## Modeling of Asphaltenes and Oil Shale Pyrolysis

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## Abstract

Pyrolysis is a key step in the conversion of carbonaceous materials into useful products. In this study, we investigate the pyrolysis of asphaltene and oil shale, both experimentally and numerically. COMSOL Multiphysics® software is used to model the combined effects of fluid flow in porous media, mass transfer of species, heat transfer, and reaction kinetics. Gas evolution and the porosity changes in the spent char are monitored and compared to experimental and literature data.

The effect of temperature and particle size parameters for both fuels is studied. The kinetic as well as physical parameters for both fuels are determined experimentally and from literature. In the case of asphaltenes, the kinetic reaction is determined by thermogravimetric analysis (TGA), giving an activation energy of 151 kJ/mol and pre exponential factor of 1.83x108 s-1. For the oil shale, data from literature was used [1], where the activation energy is 150 kJ/mol with the pre exponential factor of 2.11x108 s-1. Other physical properties are determined from literature.

A model of a laboratory gasifier shown in Figure 1 was used to for testing the kinetic model developed. A section of the gasifier used for modeling is shown in Figure 2 and the mesh used is shown in Figure 3. Validation of the COMSOL model with literature data is shown in Figure 4.

Higher conversion rates are obtained with increasing the temperature and decreasing particle size for both fuels. It is noted that the asphaltenes decomposition is slower than the oil shale when varying both parameters. The organic matter variation in the oil shale (kerogen) causes a variation in the time required for a total decomposition. It is also observed that the final porosity becomes higher, giving a lower percent of char at the end of the process. Based on Péclet Number analysis, it is established that the process is limited by diffusion, and the nitrogen flow injection into the furnace did not change the studied parameters, only the retention time of the particle fuel into the furnace.

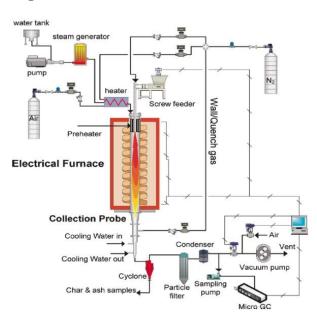


Figure 1: Experimental setup for asphaltenes pyrolysis in a laboratory gasifier.

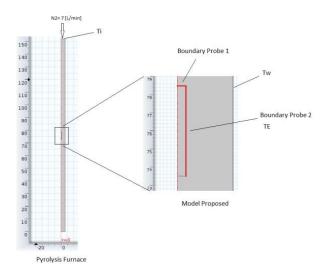


Figure 2: Physical model used for determination of boundary conditions.

## Figures used in the abstract

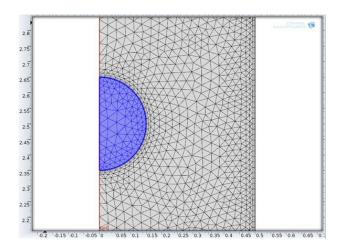


Figure 3: Meshing of the asphaltenes and furnace area under study.

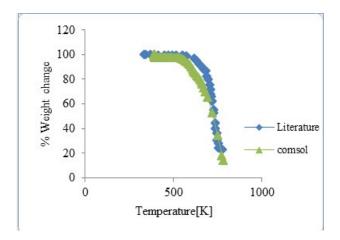


Figure 4: Validation of the model with literature.