**Soot Formation and Secondary Pyrolysis in Oxy-Coal Combustion with Large-Eddy Simulation**

Alexander J Josephson, David O. Lignell

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Recent research has been dedicated to the control carbon pollutants from energy sources. One such purposed system is the oxy-combustion of fuels. When burning fuels under oxy-fuel conditions, carbon capture techniques become more economically feasible. Computer simulations of these purposed systems have been accomplished using Large-Eddy Simulation (LES); however, until now these simulations have been incomplete and have not incorporated models for secondary pyrolysis or soot formation.

This research focuses on the oxy-combustion of coal and the challenges associated with it. Coal combustion is different from combustion of other fuels. With respect to soot, when coal pyrolyzes light gases are given off in companion with a heavier tar. This tar can transform into soot and is the principle source of soot particles in conventional coal combustion systems. Soot can also be formed by the light gas products of primary pyrolysis. These light gases may radicalize and nucleate into soot precursors which may grow into larger particles. In both cases, particle growth can occur through the agglomeration of particles with one another, or the coagulation of lighter molecules onto the surface of the soot particle. Our proposed soot formation model will include soot transformed from tar and grown from nucleated light gases along with growth mechanisms for these particles.

In addition to the formation of tar and soot, a complete model of secondary pyrolysis needs to include the destruction of tar and soot. Tar and soot are destroyed in a combustion system through a combination of gasification and oxidation. The gasification and oxidation of tar and soot is secondary pyrolysis and can contribute to overall mass/energy balance and radiation of any combustion system. Possible cracking of the particles will also be explored.

Oxy-coal combustion LES with models for secondary pyrolysis and soot will be presented with comparisons to simulations lacking those. Effects on radiation, gas temperature, and heat loss will be explored and presented. These simulations will be carried out on the Fulton Supercompter at Brigham Young University and incorporated in the LES software developed by the University of Utah, as part of a larger project exploring oxy-coal combustion in full-scale reactors.

With the development of accurate simulations, production of oxy-coal reactors with reduced pollution production could become possible. In addition, the physics, tools, and models developed in the process could be readily applicable to other research with minor to little adjustment.