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# Numerical simulations of hydrogen detonations with detailed chemical kinetics

B.D. Taylor<sup>\*,1</sup>, D.A. Kessler, V.N. Gamezo, E.S. Oran

*Laboratories for Computational Physics and Fluid Dynamics, Naval Research Laboratory, Washington, DC, USA*

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## Abstract

Time-dependent, multidimensional simulations of unstable propagating detonations were performed using a detailed thermochemical reaction model for a stoichiometric argon-diluted hydrogen–oxygen mixture at low pressures and a hydrogen–air mixture at atmospheric pressure. Detonation cells computed for the low-pressure, dilute  $H_2$ – $O_2$ –Ar systems were regular in shape, and their sizes compared reasonably well with experimental observations. The computed  $H_2$ –air cells at atmospheric conditions were qualitatively different from those observed in experiments, and their widths range from less than 1 mm to nearly 5 mm with multilevel hierarchical structures. The effective activation energy of the  $H_2$ –air mixture, based on constant-volume ignition delay times computed using the detailed thermochemical model, varies between 5 and 40 over the range of post-shock temperatures and pressures in the simulations and is, on average, significantly larger than expected based on the regularity of experimental cellular patterns. Analysis of the simulations suggests that vibrational relaxation of the gas molecules, a process which is ignored when calibrating detailed chemical reaction models, occurs on time scales similar to the ignition delay times for the detonations and may be a source of discrepancy between numerical and experimental results.

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## 1. Introduction

Predictive numerical simulations of detonations are essential to continued progress as research on high-speed reactive flows moves beyond an exploration of fundamental mechanisms towards applications. To date, significant progress has been made in understanding the

behavior of gas-phase detonations through numerical simulations with reduced thermochemical models (see, e.g. [1] and the references therein). With increasing computer speed and memory and algorithmic improvements, such as adaptive mesh refinement, it has now become possible to simulate multidimensional detonations on increasingly higher-resolution grids.

Detailed thermodynamic and chemical kinetic models play an important role in simulations, as they are expected to give more accurate results than reduced models. Detailed models may also be used in simulations to calibrate simpler, more computationally efficient models. It is important, therefore, to test whether a detailed thermochemical model can quantitatively reproduce experimental data.

\* Corresponding author. Address: Naval Research Laboratory, Code 6043, 4555 Overlook Ave. SW, Washington, DC 20375, USA. Fax: +1 202 767 4798.

E-mail address: [bdtaylor@lcp.nrl.navy.mil](mailto:bdtaylor@lcp.nrl.navy.mil) (B.D. Taylor).

<sup>1</sup> National Research Council Postdoctoral Research Associate.

In this paper, two-dimensional (2D) numerical simulations of a propagating detonation were performed with a detailed thermodynamic model and a recently developed detailed chemical kinetic mechanism for high-pressure combustion of  $H_2$ -air [2]. Simulations of several low-pressure argon-diluted (70%)  $H_2$ - $O_2$  mixtures at 300 K and a stoichiometric  $H_2$ -air mixture at 300 K and 1 atm are presented. Comparisons of computed detonation cell sizes from the simulations to prior experimental data [3–6] are discussed in terms of properties of the thermochemical model.

## 2. Background

The high cost of computing detailed chemical kinetic mechanisms has restricted their use in numerical simulations of multidimensional detonations until relatively recently. Most such research with detailed kinetics has involved stoichiometric hydrogen-oxygen ( $H_2$ - $O_2$ ) mixtures, heavily diluted with argon (Ar), at an initial pressure of less than a tenth of an atmosphere, where detonations produce very regular cellular patterns on experimental smoke foils [7]. Two-dimensional simulations of such systems [8–11] have used different numerical methods and kinetic models. The computed detonation cells in all of these cases were consistent with experiments, producing very regular cellular structures. With one exception [10], in which much smaller cells were computed, the cells were  $\sim 2$  times smaller than experimental values. Given uncertainties in experiments [9], this has been considered good agreement.

Tsuboi, Hayashi, and their collaborators studied detonations in stoichiometric  $H_2$ -air at 300 K and 1 atm in 2D and 3D using detailed chemical mechanisms. Their simulations described 3D cellular structures with rectangular [12] and diagonal [13] modes and spinning detonations in square channels [14] and round tubes [15]. The cell widths computed were much smaller than those in experiments, but the simulations were performed on computational domains on the order of the detonation cell width, which precluded the formation of multiple cellular structures. This discrepancy was discussed in [14], where cellular detonations were computed in two-dimensional channels with widths of 1, 2, 4, and 6 mm. The results in the 1 and 2 mm channels were mode locked and produced a half cell across the domain. Cells in the larger channels were quite irregular, with widths reported to range from 1 to 8 mm.

Experiments in  $H_2$ -air at these conditions found a cell width of 8–9 mm [3–6], with one outlier at 15 mm [16]. Unlike the case of low-pressure, Ar-diluted  $H_2$ - $O_2$  mixtures, where simulations and experiments agree better, there is a significant qualitative (cell regularity) and quantitative (cell

size) disagreement in  $H_2$ -air mixtures at atmospheric pressure.

## 3. Numerical model

The reactive Euler equations are solved on a structured adaptive mesh using the fully threaded tree data structure [17], as described by Gamezo et al. [18]. The code, which has been modified to handle temperature-dependent thermodynamic data and multistep chemical kinetics, uses directional splitting and an explicit, second-order Godunov scheme with the Colella–Glaz Riemann solver [19]. Mesh refinement is dynamically controlled by gradients of density, pressure, and composition.

Several different equilibrium chemical kinetic mechanisms were tested, but here we focus on the results obtained using the chemical kinetics and thermodynamic data of Burke et al. [2] for high-pressure combustion of  $H_2$ -air mixtures. This mechanism involves 27 reversible elementary reactions among the 8 species  $H_2$ ,  $O_2$ ,  $H_2O$ , H, O, OH,  $HO_2$ , and  $H_2O_2$ , with 5 nonreacting species,  $N_2$ , Ar, He, CO, and  $CO_2$ . The reacting gas mixture is assumed to be thermally perfect, and thermodynamic properties of the chemical species are evaluated from the 7-coefficient NASA polynomial representation (see [20]). The species production rates are integrated as ordinary differential equations (ODEs) in an operator-split manner using CHEMEQ2 [21], which implements an  $\alpha$ -QSS predictor-corrector method that is A-stable and second-order accurate.

The computational domain is a 2D channel of height 4 cm and length 128 cm. Adiabatic, slip-wall boundary conditions are applied on the edges of the domain. The domain is initially filled with a stoichiometric mixture of  $H_2$ ,  $O_2$ , and diluent at 300 K. In the low-pressure tests, the mixture is diluted with 70% Ar by volume, while in the  $H_2$ -air simulations the mixture is at 1 atm and contains 55.62%  $N_2$  (mole ratio  $O_2:N_2$  of 1:3.76).

The detonation is initiated by the rapid expansion of a 1 cm wide region of  $H_2O$  and diluent at high pressure and temperature at the left edge of the domain and extending across the full height of the channel. Several semi-circular regions of  $H_2O$  and diluent at these conditions are used to perturb the shock and hasten the onset of cellular instabilities. The resulting detonation is initially overdriven, but quickly slows before reaching a self-sustained velocity within a few percent of  $D_{CJ}$ .

## 4. Results

### 4.1. $H_2$ - $O_2$ -Ar tests

For this study, detonation cells in stoichiometric  $H_2$ - $O_2$  mixtures with 70% Ar dilution, ini-

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