Ignition of Methanol Droplet Groups with Detailed Chemical Kinetics in Different Flow Environments

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At the present time there are very few research studies where detailed chemical kinetics have been used to predict the ignition of liquid droplet groups under realistic thermodynamic conditions, Ref [1]. The majority of the previous studies have used global chemical kinetics, Ref [2], which global chemical kinetics were not developed to treat the sensitive conditions associated with ignition. This problem is quite important for modern IC engines and for understanding safety concerns with the handling of liquid fuels. At the present time we have considered small groups of droplets, two and three, in a fully three dimensional and time-dependent environment, where the influence of droplet relative geometry and cold walls can be brought into play, Ref. [3]. The paper shows extreme sensitivity of the ignition process to flow thermodynamics conditions as well as droplet group orientations. In general, the larger and more concentrated groups lead to a more stable ignition process.

Due to the efficiency of the overset grid method and to the use of operating splitting for the chemical reactions, we have been able to apply a detailed chemical reaction mechanism to our droplet dynamics code. The reaction mechanism for methanol consists of twenty species and ninety fundamental chemical reactions. The computation effort is still quite larger, and we have limited our calculations to droplet heat up and ignition, however we have been able to do ignition studies of droplet arrays in different configurations and wall conditions. Some results are shown in figures (1) and (2) for a time when droplets have lost 22 % of there mass. Due to the small size of the droplets, 12μm, the reaction zone is significantly larger than the computational domain, and we can not see the full ignition region. Shown in figure (4b) are the contours of H atoms and the OH radical, and there are interesting interactions between the array and flow.

A very important droplet array problem is the behavior of droplets near a cold wall, which we have previously studied experimentally. For the first time we have been able to model this situation, and the results are shown in figure (3). As can be seen from the results in figure (3) the mesh has been expanded near the wall to capture the wall/droplet interaction. The temperature contours show a strong interaction with the cold wall, and a very asymmetrical heat transfer pattern near the wall. The paper shows the influence of wall cooling on the ignition process, as well as droplet relative configuration.

References

1. Sirignano, W.A., **Fluid Dynamics and Transport of Droplets and Sprays**, Cambridge University Press, 1999.
2. Staph, P., Maly, R., and Dwyer, H.A. Dwyer, 1998, “A Group Combustion Model for Treating Reactive Sprays in IC Engines”,27th Inter. Combustion Symposium, 1857-64. The Combustion Institute: Pittsburgh, Pa.
3. Delplanque, J.P., and Sirignano, W.A., 1994, “Boundary Layer Stripping Effects on Droplet Transcritical Convection Vaporization”, Atomization and Sprays $, 325-49.

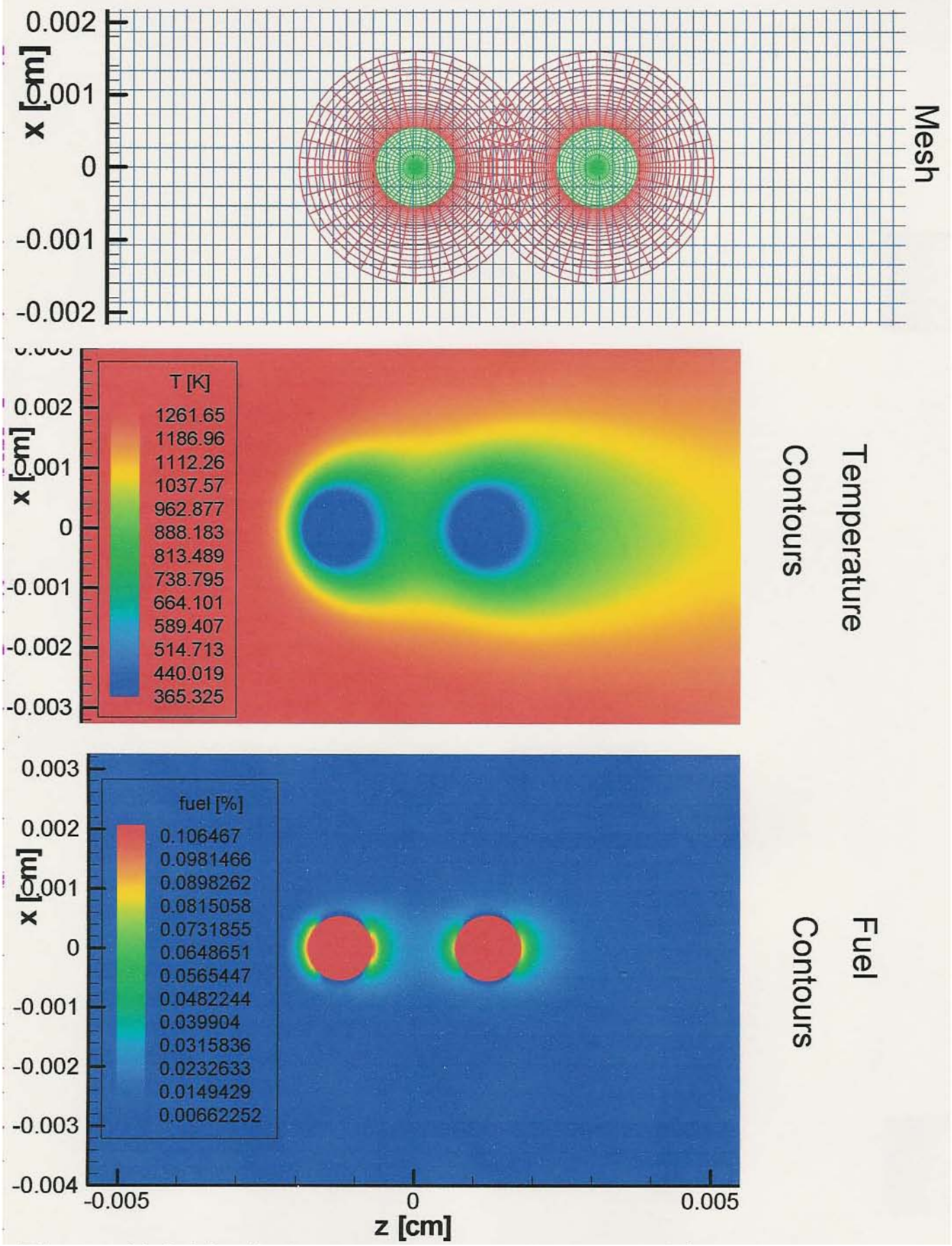

Figure (1) Mesh, Temperature Contours, and Fuel Contours

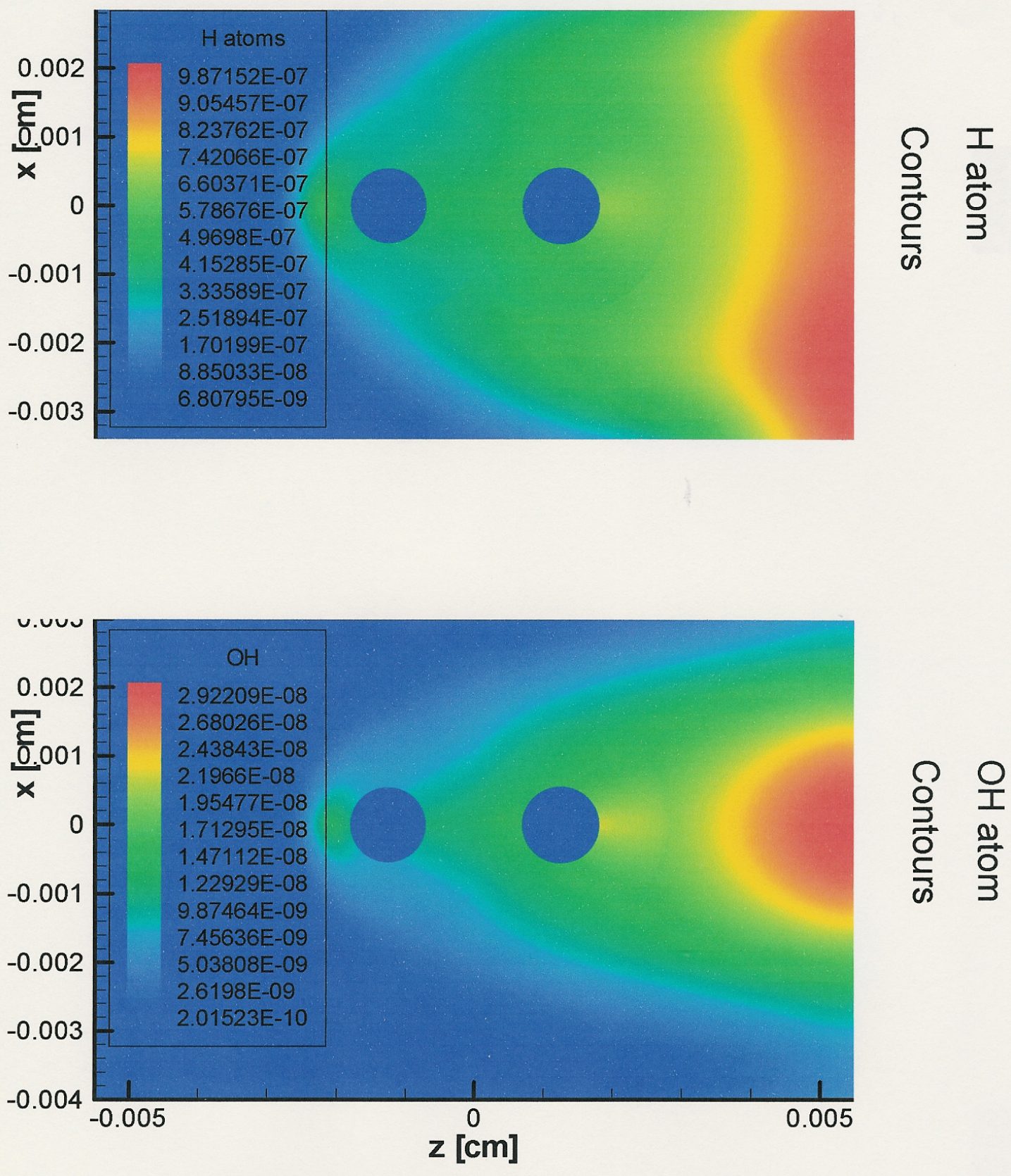

Figure (2) Distribution of Species Radical Around a Droplet Group

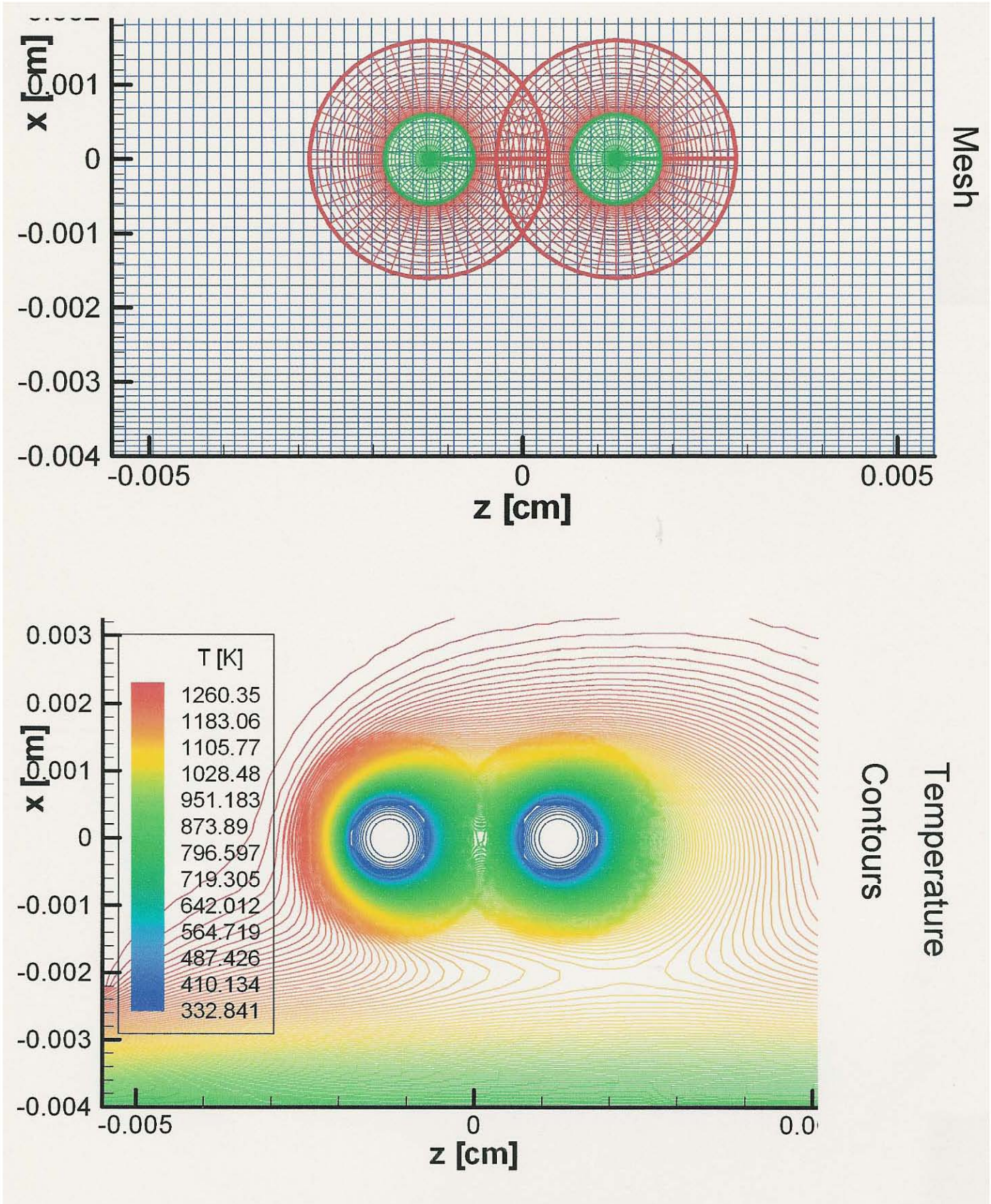

Figure (3) Mesh and Temperature Contours Around a Droplet Group Near a Cold Wall