

Development and validation of a new MATLAB/GUI based thermochemical code

Alberto Cuadra-Lara & Marcos Vera

Department of Thermal and Fluids Engineering, University Carlos III of Madrid
acuadra@ing.uc3m.es (ACL), marcos.vera@uc3m.es (MV)

MSC11, 11th Mediterranean Combustion Symposium
Tenerife, Spain | Jun 16-20 2019

Motivation

In a wide range of applications involving chemically reacting flows, thermochemical calculations involving overall mass and energy balances with chemical equilibrium are enough to estimate the overall performance of the system. This is often determined by magnitudes such as the adiabatic flame temperature or the equilibrium composition of the products. Thermochemical codes have been developed for this purpose dating back to the late 1940's at the NACA Lewis Flight Propulsion Laboratory, with the initial aim of evaluating rocket performance of various potential propellants. The use of thermochemical codes has been growing ever since, and today they are basic research tools both for combustion applications and in the analysis of the thermal decomposition of high-energy materials (HEMs), including deflagration and detonation conditions.

Introduction

As a first step towards the development of a wider-scope thermochemical tool, in this work we present a thermochemical code with application to gaseous combustion problems recently implemented by the authors in MATLAB®. The code solves six chemical equilibrium problems (TP, HP, SP, TV, EV and SV transformations; where T denotes temperature, P pressure, H enthalpy, S entropy, E internal energy and V volume), incident and reflected planar shock waves, as well as ideal detonations according to Chapman-Jouguet theory, assuming always ideal gases in all cases.

The code computes the equilibrium composition using equilibrium constants rather than by minimization of the Gibbs–Helmholtz free energy, and employs NASA's 9-coefficient polynomial fits to evaluate the thermodynamic properties. Along with the plain code, the new tool has been equipped with a Graphical User Interface (hereafter **Combustion-Toolbox**) developed in MATLAB® 2018 under AppDesigner.

Results computed with **Combustion-Toolbox** have been validated against, and are in good agreement with, NASA's Chemical Equilibrium with Applications (CEA) program [1], CANTERA, and Caltech's Shock and Detonation Toolbox [2]. Moreover, the time required for the computations is comparable to that of other existing codes. **Combustion-Toolbox** has teaching and research aspirations and will be distributed as open source package as soon as it has been fully tested.

Combustion-Toolbox

Available thermochemical transformations

1. **TP**: equilibrium composition at defined temperature and pressure.
2. **HP**: adiabatic temperature and composition at constant pressure.
3. **SP**: isentropic compression/expansion to a specified pressure.
4. **TV**: equilibrium composition at defined temperature and constant volume.
5. **EV**: adiabatic temperature and composition at constant volume.
6. **SV**: isentropic compression/expansion to a specified volume.
7. **SHOCK I**: planar incident shock wave at normal incidence.
8. **SHOCK R**: planar reflected shock wave at normal incidence.
9. **DET**: Chapman-Jouguet detonation (CJ upper state).

Database

- Employs 9-coefficient polynomial fits to evaluate the thermodynamic properties from NASA's thermodynamic database (2075 species) [3].

Features

- The reactant mixture is specified by fuel-air mixture, equivalence ratio, and/or the number of moles (or mole fraction) of the different species, which can also have different temperature.
- Parametric sweeps for different input parameters, such as the equivalence ratio ϕ .
- Solves both complete and incomplete (i.e., dissociation) combustion problems. For incomplete combustion, the minor species present in the final equilibrium can be selected at will, with some preselected subsets already defined.
- The equilibrium composition can be solved considering condensed species (graphite so far).
- Can estimate thermal NO_x for a given residence time.
- Automatic plots of the product composition and thermodynamic properties as a function of the equivalence ratio ϕ .
- Detailed results reported via the MATLAB® command window or an Excel file.
- Personalized use and modification of the plain code and routines.
- Easy access to all the results of a working session through an editable tree diagram.

Algorithms

- The equilibrium composition is computed using an iterative segregated solver that estimates first the minor species from suitable (nonlinear) equilibrium conditions and then corrects the major species to guarantee (linear) atom conservation.
- The thermochemical transformations HP, SP, EV, and SV are computed using a Steffensen-Aitken root-finding algorithm which employs the iterative segregated solver.
- Incident and reflected planar shock waves, as well as ideal detonations according to Chapman-Jouguet theory, are computed using a Newton-Raphson root-finding algorithm as [4]. It also employs the iterative segregated solver.

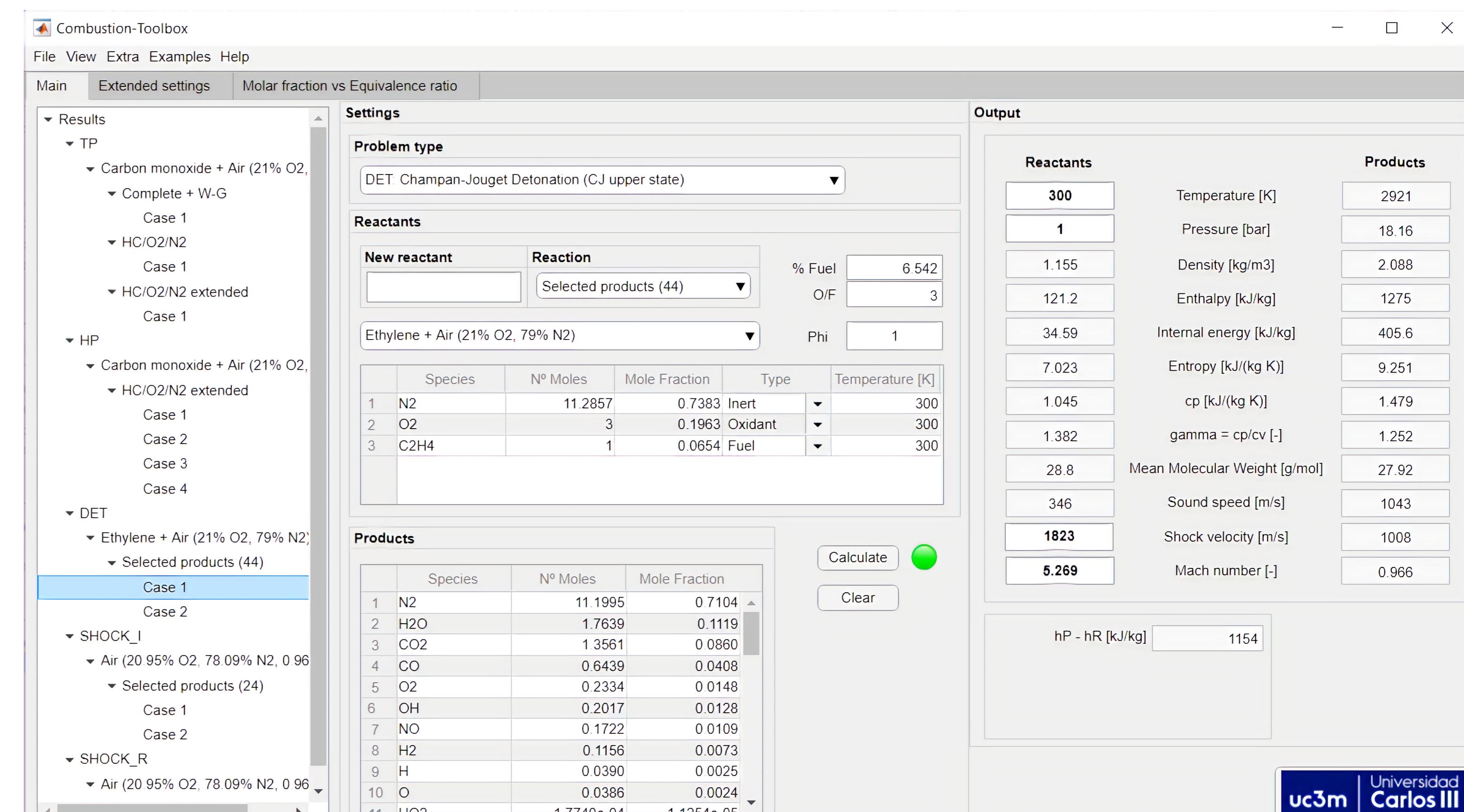


Figure 2: Current state of the GUI Combustion-Toolbox developed.

Results

In order to validate the model, Figure 3 shows the adiabatic flame temperature for different fuel-air mixtures initially at room temperature and pressure. Figure 4 shows the variation of the molar fraction of the product species with the equivalence ratio for lean to rich acetylene-air mixtures, with

$$\phi_{gr} = \frac{2}{x - z} \left(x + \frac{y}{4} - \frac{z}{2} \right), \quad (1)$$

the theoretical starting value for soot formation, and x, y, z the number of moles of carbon, hydrogen and oxygen in the fuel molecule, respectively. Figure 5 shows some results (density, detonation velocity, temperature and pressure), obtained from a Chapman-Jouguet detonation of an ethylene-air mixture.

All the results are in good agreement with NASA's Chemical Equilibrium with Applications (CEA) program, CANTERA, and Caltech's Shock and Detonation Toolbox.

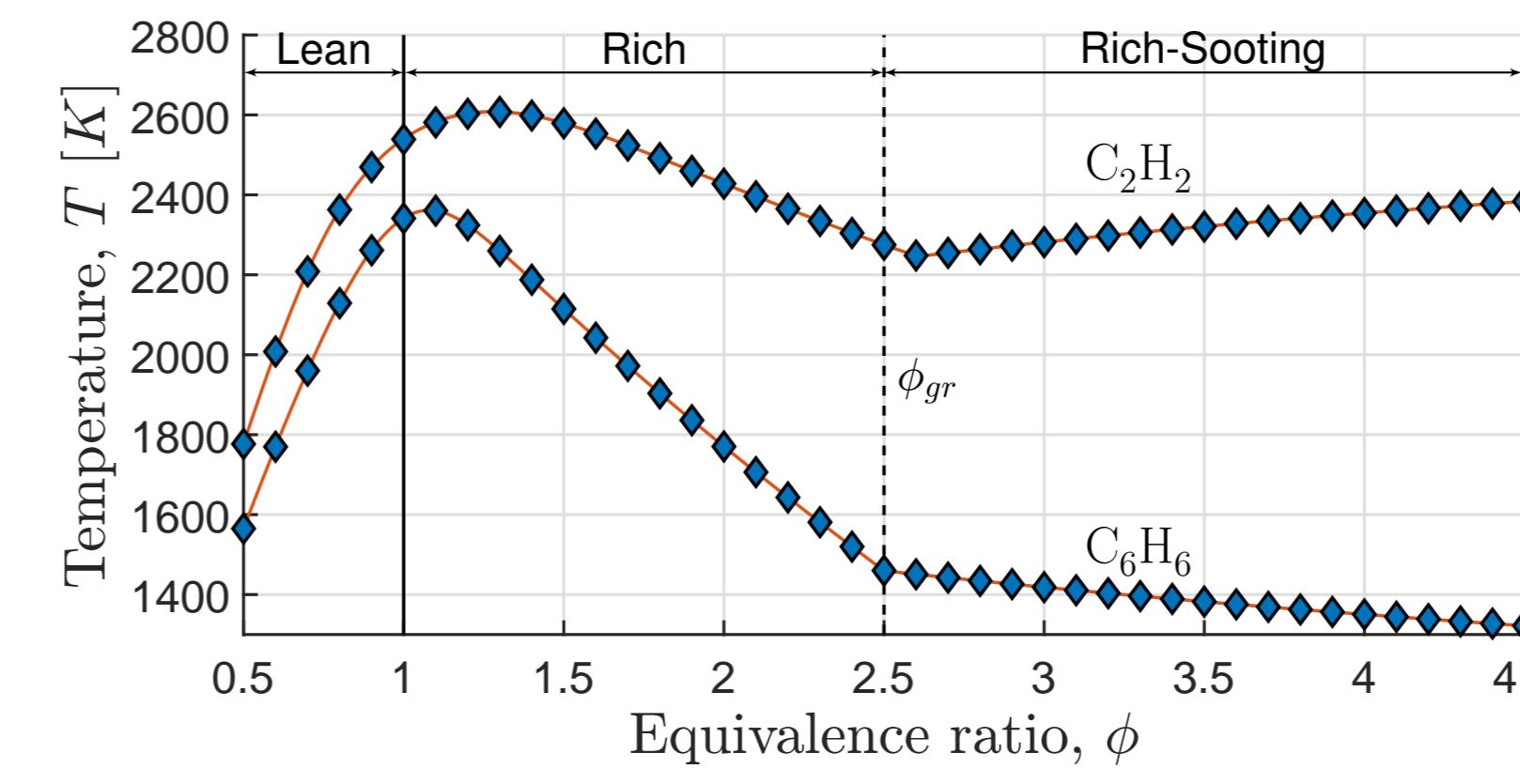


Figure 3: Adiabatic flame temperature as a function of the equivalence ratio for different fuel-air mixtures: acetylene (C_2H_2), and benzene (C_6H_6). Combustion-Toolbox (line) and CEA (diamond).

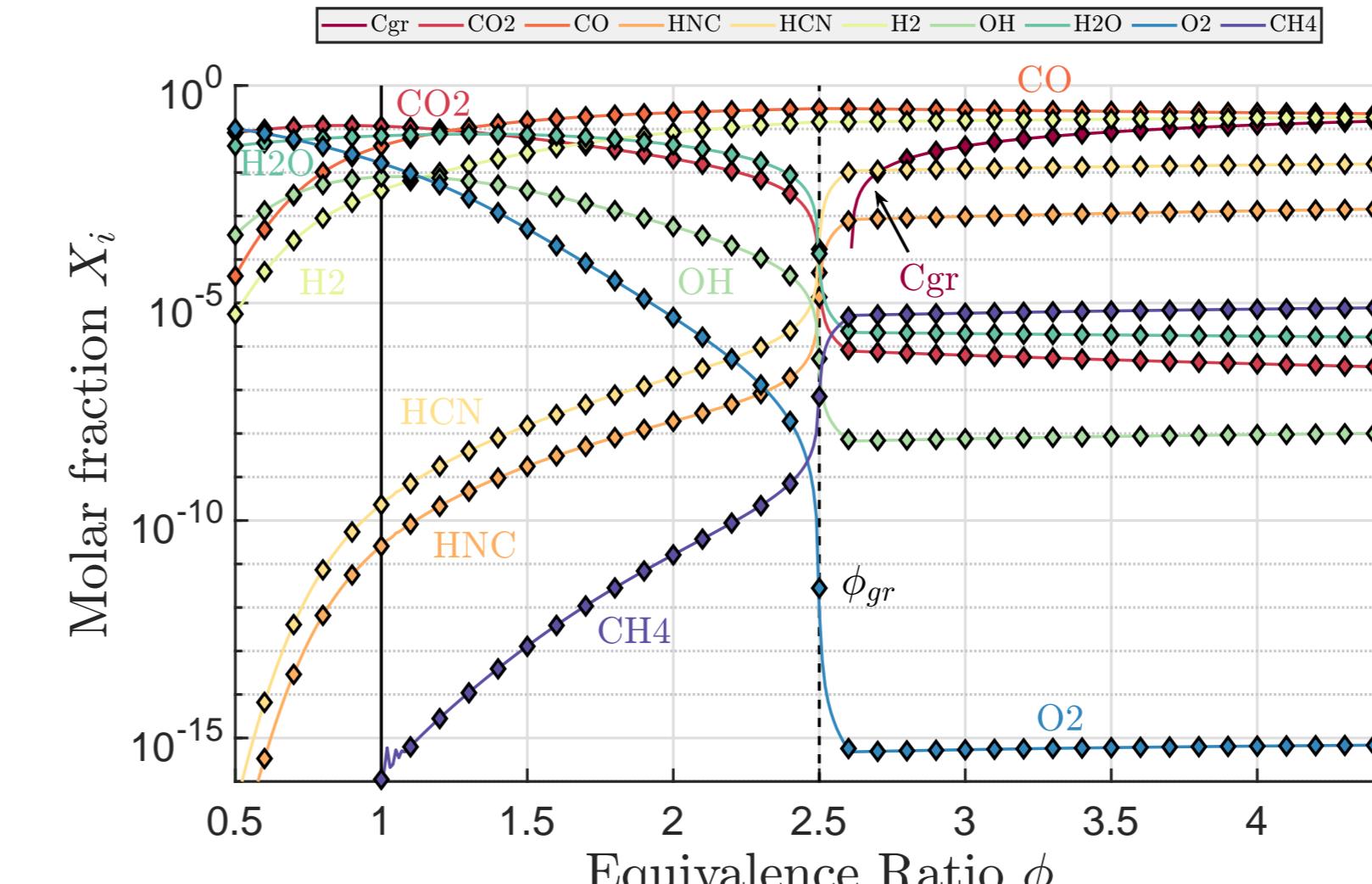


Figure 4: Variation of molar fraction with equivalence ratio for lean to rich acetylene-air mixtures. Combustion-Toolbox (line) and CEA (diamond).

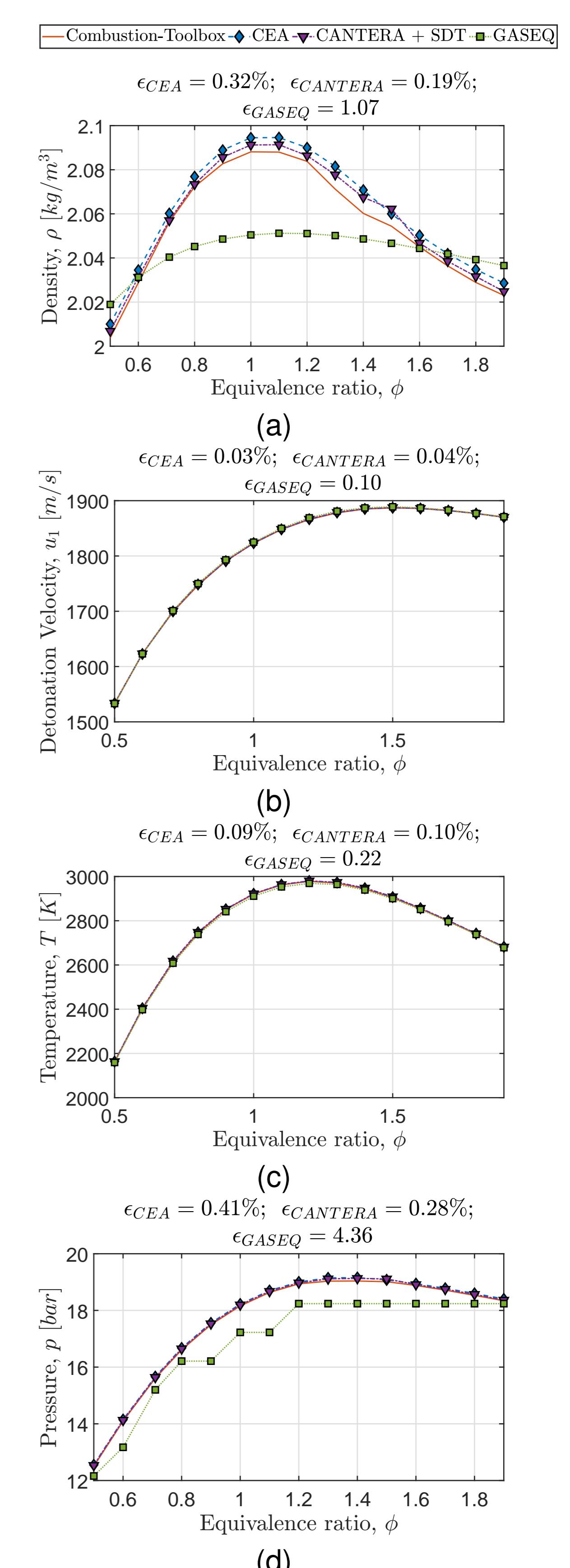


Figure 5: Chapman-Jouguet detonation properties for an ethylene-air mixture initially at room temperature and pressure as a function of the equivalence ratio: (a) density, (b) detonation velocity, (c) temperature, (d) pressure. Results validated with CEA (NASA) and CANTERA with Caltech's Shock and Detonation Toolbox.

References

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