An Open-Source, Extensible Software Suite for CVD Process Simulation

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Chemical vapor deposition processes involve a complex interplay of chemistry and transport, both in the vapor and on the surface. Arriving at a mechanistic understanding usually requires both experimental process diagnostics and numerical simulation. Just as appropriate tools (gas chromatographs, lasers, spectrometers) are required for diagnostics, suitable numerical tools are needed for simulation, including ones to compute chemical equilibrium, simulate stirred reactors or reacting flow problems with surface chemistry, carry out reaction path analysis, among others. To be most effective, these software tools should be open-source, so that their internal workings can be examined if necessary (as can be done with hardware), should be extensible, and should have easy-to-use interfaces.

This paper describes a suite of open-source software tools designed to provide a flexible, extensible toolkit for simulations involving chemical kinetics, thermodynamics, and transport processes. Known as Cantera, it can be used to efficiently evaluate thermodynamic properties, transport properties, and homogeneous and heterogeneous kinetic rates in user-written application programs, compute chemical equilibrium, simulate kinetics in networks of stirred reactors, compute steady-state reacting stagnation flows, calculate the structure of flat flames, and generate reaction path diagrams.

Cantera is object-oriented, and provides objects that represent components of a simulation — gas mixtures, reactors, flow controllers, kinetics models, surfaces, equations of state, flames, ODE integrators, reaction path diagrams, and so on. Numerical models are constructed in a physical, intuitive way, by creating and assembling components. This modular, component-based approach allows an enormous range of processes to be simulated (far more than a conventional turn-key application program with fixed capabilities can provide).

Cantera is designed to handle problems with large elementary reaction mechanisms efficiently. Mechanisms may include any number of species and reactions, and may be imported from specifications in text files in standard formats [2]. Efficient algorithms are used to evaluate reaction rates of progress and species chemical production rates, with the result that kinetics simulations with Cantera may run significantly faster than equivalent simulations with other packages.

Cantera consists of a "kernel" written in C++ that provides the core numerical capabilities, and interface packages that allow using Cantera from other languages or applications. A MATLAB toolbox, an interface to the Python scripting language, and a Fortran 90 module are provided. Using Cantera from MATLAB or Python, problems can be solved quickly by writing short scripts. As an example, a Cantera Python script to read in a reaction mechanism, carry out an adiabatic, constant-volume kinetics simulation,

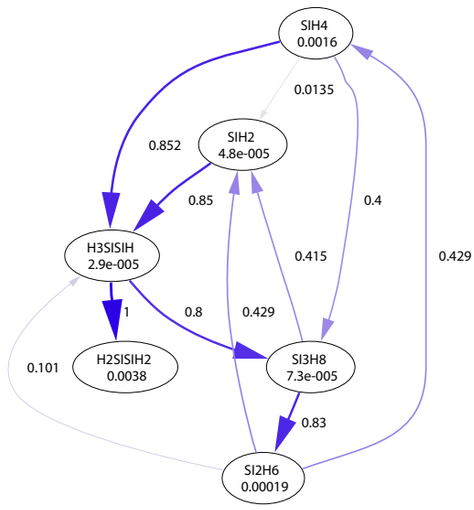

Figure 1: Example reaction path diagram tracing the flow of elemental silicon among species. Each node is labeled with the species name and mole fraction, and each path is labeled with its net relative flux. It is also possible to show arrows for the forward and reverse paths separately, and to list the reaction contributing to each path.

and print the species mole fractions is shown below.

```
gas = IdealGasMix('silane.inp')
gas.setState_TPX(1100.0, 0.1*OneAtm,
                 'SIH4:0.01,HE:0.99')
r = Reactor(gas)
r.advance(0.01)
print r.moleFractions()
```

Reaction path diagrams like that shown in Figure 1 can be generated automatically at any point in a simulation. This diagram shows the reaction paths for the gas state at the end of the above simulation, computed using the mechanism of Ho, Coltrin, and Breiland [1].

The current capabilities of Cantera, near-term development plans, and benchmark test results will be presented. Cantera may be downloaded from http://www.cantera.org.

REFERENCES

[1] P. Ho, M.E. Coltrin, and W.G. Breiland. Laser-induced fluorescence measurements and kinetic-analysis of Si atom formation in a rotating- disk chemical-vapor-deposition reactor. *J. Phys. Chem.*, 98(40):10138–10147, 1994.

[2] R. J. Kee, F. M. Rupley, and J. A. Miller. Chemkin-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics. Technical Report SAND89-8009, Sandia National Laboratories, 1989.