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Thermo-chemical Analyses of Steady Detonation Wave using the Shock and Detonation Toolbox in Cantera

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Abstract

We describe the implementation of several thermo-chemical analyses in Cantera and the Shock & Detonation Toolbox (SDT), that can be employed to investigate the chemical dynamics of planar steady detonation. A Matlab Graphical User Interface has also been developed to post-process the data provided by the detonation codes. These utilities will be made available on request and in the future releases of the SDT.

keywords: Planar steady detonation, Thermo-chemical analyses, Cantera

1 Introduction

Detonation waves are multi-dimensional, unsteady combustion waves that propagate at a super-sonic velocity [1, 2]. They are characterized by the strong coupling between the leading shock front and the chemical reaction zone behind it. The auto-ignition of the reactive mixture is ensured by adiabatic shock compression. As a result, the expansion induced by the combustion process sustains shock propagation. The simplest model considers a detonation wave consists of a steady, planar shock wave, followed by a reaction zone. At thermodynamic equilibrium, the flow becomes sonic with respect to the leading shock wave. This model was independently proposed by Zel'dovich, von Neumann, and Doering, and is referred to as the ZND model [2]. With the increase of computational resources, numerical implementation of the ZND model in Chemkin became possible [3]. The ZND model was later implemented in Cantera [4] and is currently available in the Shock and Detonation Toolbox (SDT) [5]. The SDT has become very popular over the years and is now widely employed [6, 7]. Although Cantera enables performing a number of thermo-chemical analyses, such as rate of production or sensitivity analyses, no implementation of such utilities is available in the SDT [8]. This limits the utilization of the SDT since the users have to implement such capabilities themselves. Making available such utilities in the SDT would be tremendously beneficial to the detonation community. Our goals were to describe several widely employed thermo-chemical analyses and to explain their implementation in the SDT. We also aim to provide a simple and versatile Matlab interface to post-process the data provided by the SDT codes.

2 Steady detonation model

We have considered the steady planar detonation model. The formulation is

$$\eta\frac{dw}{dt} = w\dot{\sigma};\ \eta\frac{d\rho}{dt} = -\rho\dot{\sigma};\ \eta\frac{dP}{dt} = -\rho w^2\dot{\sigma};\ \frac{dy_k}{dt} = \frac{W_k}{\rho}\dot{\omega}_k \tag{1}$$

with

$$\dot{\sigma} = \sum_{i=1}^{N}\left(\frac{\bar{W}}{W_i} - \frac{h_i}{C_P T}\right)\frac{\omega_i}{\rho}. \tag{2}$$

with t: time, w: flow speed in the detonation frame, ρ: density, P: pressure, σ: thermicity, M: Mach number, η=$1 - M^2$: sonic parameter, Y_i: mass fraction, ω_i: source term, N: number of species, $\bar{W}$: mean molar mass, W_i: molar mass, h_i: enthalpy, C_P: heat capacity at constant pressure, and T: temperature.

3 Thermo-chemical analyses

3.1 Fundamental equations

We give the equations employed to perform three different thermo-chemical analyses and explain the physical meaning of the quantities they provide.
The heat release rate of the j^{th} reaction (HRR_j) is expressed in J/kmol-m^3-s, and is given by

$$\mathrm{HRR}_j = \Delta_r H_j^{\circ} \times r_j, \tag{3}$$

where $\Delta_r H^\circ$ is the standard enthalpy of reaction, and r is the net rate of reaction. For reversible reaction, r can be positive or negative, depending on the dominant direction (forward or backward) of the reaction. The HRR enables to determine which are the dominant exo- and endo-thermal chemical processes. The HRR analysis is always relevant, and has proven especially useful to explain the origin of complex, non-monotonous heat release profiles in various chemical systems [9–13]. The HRR can also be time-integrated to provide the total heat released by each reaction during the detonation process.
The rate of production for the i^{th} species by the j^{th} reaction ($RoP_{i,j}$) is expressed in kmol/m^3-s and defined as

$$\mathrm{RoP}_{i,j} = \nu_i r_j, \tag{4}$$

where N is the total number of reactions. The RoP enables to identify the most important chemical pathways producing or consuming a given chemical species. Reaction pathway diagram can be established based on the RoP of several species.
Sensitivity analyses (Sens) enable to identify the most important reactions with respect to a given parameter of the thermo-chemical system. Such information are important to develop reduced reaction models for multi-dimensional simulation of detonation. These parameters can be species concentration but also the temperature. The normalized sensitivity coefficient of a parameter P_r with respect to the rate constant of the reaction j is defined as

$$C_j^{P_r} = \frac{\partial \ln P_r}{\partial \ln k_j} = \frac{k_j}{P_r}\frac{\partial P_r}{\partial k_j}, \tag{5}$$

where k_j is the rate constant of reaction j. The sensitivity coefficient has no unit. A positive/negative coefficient indicates that the reaction promotes/inhibits the production of i.

3.2 Numerical implementation

First, the ZND model is solved using the SDToolbox. The code calculates the Chapman-Jouguet (CJ) detonation velocity. Using this velocity, the post-shock/von Neumann state is obtained and is used as the initial state for integrating Equation 1. Details of the numerical methods can be found in [5]. It is noted that a new CJ velocity solver, based on the root solver of SciPy, was designed to improve the efficiency. Secondly, since the solution of the ZND model provides the state of the mixture at every instant, the HRR, RoP and sensitivity coefficient can be calculated accordingly. For HRR and RoP, $\Delta_r H^\circ$, r_j and ν_i can be directly obtained from Cantera. Relevant python functions are

```
def HRR(gas):
  HRR_i = - gas.net_rates_of_progress * gas.delta_standard_enthalpy
  HRR_t = np.sum(HRR_i)
  return HRR_i, HRR_t
```

```
def RoP(gas, species):
  index = gas.species_index(species)
  v_k = gas.product_stoich_coeffs()[index,:] - gas.reactant_stoich_coeffs()[
      index,:]
  RoP = gas.net_rates_of_progress * v_k
  return RoP
```

For sensitivity coefficient, the rate constant of the targeted reaction is perturbed by 1%. The perturbed reaction model is then used to solve the ZND model. The sensitivity coefficient is finally approximated with a forward difference. The essential part of this function is

```
def SEN(gas1,mech,cjspeed,Rpert,dp):
  ...
  out = zndsolve(gas, gas1, cjspeed)
  for Ri in Rpert:
    gas_p1 = PostShock_fr(cjspeed, gas1.P, gas1.T, gas1.X, mech)
    gas_p1.set_multiplier(1+dp, Ri-1) # perturb the reaction rate constant
        of Ri by dp*100%
    out_p1 = zndsolve(gas_p1, gas1, cjspeed, t_eval = out['time'][0:N1])
    N2 = len(out_p1['time'])
    SEN_i = (out_p1['T'] - out['T'][0:N2]) / out['T'][0:N2] / dp
    ...
```

3.3 Post-processing and examples

The post processing part is integrated into a MATLAB App with user interface (UI). This UI is shown in Figure 1 and offers three different types of analysis corresponding to functions described in section 3.2.

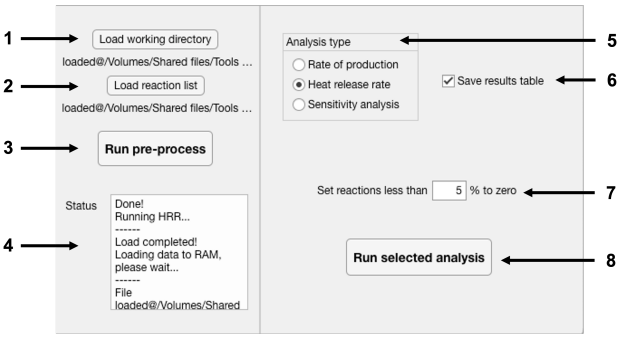


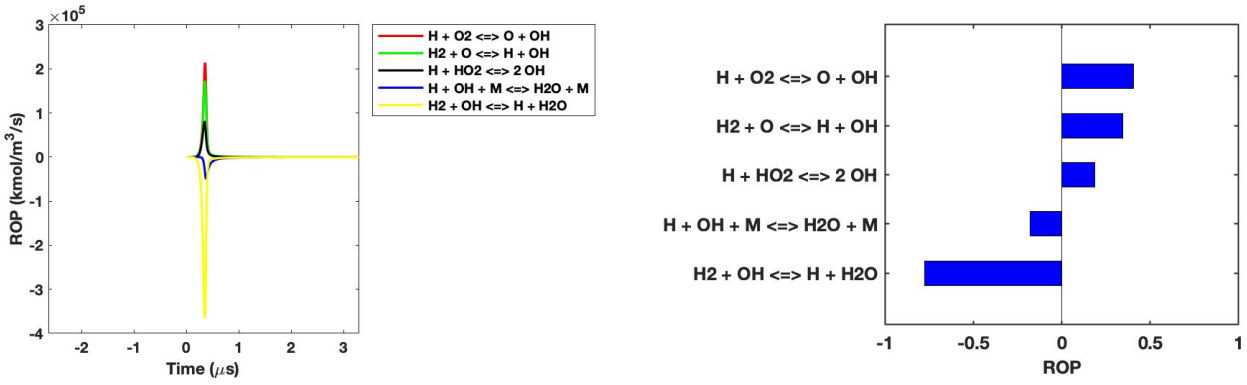
Figure 1: The UI of the post-processing MATLAB App.

The steps to follow to use the UI App are:

- I. Use buttons 1 and 2 to load the working directory (WD) and the list of reactions (LoR) used for the ZND simulation. The WD should only contain one type of file (HRR, or RoP, or Sens). No other files should be located in this directory, including the LoR file. Several files of the same type can be included and will be post-treated one after the other. The LoR can be generated from the .cti file using "reactionListGenerator.py" provided in the package.
- II. Use button 3 to load the files to the RAM. This approach is more convenient when dealing with large amounts of data.
- III. Use button 5 to select the analysis type.
- IV. Use button 8 to generate the post-processed results, which are saved in "results folder" inside the WD. By checking box 6, the data used in the figures are save in csv file in "results folder". The textbox 7 controls the number of reactions included.

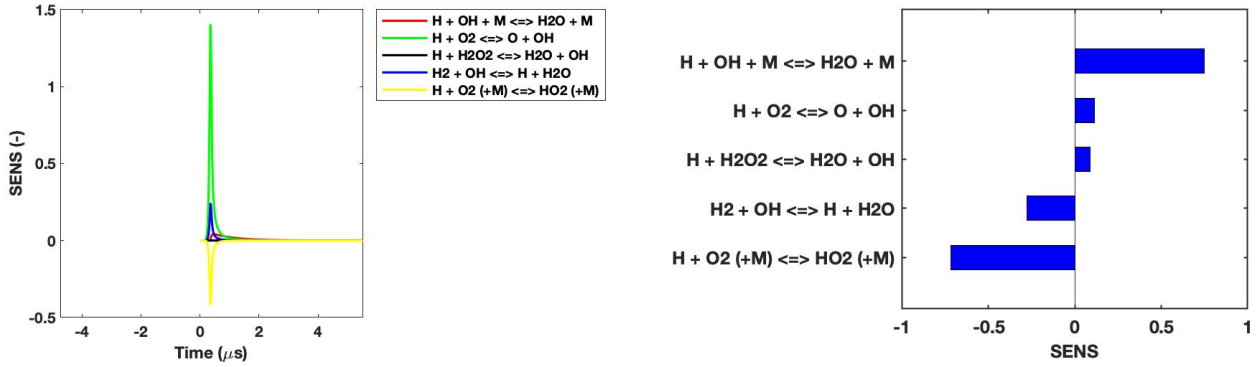
The post-processing figures are saved in two formats: JPEG and MATLAB fig file. The figures obtained after post-processing with our App are shown in Figure 2 to 4. To generate the normalized RoP and sensitivity results shown in Figure 3 b) and 4, the following approach is employed: i) the curves are integrated and sorted as positive and negative according to the sign of the area; ii) the total absolute value of the area in each group is calculated and used to normalize the area of each individual reactions in each group. Based on the value $n\%$ used in textbox 7, the reaction for which the area is lower than $n\%$ are removed from the analysis results. It is noted that the auto-scaling of the figures might not be very suitable under particular conditions. Since the data can be saved as MATLAB figures and in .xlsx files, archival quality figures can be prepared by the user.

HRR profiles for a ZND detonation propagating in a H_2-air mixture. Φ=1, P_1=100 kPa, T_1=300 K.



a) Temporal profiles b) Integrated results

Figure 2: Temporal and integrated RoP for a ZND detonation propagating in a H_2-air mixture. Φ=1, P_1=100 kPa, T_1=300 K.



a) Temporal profiles b) Integrated results

Figure 3: Temporal and integrated C_s for a ZND detonation propagating in a H_2-air mixture. Φ=1, P_1=100 kPa, T_1=300 K.

4 Conclusions

We describe the implementation of utilities to perform thermo-chemical analysis, including HRR, RoP, and sensitivity coefficients, under steady detonation conditions. These include python examples for planar detonation, as well as a Matlab UI to post-process the data from Cantera. The interface can also be used to post-process data obtained using constant volume and constant pressure adiabatic reactors, as long as the format of the input file is respected. Further extension to quasi-steady [14] and quasi-unsteady detonation models [15] is possible and would enable studying the impact of curvature and unsteadiness on the induction zone length and chemical pathway, as done in [16, 17]. The utilities are available as additional material of this paper and will be distributed in the next versions of the SDT.

Declarations

The authors have no conflict of interest. The data are available upon reasonable request.

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