

## Supplementary Material

## **1 DETONATION MODEL FOR A HETEROGENEOUS MEDIUM**

This model is based on simple principles of determining the characteristics of a Chapman-Jouguet detonation in a system of unmixed gaseous components with different initial temperatures. The pressure and velocity of all the components are equilibrated in the initial and final states (see p. 496 in Gavrilyuk and Saurel (2007)). The detonation wave is assumed to be planar. Its thickness is small with respect to the length scale of heterogeneities, so that at any point, the same component is found on both sides of the detonation wave. Mass and energy exchange between the components is neglected within the detonation wave.

The following equations can be written for the flow parameters in the moving frame attached to the detonation front:

• mass flow rate of component k

$$G_{k,1} = G_{k,2} = G_k \tag{S1}$$

• stagnation enthalpy of component k

$$G_k H_{k,1} = G_k H_{k,2}$$
  
 $H_{k,1} = H_{k,2} = H_k$  (S2)

Indices 1 and 2 correspond to the initial and final states respectively.

The mass flow rate and stagnation enthalpy of component k are expressed as:

$$G_k = A_{k,n}\rho_{k,n}u_n \tag{S3}$$

$$H_k = h_{k,n} + \frac{1}{2}u_n^2$$
 (S4)

where index n = 1 or 2 identifies the state; A is the flow tube cross-sectional area;  $\rho$  is the mass density; h is the mass-specific enthalpy; u is the flow speed assumed to be equal for all the components in the same state.

For the flow of all the components in the moving frame, the following relations are verified:

• total area

$$A_{\Sigma,1} = A_{\Sigma,2} = A_{\Sigma} \tag{S5}$$

• total mass flow rate

$$G_{\Sigma,1} = G_{\Sigma,2} = G_{\Sigma} \tag{S6}$$

• total impulse

$$G_{\Sigma}u_1 + P_1A_{\Sigma} = G_{\Sigma}u_2 + P_2A_{\Sigma} = F_{\Sigma}$$
(S7)

where each quantity with index  $\Sigma$  expresses the sum of respective quantities of all the components.

To close the problem, two conditions are imposed:

$$u_1 = D \tag{S8}$$

$$u_2 = c_2 \tag{S9}$$

where D is the detonation speed with respect to the gas in the initial state;  $c_2$  is the average speed of sound for the final state.

For a heterogeneous medium, the speed of sound can be evaluated using the following equation (Wood formula on p. 7 in Benjelloun and Ghidaglia (2021)):

$$\frac{A_{\Sigma}}{\rho c^2} = \sum_{k=1}^{N_k} \frac{A_k}{\rho_k c_k^2} \tag{S10}$$

with the average density expressed as:

$$\rho = A_{\Sigma}^{-1} \sum_{k=1}^{N_k} \rho_k A_k \tag{S11}$$

The initial condition is specified in terms of pressure,  $P_1$ , component temperatures,  $T_{k,1}$ , and component mass fractions,  $Y_{k,1}$ . Each component is defined as a mixture of chemical species with a particular composition. The remaining parameters of the components  $(h_{k,1}, \rho_{k,1})$  are found from their thermodynamic models. The initial areas,  $A_{k,1}$ , are defined proportional to the component volume fractions:

$$A_{k,1} \propto Y_{k,1} / \rho_{k,1} \tag{S12}$$

To solve the problem, the algorithm described below can be used. Starting values are set for the detonation speed,  $D = u_1$ , and final state parameters  $P_2$  and  $u_2$ . The following steps are made to determine the final state corresponding to a given parameter set  $(D, P_2, u_2)$ . Using equations S2 and S4, static enthalpies of components are:

$$h_{k,2} = h_{k,1} + \frac{1}{2} \left( u_1^2 - u_2^2 \right)$$
(S13)

A specific procedure is used to determine state parameters  $(T_{k,2} \rho_{k,2}, c_{k,2})$  and equilibrium composition for each component from  $P_2$ ,  $h_{k,2}$ , and initial component composition. The final area,  $A_{k,2}$ , is determined from equations S1 and S3:

$$A_{k,2} = A_{k,1} \frac{\rho_{k,1} u_1}{\rho_{k,2} u_2} \tag{S14}$$

The average speed of sound,  $c_2$ , is found from equations S10 and S11.

The following residuals are used to verify the final state:

$$r_u = u_2 - c_2 \tag{S15}$$

$$r_A = A_{\Sigma,1} - A_{\Sigma,2} \tag{S16}$$

$$r_F = F_{\Sigma,1} - F_{\Sigma,2} \tag{S17}$$

The problem parameters  $(D, P_2, u_2)$  are found by solving a non-linear equation system:

$$\begin{cases} r_u = 0\\ r_A = 0\\ r_F = 0 \end{cases}$$
(S18)

The method described above is implemented in the *DetonHeter* code written in Fortran 90. Thermodynamic procedures from the CHEMKIN-II library by Kee et al. (1989) together with the STANJAN equilibrium solver of Reynolds (1986) are used to determine state parameters of the mixture components. The following solution algorithm with nested iteration cycles is used:

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Iteration on D

Iteration on P_2

Iteration on u_2

Update the final state for the current parameter set (D, P_2, u_2)

Determine the residuals (r_u, r_A, r_F)

If |r_u| > \epsilon u, correct u_2 and repeat

If |r_A| > \epsilon A, correct P_2 and repeat

If |r_F| > \epsilon F, correct D and repeat
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In this pseudo-code,  $\epsilon_u$ ,  $\epsilon_A$ , and  $\epsilon_F$  are numerical tolerances.

## 2 APPLICATION TO A ROTATING DETONATION COMBUSTOR

In the present study, the *DetonHeter* code is used to evaluate the detonation speed in a heterogeneous mixture created by propellant injection in a Rotating Detonation Combustor (RDC). Different strategies exist for determining the initial state of heterogeneous mixture. One of them is detailed below.

Let us assume a 3D flowfield from a reinjection simulation for an injection element. A pre-processing step prior to detonation speed evaluation is to determine the properties of the mixture components. The volume of the simulation domain containing the mixture can be sliced at regularly distributed distances from the injection plane. Each slice is processed independently of the others.

In a processed slice, the used flowfield parameters are: static pressure, P, static temperature, T, velocity vector components  $(v_x, v_y, v_z)$ , and species mass fraction vector,  $Y_s$ . These parameters are collected from all computational cells contained in the slice. Temperature and species mass fractions from the computational cells are distributed among several bins, which are defined in terms of equivalence ratio of fresh reactants,  $\phi$ , and mass fraction of burnt gases,  $Y_B$ . An average temperature is determined for each bin from the mass-averaged static enthalpy and species fractions by assuming frozen composition of the gas. Species fractions in a bin are distributed between four components:

• burnt gases including all species but the fresh reactants;

- stoichiometric mixture including fresh reactants in stoichiometric proportions;
- unmixed fuel representing the rest of fuel;
- unmixed oxidizer representing the rest of oxidizer.

For the detonation model, the initial conditions are defined as follows. The pressure is taken equal to the volume-averaged static pressure in the whole slice. The velocity components are mass-averaged in the whole slice, they are used to calculate the detonation velocity in the laboratory reference frame by adding the detonation speed D to the fresh mixture velocity projected on the propagation direction. Given  $N_{\phi}$  bins with respect to the equivalence ratio and  $N_B$  bins with respect to the burnt gases mass fraction, the heterogeneous mixture in a slice includes  $N_{\phi} \times N_B \times 4$  components. The four components in a bin have the same initial temperature equal to the aforementioned average temperature.

In the detonation model, the heterogeneous mixture components, corresponding to the burnt gases and stoichiometric mixture in the initial state, are treated as reactive and their chemical composition is at equilibrium in the final state. The unmixed fuel and unmixed oxidizer are considered to be non-reacting, so their chemical composition must remain unchanged. It is technically possible with the equilibrium solver by introducing additional chemical elements, which are used specifically to compose the non-reacting components.

## REFERENCES

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