

CANTERA: An open-source, object-oriented software suite for combustion

David G. Goodwin
Division of Engineering and Applied Science
California Institute of Technology

Cantera is an open-source, object-oriented suite of software tools to aid in simulating problems in combustion and related fields. Some of its key features are:

1. Efficient C++ code to evaluate thermodynamic properties, transport properties, and chemical kinetic quantities for gas mixtures, liquid solutions, and surfaces;
2. Object-oriented;
3. Callable from Fortran 77 and 90 via interface libraries;
4. Backward-compatible with Chemkin-II, allowing straightforward porting of Chemkin-II-based user codes;
5. Single- and multi-phase chemical equilibrium solvers;
6. Interfaces for popular problem-solving environments (MATLAB, Python)
7. Easy-to-use tools for simulating zero-dimensional reactor networks in Python or MATLAB;
8. Efficient Newton/time-stepping solver for multi-domain, 1D reacting flows;
9. One-dimensional flames (burner-stabilized premixed, stagnation-point premixed with surface chemistry, counterflow non-premixed) ;
10. Support for electrochemistry and fuel cell modeling.

Cantera development began in 1998, with the first public release in 2000. Cantera has grown substantially since then, both in terms of the code capabilities and the number of users. Although the total number of users is unknown, the web-based users group has nearly 500 members, and the package is downloaded on average 15--20 times per day.

In this talk, I will review some of the history of Cantera, discuss the design principles that have contributed to the success of Cantera, and also describe some of the near-term challenges that must be met in order to continue to support the needs of an expanding, diverse user community.