# Reduced Order Models for Shock-Induced Combustion of Fuel Mixtures

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#### **1** Introduction

Detonation engines have been of academic interest for a very long time due to their inherent better thermodynamic efficiency compared to the commonly used Brayton cycle, but it has been difficult to realize this potential in practical combustion engines for a variety of reasons. Current work on detonation engines has focused on Rotating Detonation Engines (RDEs), where flow is pushed axially through an annular combustion chamber and a detonation wave rotates azimuthally around the annulus combusting the fuel mixture. There are many experimental and modeling challenges to investigating RDEs. Nevertheless, the feasibility of RDEs has been experimental [4] studies have shown that the RDE is worth continued investigation. We have developed a code for simulating two-dimensional and three-dimensional RDE combustion chambers using the same algorithms that have been applied successfully to PDEs and for general detonation research [5,6]. In our previous papers [7-9], we have investigated several different aspects of hydrogen-air RDEs; including pressure effects and engine sizing, hydrocarbon fuels, as well as describing in more detail the features of the flow field.

Unlike most previous detonation tubes and engines, most experimental RDE rigs inject fuel and oxidizer separately into the annular combustion chamber of an RDE. This produces a stratified mixture with local pockets of fuel-rich and fuel-lean premixture, which can significantly affect the stability and efficiency of the detonation wave. In addition, the premixture is often by design a mixture of different fuels (for example, hydrogen mixed with ethylene), which can significantly alter its reactivity and thus the stability of the detonation wave. Modeling both of these effects are challenging but necessary if modeling is to play an important role in designing RDEs. Due to the size and complexity of RDEs, detailed kinetic models are not feasible to use for simulations of RDEs. The present work develops a reduced order model based on the hydrogen-air induction-time parameter model to simulate RDEs with both stratified premixtures and other fuel mixtures. This method can easily be extended to other fuel mixtures. For this paper, the model is demonstrated for detonation tubes, however, it can be directly applied to rotating detonation engines.

#### **2** Detonation Model

The focus of this paper is on the development of an induction-time parameter model for doing stratified fuels or fuel-blends. Although ultimately this model will be used to simulate full-scale RDE rigs, this paper will focus on detonation tubes, typically on the order of 1 m long and 60 mm in height and with a resolution of 0.1-0.2 mm. Due to the time-scales, grid-scales and the speed of the detonation wave, we solve the inviscid Euler conservation equations, with additional conservation equations for species,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \mathbf{v} = -\dot{w}_{det} \tag{1}$$

where the solution variables are density,  $\rho$ , momentum,  $\rho \mathbf{v}$ , total energy, *E*, and species concentration,  $n_i$ . We use 6th order polynomial curve-fits in temperature for species enthalpy and the ideal gas law to calculate the pressure *P* from total energy *E* and species concentration  $n_i$ , as described in detail in Ref. 9.

For this work, we use a 3-species mixture model. We split the reactant into  $\rho Y_{\text{Fuel}}$  and  $\rho Y_{\text{Air}}$ . For the 3-species mixture model, the reactant densities are convected, and the product density is obtained via  $\rho Y_P = \rho - \sum \rho Y_k$ . The thermodynamic curve-fit coefficients for the product species are computed assuming CJ equilibrium species for a stoichiometric mixture which can be found by running a chemical equilibrium code such as CEA. In addition to this, we modify the heat of formation for each pseudo-species such that the zero state energy at T = 0 K is 0 for all species. This necessitates adding a heat-release term into the energy equation ( $\Delta H$ ). For stoichiometric mixtures, this is fixed by the curve-fit coefficients and will recover the correct detonation velocity, temperature and pressure.

The solution procedure is based on the FCT-algorithm [10] and domain decomposition for the parallelism. The procedure and convergence criteria used for RDEs has been detailed in Ref. 7.

#### **3** Induction-time Parameter Model

The reaction rate term,  $\dot{w}$ , in equation (1) is calculated using an induction-time parameter model [11]. The induction-time parameter model (IPM) is based on the observation that shock-induced combustion consists of two distinct steps. The first step is the build-up of radicals in the shocked gases after the shock-wave passes. After the radicals build up to a critical level, the second step starts representing release of heat from combustion. In the IPM, the first step is represented by convecting an additional conserved scalar,  $\rho\tau$ . This parameter represents the local progress toward building up a critical amount of radicals. When  $\tau = 1$  we have reached the critical point. In regions where  $\tau > 1$ , any reactant is converted to products and heat is released over a characteristic reaction time-scale. The conservation equation for the induction-time parameter is straight-forward:

$$\frac{\partial \rho \tau}{\partial t} + \nabla \cdot \rho \tau \mathbf{v} = \frac{\rho}{t_{ind}}$$
(2)

The source term is dependent on the induction-time at local temperature and pressure conditions. This induction-time can be taken either from experimental correlations (typically shock-tube experiments), or it can be calculated from detailed kinetic models. Our previous work on hydrogen/air detonations used the NRL model to determine the induction-time,  $t_{ind}$ , as a function of temperature, pressure for stoichiometric mixtures [11,12]. There are similar expressions in the literature for ethylene and propane combustion [8]. We have found that heat-release time has only a minor effect on the detonation solution; however, care

must be taken to spread the heat-release out over several time-steps so that the numerical scheme remains stable.

# 4 Extending the IPM for Non-Stoichiometric Hydrogen-Air Mixtures

The IPM's that have been used in our previous work typically assume a specific, uniform mixture. For the NRL model for hydrogen-air combustion, the mixture is assumed to be stoichiometric with diluent. However, for practical RDEs, as discussed above, we typically have a stratified mixture with regions that are fuel-rich or fuel-lean, as well as stoichiometric. We therefore propose to extend the IPM model to account for mixture composition as specified by equivalence ratio.

There are two elements of the induction-time parameter model that are critical for the model to work. The first element is the induction-time at a range of pressures and temperature of interest. For the NRL model, this range is from 1000 to 2000 K and from 0.05 to 200 atm. The induction-time is further extrapolated from 2000 to 3000 K. The reasoning behind the temperature and pressure range is that the induction-time is critical just behind the shock wave before heat-release begins, and so is at very high pressures but only moderate temperatures (i.e. not combustion temperatures). The other important elements are the heat-release time and the amount of heat-release.

The original NRL model was constructed using a detailed kinetic mechanism [13], while the newer induction-time model used in this work uses a more recent detailed kinetic mechanism from 2011 [14]. To build the table, we do a constant volume perfectly stirred reactor calculation at a given pressure and temperature and equivalence ratio, with a small amount of seed OH radicals. Seeding radicals are required to start the induction chemistry, but should not have a significant effect on the induction times. We then determine the time at which the maximum temperature gradient occurs, and assign that to be the induction-time. Figure 1 shows the induction-time for the pressure and temperature range of interest for lean and rich mixtures. Blue is the original model, red is a stoichiometric mixture with the new model, and the thinner black lines are different equivalence ratios ( $\phi$ ) varying from 0.23 to 3. There are some differences between the new model and the older model, but the trends are similar and the values are reasonably close. One of the more interesting features of this figure is that the induction-time does not vary significantly with respect to equivalence ratio over the range of temperatures and pressures that are of interest, suggesting that the induction-time parameter model should be able to be adapted to varying equivalence ratios successfully.

The above results can be constructed into a table similar to the previous NRL model. Instead of a twodimensional table based on temperature and pressure, we now have a three-dimensional table based on temperature, pressure, and equivalence ratio. We use a simple linear interpolation for equivalence ratio, and the same interpolation procedure as the original IPM for temperature and pressure.

The second element of the induction-time parameter model is the amount of heat-release. Using temperature-dependent thermodynamics and knowing the composition at the CJ point of the detonation wave fixes the amount of heat-release for stoichiometric detonations. For previous stoichiometric calculations, therefore, heat-release was completely specified by the CJ conditions. However, as the equivalence ratio varies, the composition changes. Since we are using a three-species model (Hydrogen, Air, and Product), we must scale the heat-release such that we recover the correct detonation wave velocity for a range of equivalence ratios. We use a scaling factor *f*, such that  $\Delta H = f(\phi^*)\Delta H_{st}$ . Note that we are able to do this by making the heat-release an explicit source term in the energy equation. The values are greater than one due to the lower temperatures of non-stoichiometric detonations, resulting in lower amounts of dissociation.

## **5** Results

Our ability to capture the correct CJ velocities is shown in Figure 2. If we do not scale the heat-release, we end up with detonation velocities that are off by up to 4.5%, which is reduced to less than 0.1% with scaling. Similar comparisons were done for CJ pressure and temperature (not shown). From these results, we are comfortable that the induction-time parameter model is working correctly for non-stoichiometric detonations. This is critical, because detonations in RDEs with non-premixed fuel and oxidizer can have a large range of local equivalence ratios.

The next simulations are two-dimensional detonation tube simulations. These simulations investigate the development of cellular structure as the equivalence ratio  $\phi$  is varied from 2.333 to 0.429. The domain is a simple rectangular domain that is 1.00 m long and 0.06 m high. We fill the domain with a mixture of hydrogen and air at 1 atm, 300 K. For the first set of simulations, the equivalence ratio is uniform throughout the fill region. We use the same grid resolution as for the one-dimensional cases, 0.2 mm. The results for the maximum pressure are shown in Figure 3. Here we see a very regular pattern for hydrogenair until the equivalence ratio becomes very low. Cell sizes are calculated by averaging triple point collisions with the upper wall. As shown in Table 1, the cell-size does vary dependent on the equivalence ratio, and the cells become less uniform as the equivalence ratio moves further from stoichiometric, even for the higher equivalence ratios. The result at low equivalence ratio ( $\phi = 0.429$ ) is particularly intriguing, because there appears to be a strong cell setting up at the tube height (60 mm), as well as weaker triple points that define smaller cells within the strong cells. This appears to be a stable pattern, although further computations beyond 1.0 m length are needed to confirm this.

## 4 Conclusion

This paper discussed the extension of the induction-time parameter model, a reduced-order model, to examine detonations with stratified equivalence ratios. This extension is critical for RDE computations, as most experimental RDE rigs require non-premixed injection. The IPM model was created using a detailed kinetic model and a series of perfectly-stirred-reactor calculations, and showed that a simple table extension could be made to the IPM to account for different equivalence ratios. A series of one-dimensional and two-dimensional results showed the behavior of this model under different conditions, for both CJ conditions and also detonation structure based on maximum pressure.

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Figure 1. Induction-time for H2/Air using the original model (blue) and the new model (red and black) over a range of equivalence ratios from 0.25 to 4.00. Equivalence ratio of 1.0 is red.



Figure 2. Detonation wave velocity for non-stoichiometric equivalence ratios.

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(e)  $\phi = 2.333$ Figure 3. Maximum pressure in atm for a range of equivalence ratios. Domain is 1 m x 0.06 m.  $P_{\infty} = 1$  atm,  $T_{\infty} = 300$  K.

Modified equiv. ratio, $\phi^*$	Equiv. ratio, $\phi$	Cell size, mm
0.6	0.429	32.3
0.8	0.667	18.4
0.9	0.818	17.5
1.0	1.000	15.7
1.1	1.222	16.8
1.2	1.500	17.4
1.4	2.333	18.2

Table 1. Estimated cell-sizes from Figure 3