Steady and transient one-dimensional simulations of multiphase dodecane/air detonations

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1 Introduction

Multi-phase detonations are an important area of study due to their applicability in aerospace propulsion. Most existing studies have focused on gas-phase premixed detonations. In contrast, despite their relevance, multi-phase detonations have received considerably less attention. A one-dimensional steady-state solver that accounts for detailed chemistry, two-way droplet-gas coupling, external wall friction and heat loss has recently been developed within the framework of Cantera [1]. The prediction from the steady-state solver is compared to that obtained from a transient compressible Navier-Stokes solver [2,3] in this study. The steady solver, with its low computational cost, enables fast and detailed analysis of the detonation structure and quenching limits under a multitude of equivalence ratios, droplet radii, droplet loadings, and external loss conditions. However, it cannot capture transient effects such as pulsations and detonation failure. The transient model, meanwhile, offers time-accurate analysis with molecular diffusion and viscous effects. It requires significantly more computational time to relax from the initial perturbation to a steady or quasi-steady state. Comparing the two solvers provides a unique opportunity to view the structure and phenomena of spray detonations from different perspectives, in a manner analogous to comparing a ZND solution to a transient simulation of gaseous detonation. Initial comparisons between the two solvers are presented for n-dodecane/air mixtures at equivalence ratios of 1.0 and 0.7.

2 Numerical Methods

2.1 Transient compressible Navier-Stokes solver

The compressible Navier-Stokes equations are solved using the fixed-grid massively parallel code `Athena-RFX` [2,3], a multiphase reactive-flow extension of the Athena magnetohydrodynamics code [4]. Convective fluxes are calculated with the HLLC-ADC (Anti-Diffusion Control) scheme [5], and flow integration is performed with a second-order accurate Godunov scheme employing the unsplit corner transport upwind (CTU) method [6]. A piecewise linear method (PLM) [7] is used for state reconstruction. Net diffusive fluxes are calculated with a second-order finite difference method with flux matching

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to maintain conservation [2]. Flow and chemistry are coupled through Strang splitting [8] with a global reaction-advection time-step control. This methodology is of second-order accuracy in both time and space. Chemistry is modeled using an 8-species model extracted from FFCM-1 [9] for hydrogen combustion. Chemical source terms are integrated using the non-iterative, single-step, semi-implicit ODE integrator YASS [10]. YASS employs the exact Jacobian matrix and explicitly conserves both mass fraction and total energy.

The Eulerian-Lagrangian approach is implemented in `Athena-RFX`. Massive particle equations are integrated using the Crank-Nicolson integrator with two-way coupling to the flow equations based on the predictor-corrector approach of Bai & Stone [11, 12]. Spatial interpolation of gas-phase quantities to a particle position is performed using the WENO-5 approach suitable for compressible flows with shocks [3]. Spreading of the source terms for particle feedback to the gas flow is performed with a 5-point stencil using a high-order B-spline weight function [13, 14]. The droplet model includes a treatment of the Re- and Ma-dependent drag coefficient using the correlation of Loth [15] with the Nusselt number given by the Ranz-Marshall correlation [16]. This approach was recently used to assess the accuracy of the particle imaging velocimetry in gaseous detonations [17].

On the left boundary, fuel droplets and air are injected into the domain at the CJ velocity D_{CJ}. The injection rate of fuel droplets is maintained in such a way that the overall equivalence ratio in the domain is maintained at the desired value. The fuel droplet temperature is the same as that of the ambient air. The right boundary is fixed at CJ state that is obtained from the steady state gas-phase fuel-air ZND structure. To ensure a mesh-independent solution, at least 40 grid points in the induction zone (Δ) and at least 5 points in the reaction zone (Δ_e) are used. The grip spacing in the simulations is chosen in such a way that it simultaneously satisfies both of these conditions. Table 1 summarizes the computational details for the transient simulations.

Table 1: Computational parameters for the transient simulations at P_0=1 atm and T_0= 298 K.

ϕ	D_{CJ}, ms^{-1}	Δ, cm	Δ_e, cm	dx, cm	D_d, ms^{-1}	Droplet Diameter, μm
1.00	1801.36	0.1965	0.0218	0.00437	1801.36	5.00 10.00
0.70	1668.77	0.5300	0.0410	0.00820	1668.77	5.00 10.00 20.00

2.2 Steady multiphase ZND solver

A steady-state one-dimensional spray detonation solver is constructed as detailed in a previous study [1]. The Eulerian-Lagrangian approach is implemented where the droplets are monodispersed and uniform. The two phases are two-way coupled through source terms in droplet number density, mass, momentum, species and energy equations. D^2 laws for droplet heating and vaporization are adopted in the model with Ranz-Marshall corrections [18], as shown below.

$$\dot{m}_v = 4\pi r_d n_d \rho_g D_g \ln(1+B_Y)\frac{1}{2}(2+0.552Re_d^{1/2}Pr^{1/3}) \,, \tag{1}$$

$$q_d = 4\pi r_d n_d \frac{\lambda_g}{c_{p,g}} L_v \ln(1+B_H)\frac{1}{2}(2+0.552Re_d^{1/2}Pr^{1/3}) \,, \tag{2}$$

$$B_Y = \frac{Y_{f,s} - Y_f}{1 - Y_{f,s}} \,, \tag{3}$$

$$B_H = \frac{C_{p,g}(T_g - T_d)}{L_v} \,. \tag{4}$$

Here, $\dot{m}_v$ is the rate of droplet mass vaporization per unit volume of gas, r_d is the droplet radius, n_d is the droplet number density, ρ_g is the gas density, D_g is the gas mixture-averaged diffusion coefficient for fuel, λ_g is the gas thermal conductivity, $C_{p,g}$ is the gas specific heat at constant pressure, T_g and T_d are the gas and droplet temperatures, and B_Y and B_H are the Spalding mass and heat transfer numbers. The surface mass fraction, $Y_{f,s}$, is calculated using the Antoine equation.

This model is a simplified model compared to the vaporization method used in `Athena-RFX`. Both models are described in [19], with the steady solver currently using the M1 model in Table 1 of [19], and the compressible Navier-Stokes solver using the M7 model. The droplet drag equations, however, are identical to those in `Athena-RFX`. Future work will adopt identical vaporization methods in both solvers to ensure fair comparison.

The steady-state solver implements a model similar to the traditional ZND model. The non-linear boundary value problem is solved using the shooting method. An initial detonation velocity is first guessed. The Von-Neumann state is then calculated using normal shock relations. Finally, the detonation structure is calculated using a system of non-linear ordinary differential equations [1, 18]. This method is repeated until the downstream Mach number reaches unity as all the gas energy source terms balance. The system of equations contains 30 dependent variables: three for the gas phase, three for the liquid phase, and one for each species in the 24-species chemical mechanism. The chemical mechanism is identical to that used in `Athena-RFX` [20]. The ODEs are solved using the SciPy open sourced Python library known as solve_ivp with the LSODA integration algorithm for stiff and non-stiff systems [21]. Molecular diffusion and viscous effects are not modeled in the steady model.

3 Preliminary results

Figures 1 and 2 compare the density, pressure, temperature, fuel mass fraction, velocity and heat release rates (HRR) obtained from the steady-state and the transient simulations at equivalence ratios of 0.7 and 1, respectively. The transient solution is obtained at a single time step between 10 and 15 ms to allow the detonation to relax. All quantities are normalized using the maximum values in the gaseous ZND domain. The two models show very similar detonation structure across all equivalence ratios and droplet diameters for the 10 μm and 20 μm droplets. Small differences are noted in the post-shock conditions, the onset of thermal runaway, and the downstream states. Preliminary parametric studies show that these differences can result from the differing droplet vaporization models and not fully relaxed nature of the transient detonation. Future work will improve on both of these aspects.

Post-shock temperatures and pressures were different than gaseous ZND due to the absence of fuel in the initial gaseous state. Larger droplets require longer vaporization time, which results in delayed thermal runaways when compared to smaller droplets. This delay reduces the peak heat release rates and expands the heat release region. Droplets of differing sizes all resulted in identical downstream states equal to the CJ state in both steady and transient simulations (cf. Table 1). This is expected for small droplets with all effects included except for droplet secondary atomization [18].

Another interesting observation is that the corresponding transient gaseous detonation with prevaporized dodecane undergoes failure in a 1D calculation. However, the multi-phase detonation front propagates

in a stable manner for sufficiently large droplets $> 5\mu$m. The expansion in heat release rate region might play a role here, which will be further investigated.

Finally, it is noted that the transient $d_0 = 5\mu m$ case with ϕ=0.7 deviates significantly from the steady-state model. This oscillation is believed to be physical, and can be captured by the transient model. Intriguingly, this oscillation becomes more powerful with smaller droplet sizes and smaller equivalence ratios. Further study may provide additional perspective on this effect.

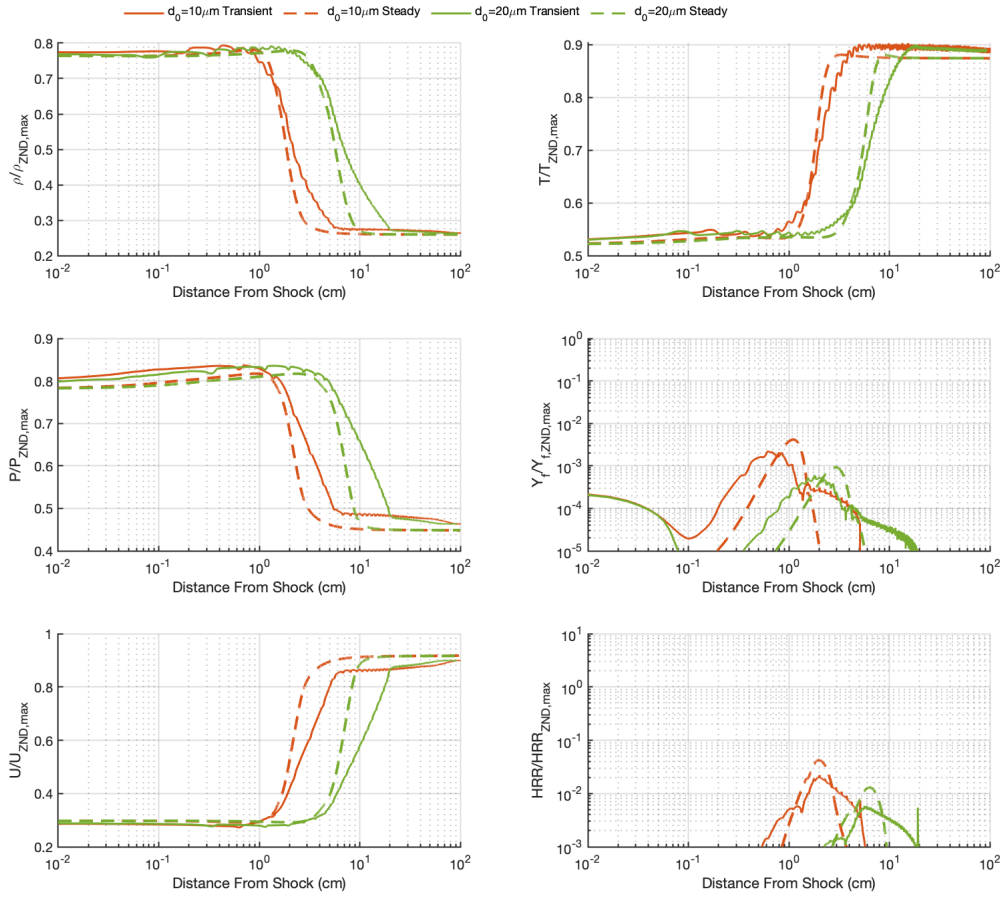

Figure 1: Transient and steady 1-D spray results at ϕ=0.7, $P_0 = 1$ bar, $T_0 = 298$ K. Figures are normalized by maximum values obtained from gas-phase ZND solutions.

3 Acknowledgements

NT and XZ acknowledge funding support through the Air Force Office of Scientific Research (AFOSR) under Grant FA9550-18-1-0173 (Attn: Dr. Chiping Li). AG, SSD and AYP acknowledge funding support through AFOSR under Grant FA9550-21-1-0012. The computational resources are provided in part by the DoD High Performance Computing Modernization Program.

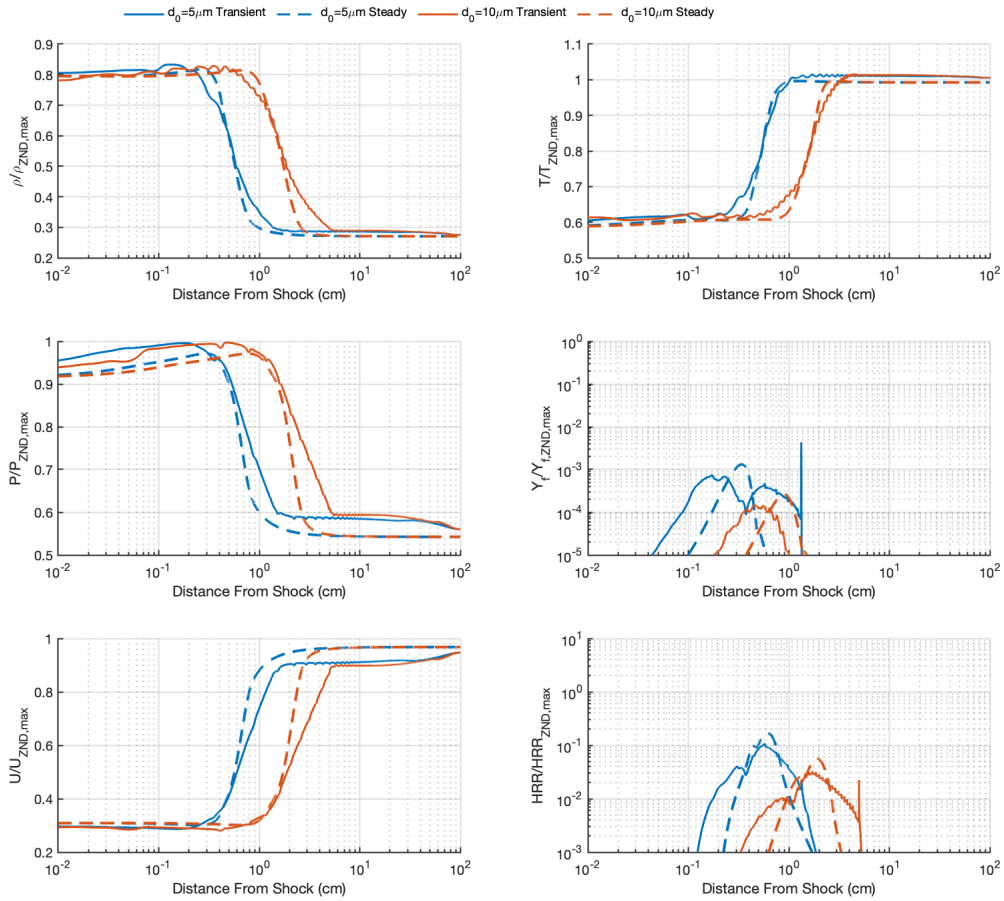

Figure 2: Transient and steady 1-D spray results at ϕ=1.0, $P_0 = 1$ bar, $T_0 = 298$ K. Figures are normalized by maximum values obtained from gas-phase ZND solutions.

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