Computer Simulated Multi-component Aerosol Thermodynamics and Chemistry

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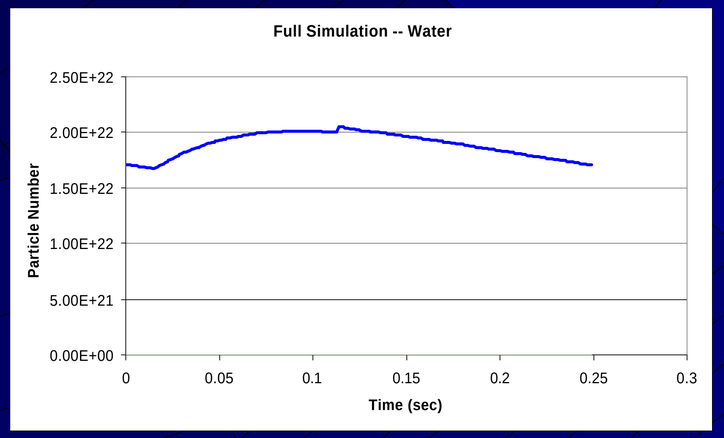
Objective

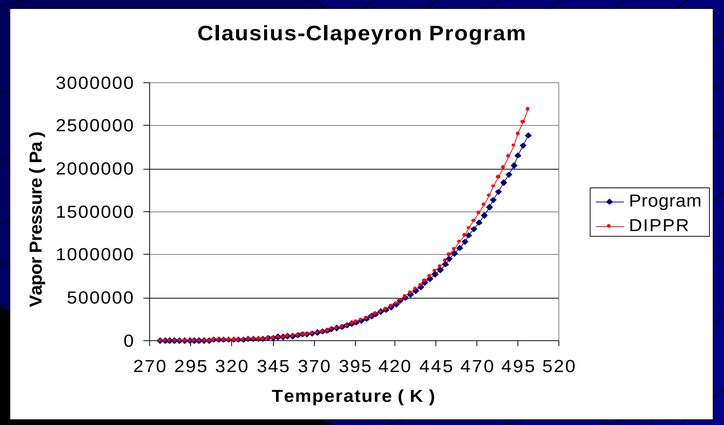
This project is intended to produce a predictive computer simulation of aerosol formation and behavior in industrial boilers.

Aerosol species, particularly sulfates and other species formed during pyrolysis of black liquor, pose serious threats as fouling agents in boilers and as pollutants in the environment. For this reason, it would be beneficial to have an accurate, predictive method of determining aerosol formation and behavior.

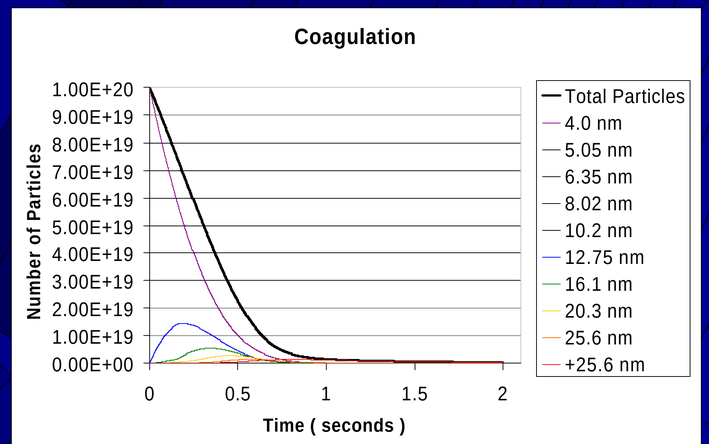
With this simulation, it will be possible to fully predict the condensed phase of the flow stream, given gas-phase data from a CFD program.

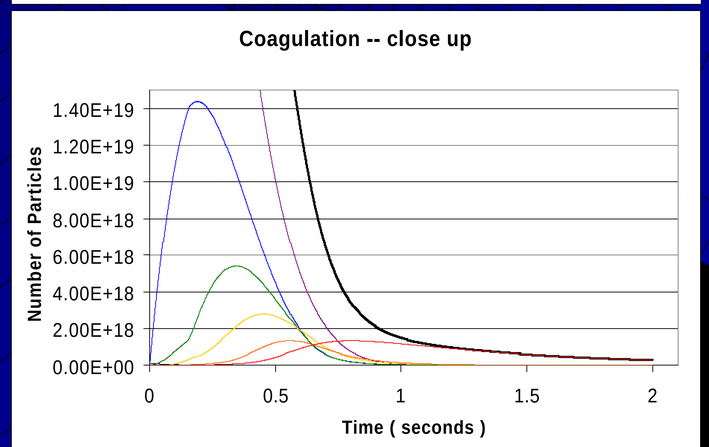


Prediction after one-quarter seconds for coagulation, nucleation and condensation – single component system.

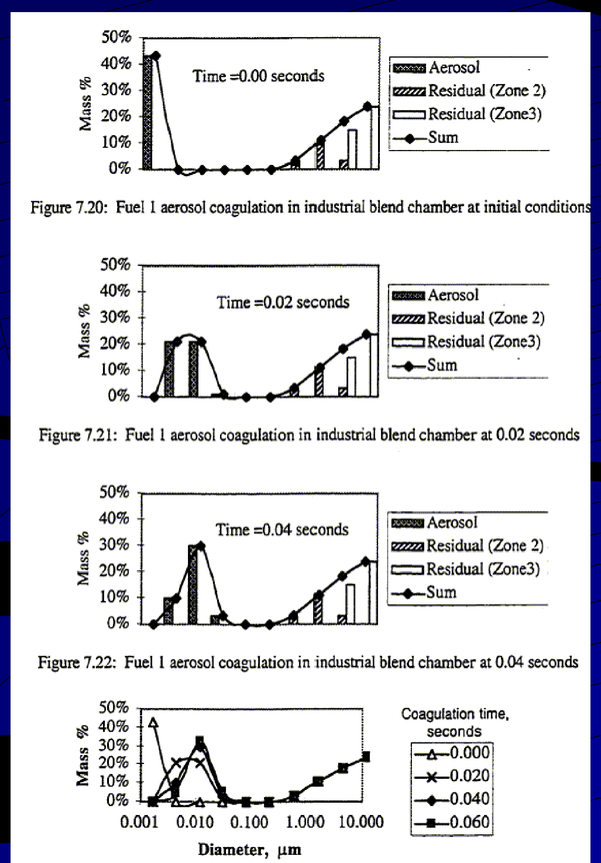


Vapor Pressure Predictions based on NASA coefficients





Predicted coagulation effects during a two second interval for a single component system.



Results of Chenevert's work

Experiment

The program has been tested against experiments performed by Blake Chenevert at the University of Washington (his results are shown at left. The simulation's predictions are shown at right).

The data follow similar trends, indicating that the simulation is correctly predicting some experimental work.