Role of Viscosity in the Detonation Cell Cycle

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1 Introduction

Historically, the regularity of the detonation cellular structure has been attributed to the sensitivity of the exothermic chemical reactions to perturbations in shock strength [1]. The sensitivity is typically quantified with the explosive parameter,

$$\chi = \epsilon_{\mathrm{i}} \frac{\Delta_{\mathrm{ind}}}{\Delta_{\mathrm{exo}}} \frac{Q}{RT_{\mathrm{vN}}}, \tag{1}$$

where ϵ_{i} is the apparent activation energy of ZND ignition, and Δ_{ind} is the distance to peak thermicity rate $\dot{\sigma}_{\mathrm{max}}$ of the ZND solution (i.e. the ZND induction length) [1, 2]. Δ_{exo} is the thickness of the heat release layer, estimated as $u_{\mathrm{CJ}}/\dot{\sigma}_{\mathrm{max}}$, where u_{CJ} is the gas velocity relative to the leading shock at the CJ state. The third term is the heat of combustion Q normalized by the gas temperature at the von Neumann state T_{vN} and specific gas constant R. While it has been demonstrated that the stability of 1D pulsating detonations is described by χ [2,3], and when controlling for other parameters increases in χ are correlated with more irregular detonation cellular structures [4], the χ parameter alone is deficient to describe all pathways to the formation of an irregular cellular structure [4–6].

An alternative mechanism for the formation of an irregular detonation cellular structure is the Mach stem bifurcation mechanism first proposed by Mach and Radulescu [5]. Mach stem bifurcations are characterized by the deformation of the nascent Mach stem due to the impingement of a strong forward jet onto the Mach stem. As the ratio of specific heats γ decreases, the forward jet is strengthened, eventually leading to the "kinking" of the Mach stem and the formation of a secondary triple point on the Mach stem. A perfect correlation was observed between γ and the onset of cell irregularity as part of the mixtures surveyed by Mach and Radulescu, however at the time they were unable to isolate γ from χ [5]. In Fig. 1a, the challenge in isolating γ from χ becomes apparent: mixtures with regular cellular structures (black circles, e.g. hydrogen mixtures dilute with noble gasses) typically have larger γ values and much χ values than mixtures which display irregular cells (red crosses, e.g. hydrocarbons). This was first addressed through parametric simulation of idealized mixtures [6], and then combined experiments and simulations of carefully engineered mixtures designed to isolate γ from χ [4]. In both studies, the reduction in γ saw the onset of Mach stem bifurcations and an irregular cell structure [4, 6].

Beyond the Mach stem bifurcation and chemical mechanisms, it has also been postulated that viscous phenomena may be critical to the propagation of cellular detonations and the onset of cell irregularity.

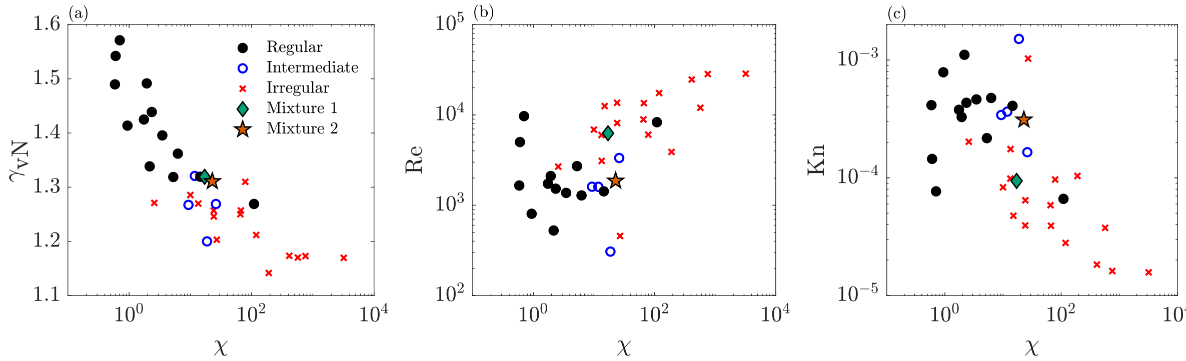

Figure 1: Survey of the explosive parameter χ with the (a) the ratio of specific heats at the von Nuemann state γ_{vN}, (b) Reynolds number Re, (c) Knudsen number Kn for a series of previously studied mixtures [2, 4, 5]. The diamond and star markers indicate Mixture 1 ($2H_2$-O_2-$3.76N_2$) and Mixture 2 ($2H_2$-$3.44O_2$), respectively.

Simulations of viscous triple-point reflections suggest that the onset of Kelvin-Helmholtz instabilities in the shear layer emanating from the triple-point may contribute to the formation of an irregular cellular structures, particularly in hydrocarbons [7, 8]. The dynamics of mixing and ignition in the shear layer and forward jet are also substantially different between regular and irregular mixtures, further suggesting that the onset of “turbulent” flow structures behind the nascent Mach stem may produce an irregular cellular structure [7, 9, 10].

We can characterize the balance of viscous and inertial forces behind the detonation wave through the Reynolds number,

$$\text{Re} = \frac{u_{\text{vN}} \Delta_{\text{ind}}}{\nu_{\text{vN}}}, \tag{2}$$

where u_{VN} is the velocity in the shock frame at the von Neumann state, and ν_{VN} is the kinematic viscosity at the von Neumann state. In Fig. 1b, we observe that mixtures with smaller Reynolds number typically have more regular cell structures, where larger Reynolds numbers correlate with more irregular cell structures. However, it is also true that the Reynolds number is typically correlated with the explosive parameter χ, that is mixtures with large values of χ typically also have larger Re. Thus it remains unclear if trends in cell regularity are associated with chemical or flow instabilities.

Of relevance to simulation is the separation of physical length scales which must be resolved to accurately capture the detonation cellular structure. It is known that simulations of all but the most regular mixtures produce spuriously small cells [8, 11–13]. Thus, we decompose the Reynolds number into a Knudsen number $\text{Kn} = \lambda_{\text{vN}}/\Delta_{\text{ind}}$ and a Mach number $\text{Ma} = u_{\text{vN}}/c_{\text{vN}}$, where λ_{vN} and c_{vN} are the mean free path and sound speed at the von Neumann state, respectively. Using the molecular definition of viscosity, the Reynolds number can be rewritten as,

$$\text{Re} = \frac{\text{Ma}}{\text{Kn}} \sqrt{\frac{\gamma_{\text{vN}} \pi}{2}}, \tag{3}$$

where γ_{vN} is the ratio of specific heats at the von Neumann state [14]. Considering typical detonable mixtures (e.g. those in Fig. 1), the Mach number at the von Neumann state is typically in the range of $(0.3, 0.5)$, and thus variations in the Mach number cannot account for the observed range of Reynolds numbers. A similar conclusion can be drawn for the $\sqrt{\gamma_{\text{vN}}\pi/2}$ factor. It follows that the Knudsen number (i.e. the separation of length scales between the molecular scale and the ignition scale) is what drives the increase in Reynolds numbers. Figure 1c compares χ to the Knudsen number for the mixtures surveyed. As expected, the observations for Reynolds number are consistent with those regarding

Table 1: Detonation parameters for mixtures simulated. Both mixtures have a quiescent temperature and pressure of 300 K and 40 kPa respectively.

Designation	Composition	γ_{vN}	χ	Re	Kn	Ma	Δ_{ind} (μm)
Mixture 1	$2H_2$-O_2-$3.76N_2$	1.32	17.1	6.24×10^3	9.41×10^{-5}	0.409	526
Mixture 2	$2H_2$-$3.44O_2$	1.31	22.8	1.86×10^3	3.11×10^{-4}	0.404	170

the Knudsen number. Larger Knudsen numbers correlate to more regular detonation cells and smaller values of χ, where smaller Knudsen number see more irregular cells and larger values of χ. At smaller Knudsen numbers, it is expected that the Kelvin-Helmholtz instabilities in the shear layer emanating from the triple-point will trigger the onset of a "turbulent" shear layer behind the nascent Mach stem, drastically altering the local mixing dynamics [7, 10]. Isolating this effect from χ suffers from the same deficiency as isolating γ, that is a correlation between Kn and χ is typically observed. Regarding simulation resolution, the reduction in separation of scales (i.e. larger Kn) for regular mixtures may have fortuitously allowed for the adequate resolution of the shear mixing layer. The failure to capture the cell size in irregular mixtures may arise from a failure to adequately resolve the shear mixing process at greater scale separations, rather than from an inaccuracy in the physical models (e.g. vibrational non-equilibrium [12]).

To address questions about the role of molecular viscosity in the detonation cellular structure, we have identified two mixtures from Ref. [4] where both χ and γ_{vN} are constant, but the Reynolds and Knudsen numbers differ. These two mixtures consist of $2H_2$-O_2-$3.76N_2$ (Mixture 1) and $2H_2$-$3.44O_2$ (Mixture 2), respectively. For both mixtures detonations propagate into a quiescent gas with a temperature and pressure of 300 K and 40 kPa, respectively. Additional parameters for these mixtures is found in Table 1. In Fig. 1 it is apparent that Mixture 1 and Mixture 2 lie at the boundary between typically regular and irregular mixtures in the (χ, γ) space, however the Reynolds number and Knudsen number vary by a factor of three. Thus, it is expected that Mixture 1 will be more prone to hydrodynamic instabilities behind the nascent Mach stem which may trigger a more irregular cellular structure. Through high-fidelity 2D simulation, this study first tests the hypothesis that when controlling for other parameters the increase in Reynolds number produces a more irregular cellular structure. Additionally, the nature of the mixing behind the nascent Mach stem, the role of the onset of Kelvin-Helmholtz instabilities, and implications of these mechanisms on numerical grid resolution will be addressed.

2 Numerical Methods and Computational Configuration

The compressible Navier-Stokes equations are solved using the fixed-grid massively parallel code Athena-RFX [15, 16], a reactive-flow extension of the Athena magnetohydrodynamics code [17]. Transport and chemistry are solved in a Strang splitting manner [18]. The convective flux is computed using the HLLC-ADC approximate Reimann solver [19]. Diffusive fluxes are computed with a second-order finite difference method with flux matching to maintain conservation [15]. Chemistry is modeled with a hydrogen submodel derived from FFCM-1 [20]. Simulations are conducted in a 2D domain $110\Delta_{\text{ind}}$ wide, to minimize the impact of mode locking. Simulations are conducted for an initial $1000\Delta_{\text{ind}}$ of propagation to allow the detonation to relax to the natural cellular structure [21], with results shown for $x \geq 1000\Delta_{\text{ind}}$. Note that for both mixtures, a grid resolution of $\Delta = \Delta_{\text{ind}}/50$ was employed. While this resolution was sufficient to capture the macroscale detonation dynamics [4], a resolution study is underway to evaluate the impact of grid resolution on the dynamics of the nascent Mach stem. Further details of the numerics and simulation configuration are provided in Ref. [4].

3 Results and Discussion

Figure 2 presents the numeric soot foils based on the maximum pressure in the laboratory frame for both mixtures. The detonation cell size from simulation is in good agreement with experimental measurements [4]. Despite the factor of 3 difference in Reynolds and Knudsen numbers, the detonation cellular structure is qualitatively very similar between the two mixtures. Quantitatively, it is found that the coefficient of variation of the detonation cell length is somewhat larger in Mixture 1 (0.271) compared to Mixture 2 (0.233) [4], indicating a broader distribution of detonation cell sizes in Mixture 1 compared to Mixture 2. This is consistent with the experimental findings [4], and suggests a weak dependence of the detonation cell regularity on the Reynolds number of a mixture.

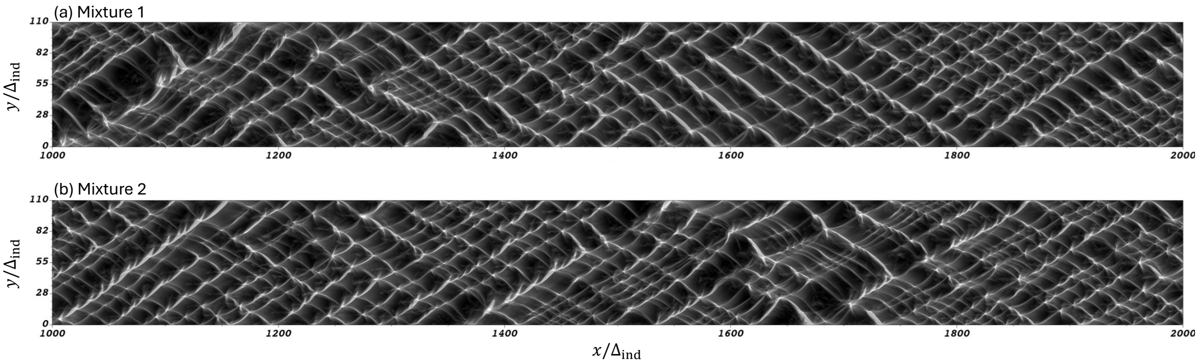

Figure 2: Numeric maximum pressure soot foils for (a) Mixture 1 and (b) Mixture 2. Spatial scales have been normalized by the ZND induction length Δ_{ind} for both mixtures.

The nature of the flowfield behind the detonation wave is demonstrated in Fig. 3, where instantaneous temperature and normalized vorticity fields are plotted for Mixture 1 and Mixture 2. The spatial domain has been normalized by the induction length to make a representative comparison between the two mixtures. Comparing the temperature fields for Mixture 1 (Fig. 3a) to Mixture 2 (Fig. 3c), in the near shock region both simulations display similarly laminar shear mixing layers emanating from the triple-point. However, moving into the burnt products Mixture 1 displays substantially more fine scale mixing as compared to Mixture 2, which is consistent with the larger Reynolds number of Mixture 1. In Mixture 1, a Kelvin-Helmholtz instability is present (1), apparent in both the temperature and vorticity fields. In Mixture 2, a similar length shear layer (2) remains stable and laminar. This is again consistent with the larger Reynolds number for Mixture 1. While the present Reynolds numbers and grid resolution are insufficient to observe the onset of Kelvin-Helmholtz instabilities behind the nascent Mach stem, the "turbulent" structure of the temperature field in the product zone will refract the transverse shock waves. The resulting acoustic waves can then perturb the Mach/incident shock structure, possibly forming additional triple points. This mechanism, along with simulations at higher grid resolutions and larger Reynolds numbers, will be presented at the confrence.

4 Concluding Remarks and Ongoing Work

Preliminary findings from simulation indicate that an increase in the Reynolds number of a mixture (i.e. a relative reduction in the viscous dissipation forces) produces a more irregular detonation cellular structure, quantified by the coefficient of variation for detonation cell length. Analysis of the flow field from simulations suggests that the increase in Reynolds number sees the onset of Kelvin-Helmholtz instabilities in the near shock region. While these instabilities appear to be isolated to the product region, the variations in local density are expected to refract the transverse shock waves, leading to perturbations

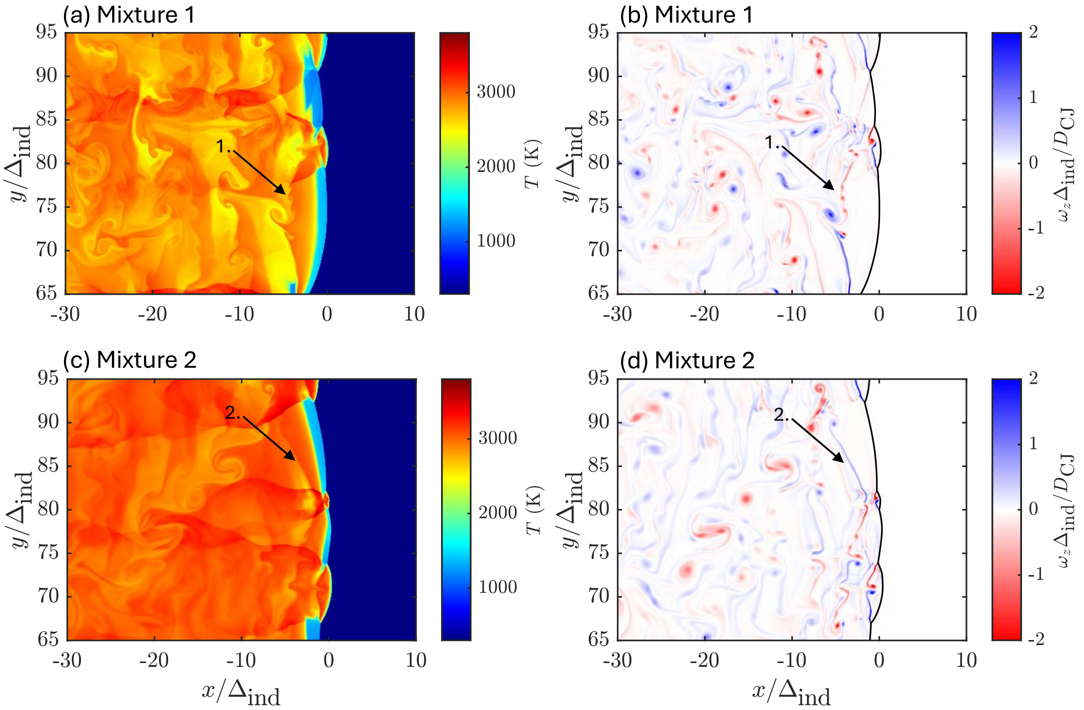

Figure 3: Instantaneous temperature (a,c) and normalized vorticity (b,d) fields for Mixture 1 (a,b) and Mixture 2 (c,d).

of the cellular structures. Note that the range of Reynolds numbers presented in the manuscript are limited and may not be sufficient to capture the onset of "turbulent" phenomena behind the nascent Mach stem. Further, the present grid resolution may be introducing excessive numeric viscosity and suppressing the formation of instabilities in Mixture 1. Simulations of Mixture 1 and Mixture 2 at higher resolutions, as well as additional parametric simulations of mixtures with idealized transport properties, are underway. Results from these simulations will be presented at the conference.

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