Gravitational Effects in Reactive Flows: From Physics to Large Eddy Simulation Modeling

Sergei Chumakov, T-CNLS; Natalia Vladimirova, University of Chicago

We use direct numerical simulations to investigate the effects of gravity in reacting flows. We consider two miscible fluids with small density difference; a reaction mechanism transforms one fluid into the other. We use a simple reaction model that is described by a single reaction progress variable, and the Boussinesq approximation for gravity. The combination of these two models allows us to focus on the interaction between gravity and reaction without interference of thermochemistry, compressibility, shock waves, density stratification, and other phenomena that make numerical simulations and interpretation of results much more complicated. The system is amenable to rigorous analysis [1] and yet is realistic enough for comparison with experiments, for instance, experiments with auto-catalytic reactions [2].

Here we describe the numerical setup that models a bubble of reaction products rising in reactant fluid. This setup has an astrophysical application. Several explosion scenarios of Type Ia supernovae involve a bubble of nuclear reaction products that rises towards the surface of the white dwarf star. Unlike regular hydrocarbon flames, the density change across the reaction front is very small and thus the Boussinesq approximation is justified. On the scale of the star the flame is very thin, and resolving the detailed reaction network at the flame scale is impractical; the simplified reaction model captures the most important effects.

The reaction at the surface of the bubble transforms “cold” material surrounding the bubble into “hot” reaction products. As the bubble grows in volume, its buoyancy increases. (See Fig.1.) When the bubble becomes large enough, the Rayleigh-Taylor instability (RTI) develops on the upper surface of the bubble. (See Fig. 2.) The instability stretches the reacting surface of the bubble and enhances the total reaction rate, further increasing the buoyancy.

The continuing efforts to follow the evolution of the bubble as a part of whole-star simulations [3–5] encounter the problem of tremendous separation of scales: millimeters (the flame front thickness) to thousands of kilometers (size of the star). All such simulations are initialized with relatively large bubbles and rely on assumptions about the state of such bubbles. Due to RTI, later bubble development is extremely sensitive to the subgrid (LES) model for reaction. Numerical simulations of small standalone bubbles are restricted to 2-D and axisymmetric bubbles [6,7]. Important 3-D effects, such as the development of the RTI on the top surface of the bubble, are not yet understood.

In our simulations, we study the effect of initial perturbations on the surface of a 3-D reacting bubble. The goal is to quantify the effect of the perturbations on the bubble growth rate and speed and how the induced flow influences the RTI on the surface of the bubble. The simulations are performed with the 3-D spectral code [8]; the 3-D spectral elements code [9] and axisymmetric finite difference code [7] are used for cross-code comparison. All three codes are parallelized using MPI and perform well on distributed supercomputers.

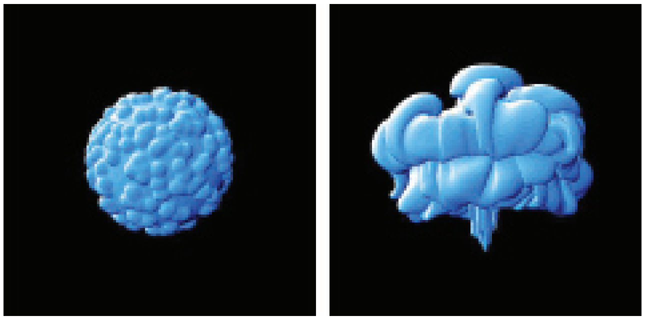

Fig. 1.
Initially perturbed surface of the bubble (left) and the surface of the bubble at later time (right).

The application of the DNS database is an *a priori* evaluation of the subgrid-scale models for Large Eddy Simulation (LES). The models in development include SGS scalar flux, SGS scalar dissipation, and SGS energy dissipation. An important extension of the existing set of models is the ability to predict the effect of SGS front stretching and curving on the gross reaction rate.

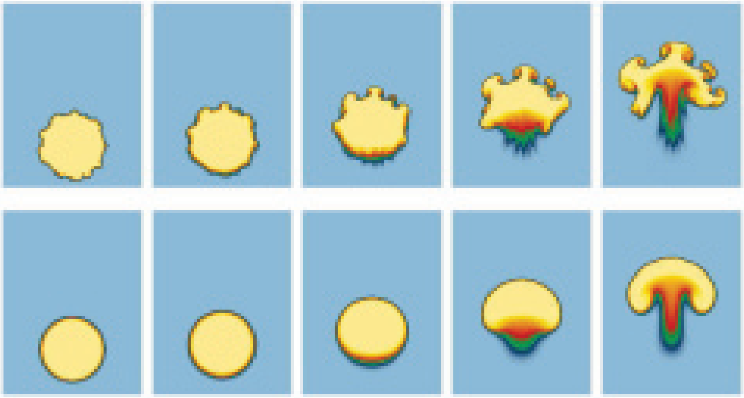

Fig. 2.
Comparison of bubbles with initially perturbed and smooth surfaces; the images show the vertical slice of 3-D bubbles at equal time intervals.

For more information contact Sergei Chumakov at chumakov@lanl.gov.

[1] H. Berestycki, et al., *Analyse Non Lineaire* **23**, 407 (2006).
[2] M.C. Rogers and S.W. Morris, *Phys. Rev. Lett.* **95**, 024505 (2005).
[3] F.K. Roepke, et al., *arXiv:astro-ph*/0609088 (2006).
[4] T. Plewa, et al., *Astrophys. J.* **612**, L37 (2004).
[5] A.M. Khokhlov, *Astrophys. J.* **449**, 695 (1995).
[6] M. Zingale and L.J. Dursi, *arXiv:astro-ph*/0610297 (2006).
[7] N. Vladimirova, *Combustion Theory and Modelling* (2007), in press.
[8] S.G. Chumakov, *J. Fluid Mech.* **562**, 405–414 (2006).
[9] H.M. Tufo and P.F. Fischer, *J. Parallel and Distributed Comput.* **61**, 151 (2001).

Funding Acknowledgements
NNSA's Campaign 4, Secondary Assessment Technology; and University of Chicago Center for Astrophysical Thermonuclear Flashes.