Simulating the Gasification of a Urea-Water-Solution Droplet

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Motivation and Objectives

- For UWS droplets, which are used in combustion after treatment in SCR systems, a more accurate view of the evaporation will lead to more accurate modeling, and more efficient construction and injection practices.
- Our previous full spray in crossflow results demonstrate the capabilities of the 3D numerical method, however the UWS droplet model was ad hoc implementation from the literature.
- A method is created based on an interface tracking procedure (Arbitrary-Lagrangian-Eulerian) and exploits the spherical symmetry of the problem.
- More importantly, the current study provides a detailed view of the evaporation of urea.
- The method couples heat transfer and phase change jump conditions while also incorporating the species diffusion at the interface.

Validation

- Validation is performed against the gaseous urea vapor results of Bernhard et al. and Emelyanenko et al., and subsequently the D2 results of Nomura et al.
- Good matching is observed between the two results.

Main Results

- Matching is seen between the experimental results of Wang et al. and the computational results of this study.
- The fully coupled boundary conditions help to capture both the initial curvature of the data, as well as the transition between the water dominated evaporation regime and the urea dominated evaporation regime.
- These results show that we are matching correctly to the experimental results.
- Discussion of the internal results follow.

Discussion/Future Work

- Internal views of the water and urea show interesting results.
- The figure on the left shows that there is a water mass fraction leftover on the inside of the droplet after the external temperature rises above the water vaporization temperature.
- This could allow for superheated water and the possibility of micro explosions.
- The figure on the right shows how the eutectic region is defined for the UWS droplet.
- It is visible that the droplet surface goes through the crystallization region, which we do not model.
- Future results would include implementing this model into a fully 3-D code, in order to accurately capture the UWS droplet vaporization process.