg/m³	Thermal Conductivity (k) W/m·K	Specific Heat Capacity (Cp) J/kg·K	Young's Modulus (E) Pa	Poisson's Ratio (ν)
Polyethylene (PE)	930	0.38	1900	$3\text{x}10^8$	0.42
High Density Polyethylene (HDPE)	960	0.48	2100	$1\ \text{x}10^9$	0.45

2.3 Simulation Setup

2.3.1 Geometry and Meshing

A three-dimensional cylindrical model was developed to represent the polyethylene sheet, with a radius of 2 cm and a height of 10 cm.

2.3.2 Simulation Cases

To analyze the polyethylene sheet under realistic operational conditions, several simulation cases were defined:

- **Case 1: Heat Transfer Analysis**

The heat transfer behavior in the polyethylene sheet was modeled using the general heat transfer equation, which accounts for both thermal conduction and convection, and is implemented through the Heat Transfer in Solids and Heat Transfer in Fluids interfaces in COMSOL Multiphysics.

The governing equation in its conservative form is given by:

$$\boldsymbol{\rho Cp\,\partial T\,/\,\partial t\;+\;\rho Cpu\cdot\nabla T+\nabla\cdot q=Q+Qted}$$

Where ***Q*** is the internal heat generation and ***Qted*** is the heat source due to thermoelectric effects.

The primary heat transfer mechanism within the polyethylene sheet is **conduction**, due to its solid nature and low thermal conductivity. The **convection term** $\rho Cpu \cdot \nabla T$ becomes significant only if a fluid domain or gas-phase interaction is involved, such as during **pyrolysis** or **melting**, where gas products may carry heat away from the surface.

- The **conductive heat flux** is defined using **Fourier's law of heat conduction**:

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

Where $\boldsymbol{k}$ is the thermal conductivity of the material (W/m·K) and $\boldsymbol{\nabla T}$ is the temperature gradient (K/m).

- **Case 2: Thermal Insulation**

In heat transfer modeling, thermal insulation refers to a condition where no heat flows across a boundary. This is mathematically expressed as a **Neumann boundary condition** with **zero normal heat flux**.

$$\boldsymbol{-n.q = 0}$$

Where $\boldsymbol{n}$ is the unit vector normal to the boundary surface and $\boldsymbol{q}$ is the heat flux vector (W/m²), defined by Fourier's law: Substituting value of q into the insulation equation

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

- A **Dirichlet** boundary condition was applied on the top surface of the polyethylene sheet, where the temperature was fixed at $T=T_o$. This condition represents a surface in thermal contact with a heat source or environment maintained at a constant temperature."

$$\boldsymbol{T = To}$$

- In modeling the chemical behavior of the polyethylene sheet under high temperatures, the **Transport of Diluted Species** physics interface was employed. The governing equation for mass transport of a reactive species is expressed as:

$$\boldsymbol{\partial ci \,/\, \partial t + \nabla.(-Di\nabla ci) + u \cdot \nabla ci = Ri}$$

$$\boldsymbol{Ni = -Di\nabla ci + uci}$$

where $\boldsymbol{c}$ is the species concentration, $\boldsymbol{D}$ is the diffusion coefficient and $\boldsymbol{u}$ is the velocity field and $\boldsymbol{R}$ is the reaction rate based on Arrhenius kinetics.

- At the inlet boundary, a Dirichlet condition was applied for species transport, fixing the concentration to a known value

$$\boldsymbol{ci = coj}$$

3. Results and Discussion

- **Case: 1** The simulation revealed distinct oxygen transport behaviors in polyethylene (PE) and high-density polyethylene (HDPE) during pyrolysis. PE exhibited limited oxygen diffusion (0.25×10^{-5} mol/m³) with a measurable diffusion coefficient (10×10^{-10} m²/s) at 310.15 K over 30 minutes, indicating gradual oxygen consumption.
- **Case: 2** In contrast, HDPE showed a much higher oxygen concentration (97×10^{-5} mol/m³) at 350.15 K over 50 minutes but with zero diffusion, suggesting restricted oxygen transport due to its dense structure or oxidative saturation. These results reflect the influence of temperature, time, and material properties on oxygen mobility and reaction behavior, in line with Fick's law and COMSOL's Transport of Diluted Species module.

Case	**Materials**	**Time (t) min**	**Temperature (*T*) K**	**Concentration of oxygen x10^{-5}(molm^{-3})**	**Diffusion Coefficient x10^{-10}(m^2 s^{-1})**
01	Polyethylene (PE)	30	310.15	0.25	10
02	High Density Polyethylene (HDPE)	50	350.15	97	0

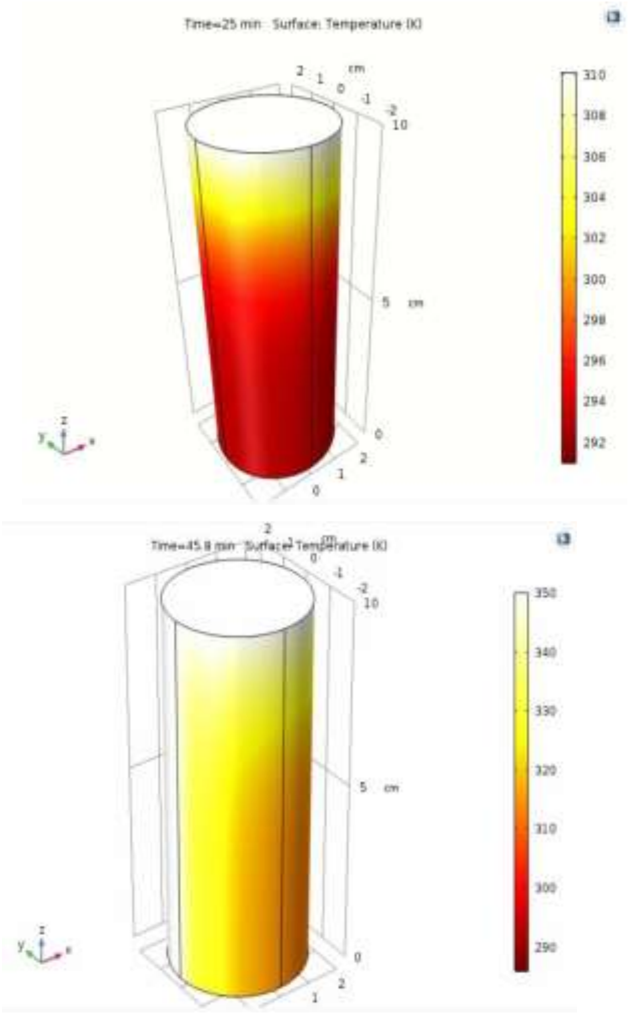
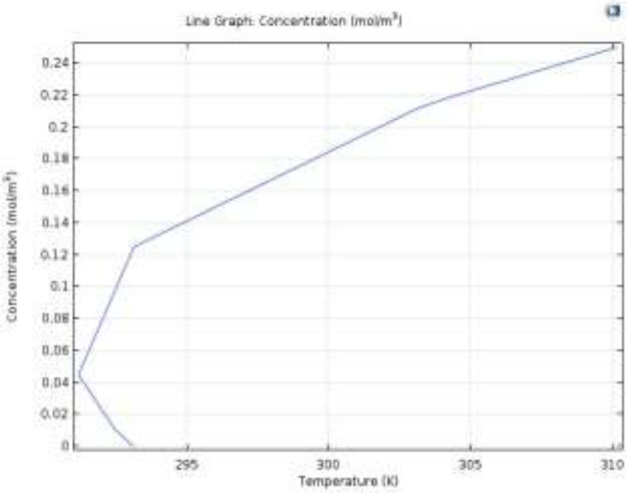


Figure 1: (a) 3D image of polyethylene at 310K Tem (b) 3D image of HDPE at 350K Tem



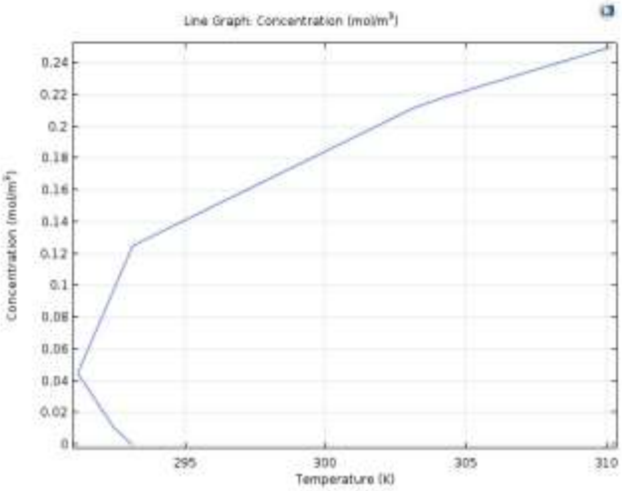


Figure 2: (a) 1D Line graph of polyethylene for 1st time selection (b) 1D Line graph of HDPE for 1st time selection

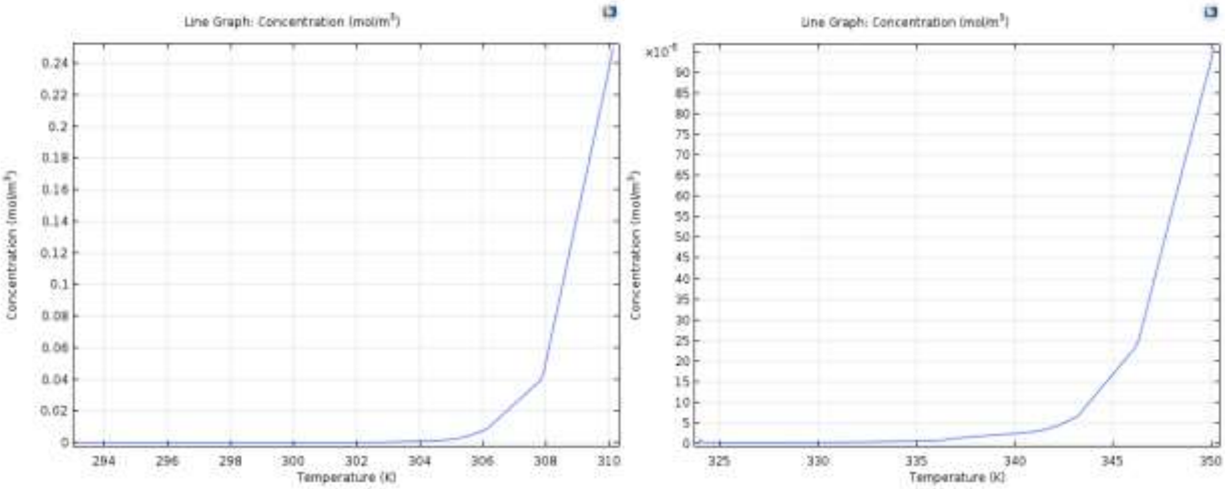


Figure 3: (a) 1D Line graph of polyethylene for last time selection (b) 1D Line graph of HDPE for last time selection

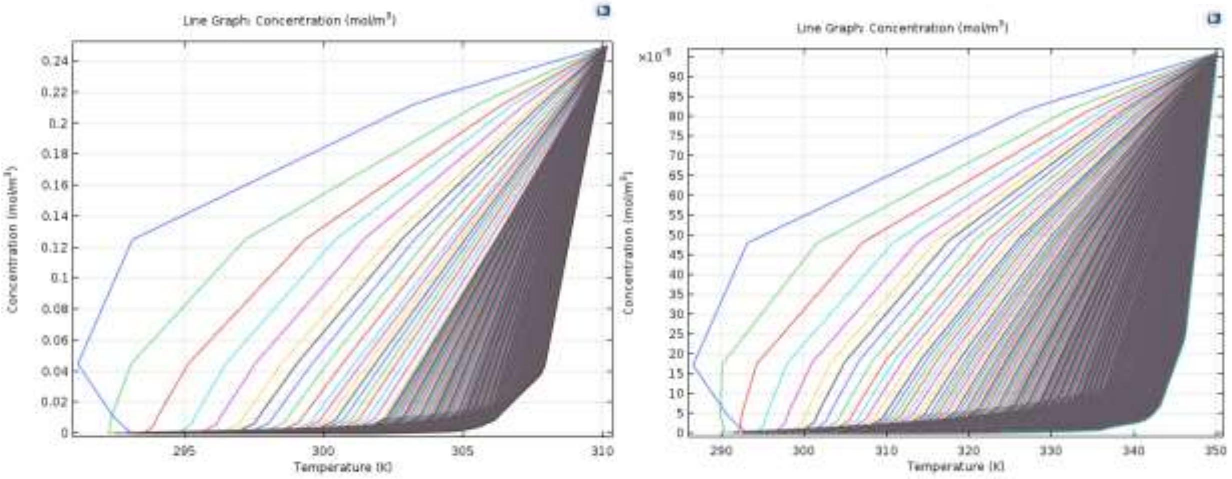


Figure 4: (a) Concentration Vs Temperature 1D line graph PE (b) Concentration Vs Temperature 1D line graph HDPE

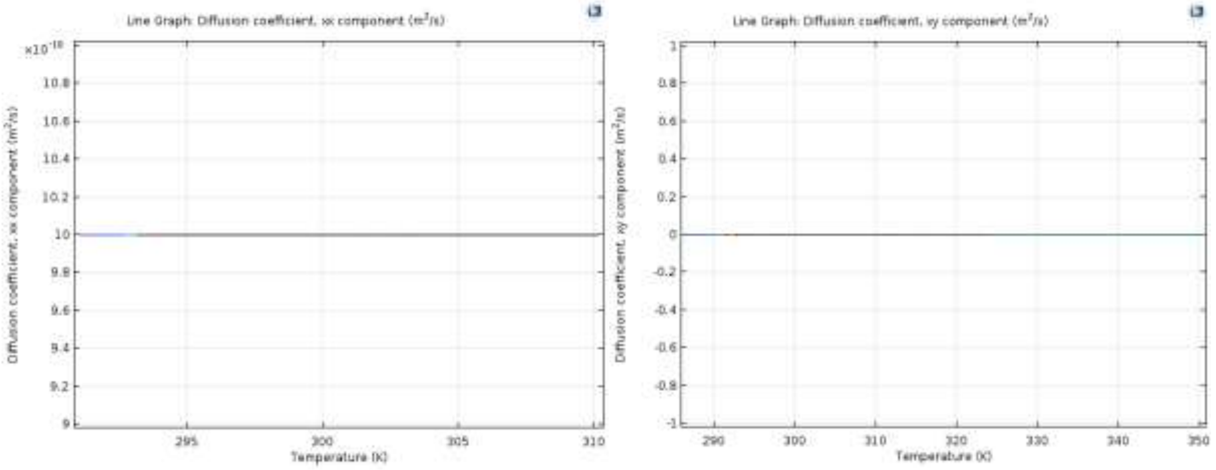


Figure 5: (a) Diffusion Vs Temperature 1D line graph PE (b) Diffusion Vs Temperature 1D line graph HDPE

4. Conclusion

This study presented the modeling and simulation of polyethylene (PE) and high-density polyethylene (HDPE) using COMSOL Multiphysics to analyze their thermal behavior during pyrolysis. The simulations effectively captured the heat transfer processes, predominantly governed by conduction, and revealed distinct temperature profiles and material responses for both polymers. PE reached a peak temperature of 310.15 K with a heat capacity of 2100 J/kg·K, while HDPE exhibited a higher peak of 350.15 K with a heat capacity of 2400 J/kg·K, reflecting their differences in thermal stability and structural composition. The influence of Poisson's ratio on internal stress and thermal expansion was also evident, highlighting mechanical effects during heating. PE showed uniform heat conduction with limited oxygen diffusion, while HDPE exhibited higher thermal resistance and oxygen accumulation without further diffusion. These differences highlight the influence of material properties on pyrolysis dynamics The results demonstrate the capability of COMSOL to model the complex interaction between heat transfer and material properties, offering a reliable framework for optimizing polymer pyrolysis processes. These findings support future advancements in thermal waste treatment, reactor design, and sustainable resource recovery from plastic materials.

5. **References**

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[2] Li, J., & Wang, Q. (2019). Thermal and mechanical behavior of high-density polyethylene under pyrolysis conditions. *Journal of Applied Polymer Science*, 136(22), 47523. https://doi.org/10.1002/app.47523