Detonability and Propagation Limits of Spray Detonations in Jet Fuel-Air Mixtures

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1 Introduction

Recent years have seen renewed interest in the detonations of liquid sprays due to their wide range of applications, ranging from detonation-based engines such as Rotating Detonation Engines (RDEs), to explosions in chemical storage facilities [1], etc. However to date, our understanding of the detonation characteristics in liquid sprays, in comparison with their pre-vaporized, premixed mixtures, is far from complete. Although several theoretical, experimental, and numerical studies [1] have demonstrated the detonability and characteristics of spray detonations in high vapor-pressure, volatile fuels, such as hexane and *n*-heptane, fundamental questions of detonability, propagation limits, and cellular structure of spray detonations in practically relevant, non-volatile, low vapor-pressure heavy hydrocarbon fuels, such as JP10, n-dodecane, or JetA2, remain far less explored and understood.

The detonability of jet fuel droplets in air (without any prevaporized fuel) at atmospheric pressure is still an open question in the community. Although several experiments [1] in the past attempted to propagate a detonation in jet fuel/air mixtures, such as JP10 and *n*-dodecane, either they were unsuccessful due to weak charge strength, narrow channel sizes (geometric limits), etc., or they required a substantial amount of pre-vaporized fuel in the upstream air, even for smaller droplets $\lesssim$ 10 µm. Recently, experimental work by Brown et al. [6] also reported unsuccessful propagation of a detonation in 5 µm Jet A2 droplets in air under atmospheric conditions, while successful propagation was observed in pure O_2 stream. At the same time, the channel size in this study is only 45 mm, which may be smaller than the critical channel size for detonation propagation in air. Finally, in the context of numerical modeling, although there have been few numerical studies [2] of spray detonations in JP10 and n-dodecane fuels, these studies were carried out in pure O_2 rather than air.

This naturally raises two fundamental questions, which are central to the present work: 1) Can detonations propagate in jet fuel droplets in air, at least for small droplets $\lesssim$ 10 µm?; and 2) What is the minimum channel size necessary for propagation at atmospheric conditions? Currently, the only answer to these questions is suggested by the experimental work of Veyssiere et al. [3], who observed a spinning near-limit detonation in 8 µm *n*-dodecane droplets in air under atmospheric conditions in a 53 mm channel.

In this work, our aim is to discuss the questions raised above using numerical simulations. This crucially requires accurate modeling of the complex spray-flow interactions through a realistic spray break-up

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model applicable in the detonation-relevant conditions. In particular, the underlying spray model should incorporate the following key characteristics:

1. *Chemistry model:* Detonations result in a wide range of thermodynamic conditions, characterized by extreme pressures and temperatures. Therefore, a realistically complex chemical kinetics model is required to accurately capture the temperature sensitivity and the resultant reaction rates over a wide range of conditions. In addition, jet fuels undergo endothermic pyrolysis prior to oxidation, which must be properly captured by the chemistry model.

2. *System geometry:* As detonations, both gaseous and spray, are inherently three-dimensional (3D), it is natural to study their properties in 3D channels instead of two-dimensional (2D) channels. Furthermore, recent numerical studies of premixed detonations in hydrocarbon mixtures, such as C_2H_4/air [4], have demonstrated that 3D detonations are much more stable and regular than their 2D counterparts. Moreover, the 3D detonation characteristics, including their cellular structure and stability, are observed to be closer to experiments than the 2D characteristics.

3. *Break-up and evaporation:* The final and most important physical process that must be captured accurately is the conversion of a liquid droplet into fuel vapor. In a spray detonation, the droplet interaction with the gas phase begins with its impact by the shock at the detonation front. Upon impact, a transmitted shock is propagated inside the droplet, which simultaneously heats and breaks the parent droplet into smaller droplets, which eventually undergo further break-up and evaporation in the surrounding gas. Crucially, both atomization and evaporation can occur under trans- and super-critical conditions, which must be properly accounted for in the model. Since the conversion of liquid fuel to vapor in a detonation front controls local fuel mass loading, which ultimately controls the resultant detonation properties, an appropriate shock-droplet interaction (SDI) model developed for detonation-relevant conditions is necessary to capture all of these complex processes and the associated time and length scales accurately.

At present, there are no droplet evaporation and breakup models developed specifically for the detonation conditions. In addition, models, which are currently used for spray detonation studies, are developed primarily for low-speed, unshocked flows using the classical d^2-law of evaporation [7]. Such models often result in very different evaporation characteristics when applied to shocked flows. For example, Fig. 1 shows the time it takes for a 10 μm *n*-dodecane droplet to completely evaporate upon impact by a Mach 5 shock, as predicted by different evaporation and breakup models with increasing complexity: a) Model I considers only evaporation [7] and no atomization of the droplet, b) Model II considers the same droplet evaporation model but with droplet break-up prescribed by Apte et al. [8], c) Model III also considers the same droplet evaporation model but with breakup prescribed by Ranger and Nicholls [9], and d) Model IV is a recently developed shock-droplet interaction (SDI) model (Wang et al. 2024, Stanford University; also see [12]) for strong shocks. The characteristic evaporation time of a droplet changes from $\sim$ 100 μs to as low as tens of nanoseconds, depending on the choice of the evaporation and breakup models. Ultimately, this would result in very different detonability and propagation limits for a given droplet/air mixture.

Since it is not clear a priori which of these models, if any, approximates the actual spray detonation properties with any accuracy, we carry out a sensitivity study using the above four models. In particular, we first carry out numerical simulations in 2D channels using Model I (no atomization case). Since the 'no atomization'case results in the largest evaporation time scale (or slowest fuel mass loading), it is expected to produce the largest cell size, which should give a conservative estimate of the minimum channel size and thus of the overall detonability. Further, only 2D channels are considered for this model, as there is no atomization, and this would also allow us to explore wider channels while keeping

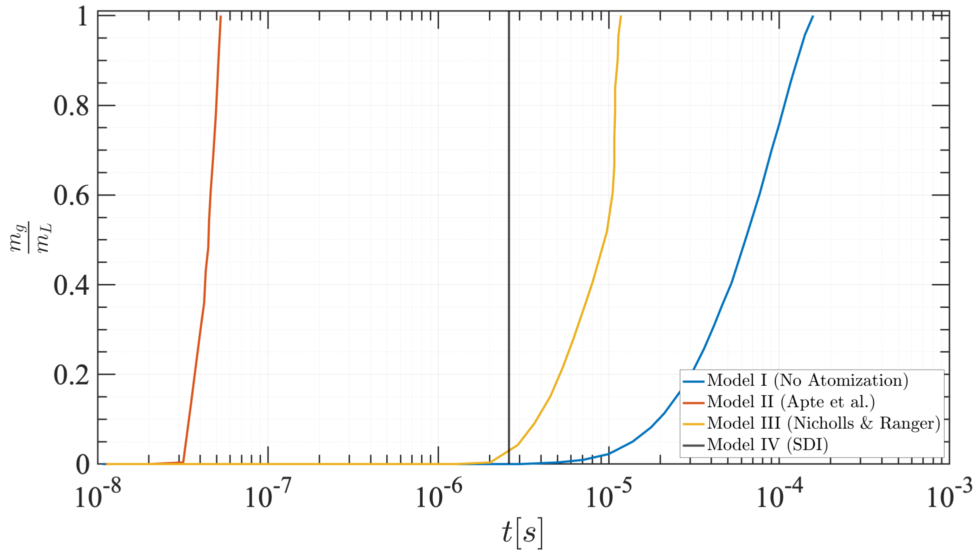

Figure 1: Time taken by a 10 µm n-dodecane droplet to completely vaporize from liquid to gaseous state after impact by a Mach 5 normal shock wave for different evaporation and break-up models.

the computational cost reasonable. Next, we carry out simulations in a 3D channel using models II-IV, which include the effects of droplet break-up and SDI. Using the results from these simulations, we aim to understand the detonability and minimum channel size required to propagate a spray detonation in a jet fuel/air mixture at atmospheric conditions.

2 Physical Model and Numerical Method

A hybrid Eulerian-Lagrangian method is used to simulate the two-way coupled gas-droplet system, in which the gas-phase equations are solved on a Eulerian grid, while the droplets are treated as point Lagrangian particles with a given density and radius. The droplet spray is assumed to be dilute and thus droplet-droplet interactions are neglected. The coupled gas-droplet equations along with the appropriate source terms can be found in Dammati et al. [12].

In the case of models I-III, the droplet drag is calculated using a Reynolds- and Mach-number-dependent drag law prescribed by Loth [10], while the droplet evaporation model of Miller et al. [7] is based on a classical d^2-law. The droplet break-up model used in models II and III is prescribed by Apte et al. [8] and Ranger and Nicholls [9], respectively. In model IV, droplet drag, break-up, and evaporation on shock impact are described using a recently developed tachyothesis mechanism (see Dammati et al. [12]).

The numerical simulations in this study solve the unsteady, reactive, compressible Navier-Stokes equations for a thermally perfect gas on a uniform grid using a fully compressible, reactive, finite-volume, multi-phase flow solver `Athena-RFX` [4, 5, 12]. The molecular transport is treated with a mixture-averaged formulation, and the gas thermodynamic properties are computed using NASA seven-coefficient format. Pyrolysis and oxidation reactions of *n*-dodecane combustion are described with the reduced versions of the HyChem (for Models I - III) and FFCM-2 (Model IV) family of chemical mechanisms for *n*-dodecane [13]. Chemical source terms are integrated using the semi-implicit, non-iterative, single-step ODE integrator YASS [11].

In the case of Models I-III, the Lagrangian droplet equations are integrated using the second-order Crank-Nicholson method [15] via a predictor-corrector approach [16]. In the case of Model IV, explicit

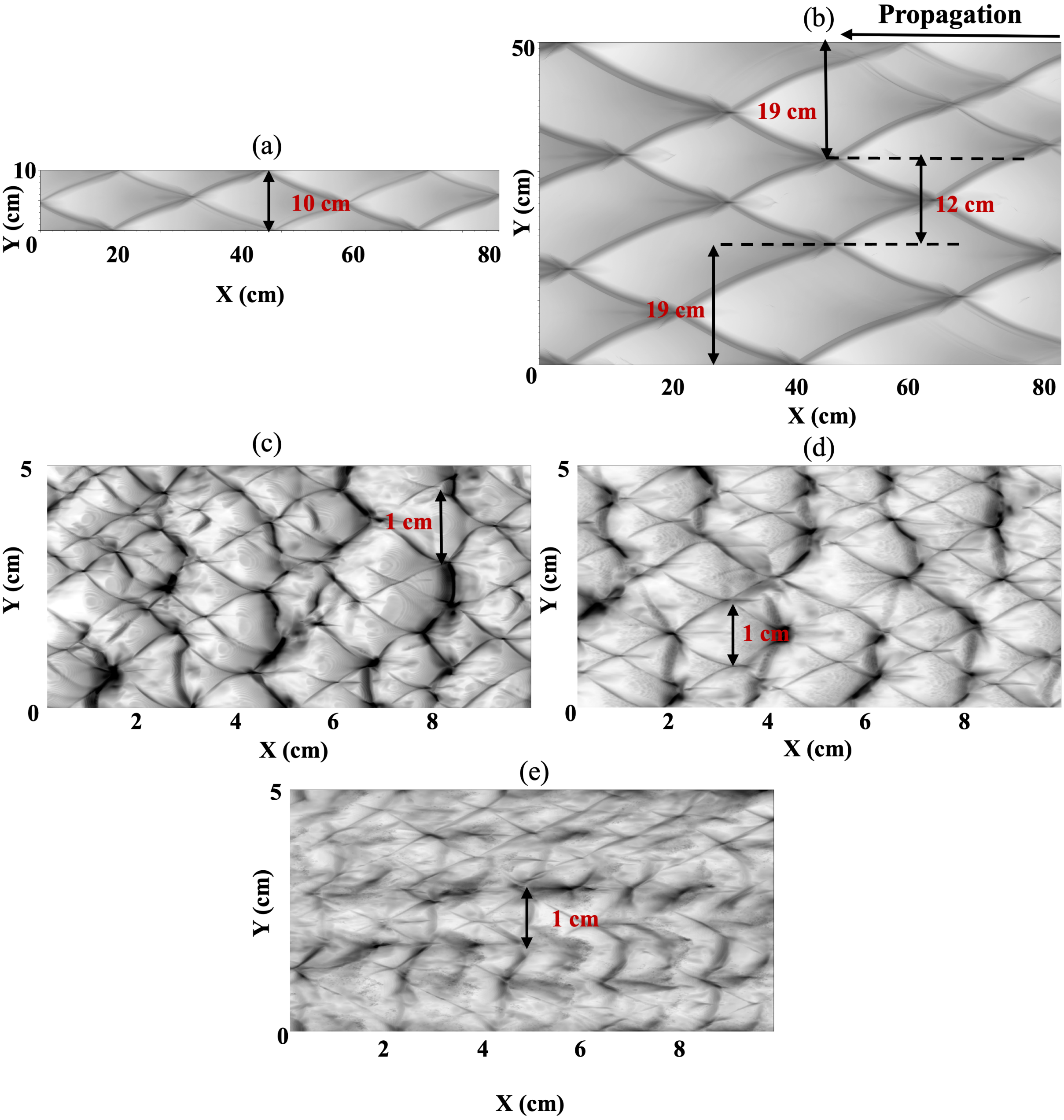

Figure 2: Numerical soot foil for a) Model I (10 cm) 2D channel, b) Model I (50 cm) 2D channel, c) Model II (5 cm) 3D channel, d) Model III (5 cm) 3D channel, and e) Model IV (5 cm) 3D channel.

expressions for the droplet position, break-up time, and slip velocity are directly prescribed, and thus no time integration is necessary. In all models, the gas-phase quantities are interpolated to the droplet position using a high-order WENO interpolation scheme [5], while the coupled source terms from the droplet to the gas are distributed using a high-order B-spline method [14].

3 Problem Setup

Numerical simulations using model I are carried out in a 2D channel 10 and 50 cm wide with adiabatic, slip walls, while simulations using models II-IV are carried out in a 3D rectangular channel with 1×5 cm cross-section and isothermal, no-slip walls, resulting in a total of five cases. The numerical resolution in the 2D cases is 40 cells per induction length and 6 cells per reaction zone width of the premixed, gaseous ZND solution. In the 3D cases, the resolution is decreased by a factor of 2 to reduce the computational cost. The flow field in the domain is initialized by sinusoidally perturbing the gaseous ZND solution, and the downstream boundary is held at a constant state with pressure below the gaseous Champan-Jouguet pressure in the ZND solution, which allows the detonation to relax naturally to its freely propagating state.

Monodisperse 10 μm *n*-dodecane droplets at 300 K are injected from the left end of the domain along with air at atmospheric pressure and 420 K at the Chapman-Jouguet (CJ) velocity, D_{CJ}, of a gaseous detonation, and at a specific seeding density of 1.429×10^5 cm^{-3}, which corresponds to a globally stoichiometric *n*-dodecane/air mixture. To randomize droplet seeding, Gaussian velocity perturbations with zero net momentum are added to the droplets injected through the left domain boundary. The problem is solved in the detonation frame of reference.

4 Results and Discussion

Regardless of the evaporation and break-up models used, in all cases a stable propagation of a detonation is observed for the channel sizes studied. Furthermore, we find that the detonation speed is within $< 1\%$ of D_{CJ} in all the cases considered.

To determine the detonability limits or the minimum channel size required for propagation, we determined the characteristic cell size in each case. To achieve this, the numerical soot foils are generated by recording the maximum pressure at each location. The resulting soot foils are shown in Fig. 2 along with the average characteristic cell size marked for each case. For Model I (no atomization), mode locking is observed in a 10 cm wide channel with a single 10 cm wide cell, while the 50 cm wide channel produced multiple cells of sizes $12 - 19$ cm. Interestingly, all three 3D cases produced a very similar average cell size of ~ 1 cm, though their morphology was different. Therefore, multiple cells were present in a 5 cm 3D channel.

These results demonstrate the detonability of jet fuel droplets in air under atmospheric conditions for 10 μm droplets. Based on the 2D results with no droplet atomization, the conservative estimate of the minimum channel size appears to be in the range of $10-20$ cm, which is consistent with the experimental observations of Veyssiere et al. [3], who observed a single-headed detonation in their 5.3 cm channel. At the same time, in the 3D cases, in which different atomization and shock-droplet interaction models were employed, irrespective of the model used, an average cell size of 1 cm was observed, with multiple cells across a 5 cm wide channel. This result is in contrast to the above 2D calculations without atomization, and it also appears to be inconsistent with the experiments [3]. These results are counterintuitive, as the 3D models, which include the physics of droplet break-up and SDI, appear to be in worse agreement with experiments than the much less realistic 2D calculations. These findings require further analysis in future work.

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