

Supplementary Document to “Numerical studies on detonation propagation in inhomogeneous mixtures with periodic reactant concentration gradient”

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1. Grid convergence

To check the grid convergence, we conducted detonation propagation simulations through inhomogeneous mixture for three mesh resolution levels. The numerical soot foils for these three mesh resolution levels are compared in figure A1. It is seen that the result for the finest mesh size of 3.9 μm (48 pts/li) is nearly the same as that for the mesh size of 1.95 μm (96 pts/li), while it significantly differs from that for the finest mesh size of 7.8 μm (24 pts/li). Therefore, we used the finest mesh size of 3.9 μm (48 pts/li) in the present simulations.

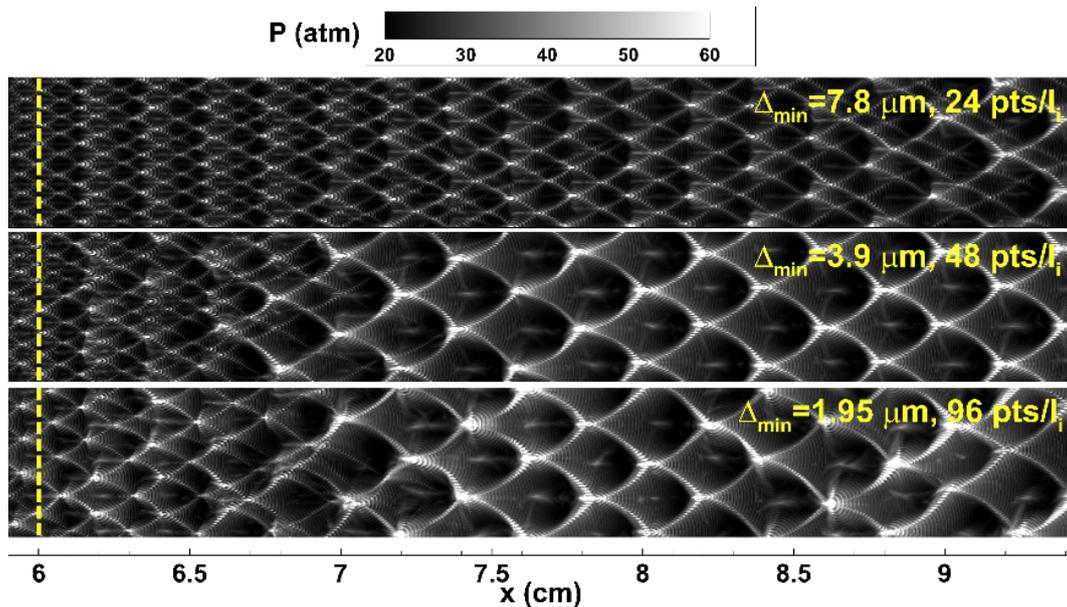


FIGURE A1. Numerical soot foils for three different resolution levels.

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2. Station structure

To demonstrate that a sufficient distance is allowed for the cellular structure to form of stationary structure, we conducted simulations for detonation propagation with a sufficiently long propagation distance. As shown in the figures A2 and A3, the original and large cellular structure does reach a quasi-stationary pattern in homogeneous as well as in inhomogeneous mixtures. Consistent results in figures 7 (in the manuscript), A2 and A3 can be observed, indicating that the present computational domain size is sufficient large.

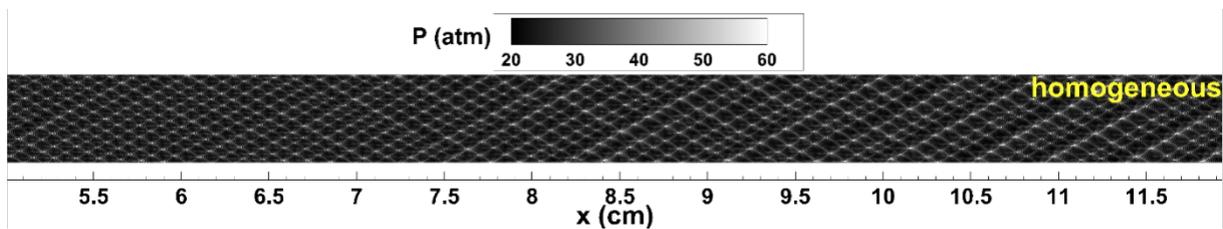


FIGURE A2. Numerical soot foils for homogeneous mixtures in a domain of length 12 cm.

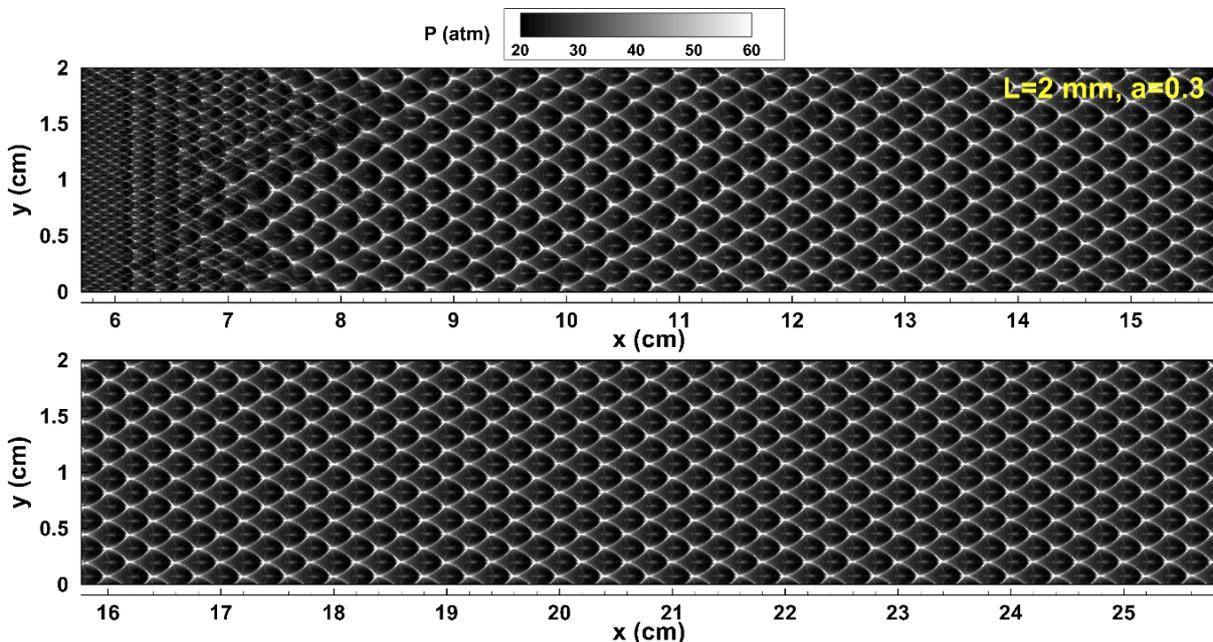


FIGURE A3. Numerical soot foils for inhomogeneous mixtures ($L=2$ mm and $a=0.3$) in a domain of length 26 cm and width 2 cm.

3. On diffusion terms

In all simulations, the diffusion terms in the governing equations were considered, i.e., the Navier-Stokes (NS) equations rather than the Euler equations were solved. The CHEMKIN packages were incorporated into A-SURF and AMROC to evaluate the temperature and component dependent transport properties. The mixture-averaged model was used for diffusion, and the Soret and Dufour effects were not included in this study. The detailed governing equations of the diffusion terms can be found in the appendix at the end of this section.

Simulations for one or the two representative cases have also been conducted for both NS and Euler simulations, as the numerical viscosity might exceed the physical viscosity of the problem [1]. The results from simulations based on Euler and Navier-Stokes are compared in figure A3. It is seen that the large cell size is consistent in both simulations with and without diffusion terms, which is in agreement with previous studies that have indicated that diffusion has little effect on the global characteristics of detonation propagation such as detonation speed and cell size. Although there is slight difference in the transition process ($6.5 < x < 7$ cm), the diffusion has little influence on the transition length. Therefore, the consideration of diffusion terms does not affect the main results and conclusions.

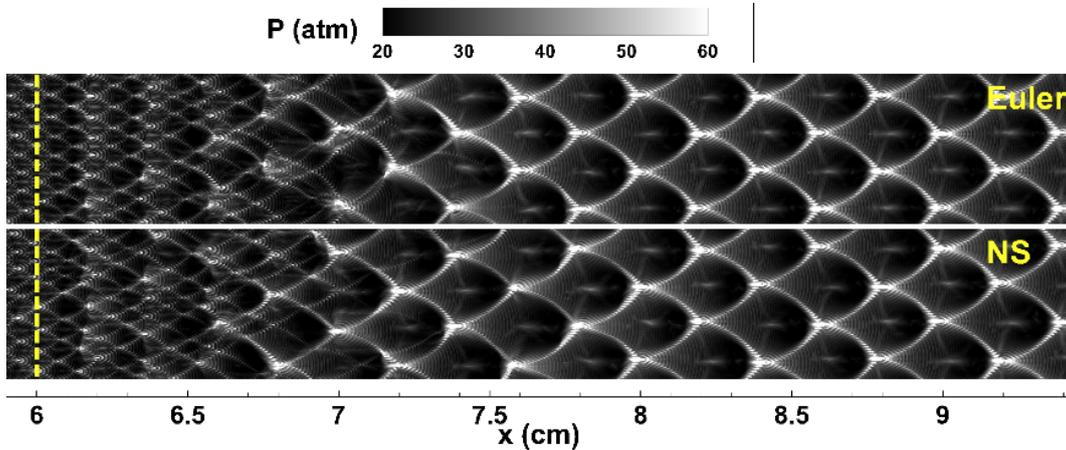


FIGURE A4. Numerical soot foils for inhomogeneous mixtures ($L=2$ mm and $a=0.3$, mixture 1) obtained with Euler and Navier-Stokes equations.

Appendix: governing equations for 1D case

A-SURF solves the conservation equations (including the unsteady Navier-Stokes equations as well as the energy and species conservation equations) for one-dimensional, adiabatic, multi-component, reactive flow in planar coordinates:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = F_v(U) + S_R, \quad (S1)$$

where t and x are respectively the temporal and spatial coordinates (x should be replaced by r for spherical configuration). In Eq. (S1), the vectors U , $F(U)$, $F_v(U)$, and S_R are defined as:

$$U = \begin{pmatrix} \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_n \\ \rho u \\ E \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u Y_1 \\ \rho u Y_2 \\ \vdots \\ \rho u Y_n \\ \rho u^2 + P \\ (E + P)u \end{pmatrix}, \quad F_v(U) = \begin{pmatrix} -(\rho Y_1 V'_1)_x \\ -(\rho Y_2 V'_2)_x \\ \vdots \\ -(\rho Y_n V'_n)_x \\ (\tau)_x \\ q_x + \Phi \end{pmatrix}, \quad S_R = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_n \\ 0 \\ 0 \end{pmatrix} \quad (\text{S2})$$

In Eq. (S2), ρ is the density, Y_k the mass fraction of species k , u the flow velocity, and E the total energy per unit mass. The subscript x in $F_v(U)$ stands for the partial derivative with respect to x . Instead of solving the continuity equation, the species conservation equations for all n species are solved in A-SURF. The continuity equation is recovered from the summation of all species conservation equations.

In the species conservation equations, ω_k and V'_k are the production rate and diffusion velocity of species k , respectively. The production rate ω_k is specified via collection of elementary reactions

$$\omega_k = M_k \sum_{j=1}^{n_r} \left\{ (v''_{k,j} - v'_{k,j}) \left[K_{f,j} \prod_{k=1}^n \left(\frac{\rho Y_k}{M_k} \right)^{v'_{k,j}} - K_{b,j} \prod_{k=1}^n \left(\frac{\rho Y_k}{M_k} \right)^{v''_{k,j}} \right] \right\}, \quad (\text{S3})$$

where M_k is the molecular weight of species k ; n_r is the total number of elementary reactions; $v'_{k,j}$ and $v''_{k,j}$ are the molar stoichiometric coefficients of species k in reaction j ; and $K_{f,j}$ and $K_{b,j}$ are the forward and reverse reaction rate of reaction j . The forward reaction rate for each elementary reaction is usually modeled using the empirical Arrhenius law

$$K_{f,j} = A_{f,j} T^{\beta_j} \exp\left(-\frac{E_j}{RT}\right) \quad (\text{S4})$$

where $A_{f,j}$ is the pre-exponential constant, β_j the temperature exponent, and E_j the activation energy. The reverse reaction rate can be obtained from chemical equilibrium constant and the forward reaction rate. These parameters ($A_{f,j}$, β_j , E_j) are given in the chemical mechanism and the reaction rates are calculated using the CHEMKIN package [2].

The diffusion velocity of species k is composed of three parts:

$$V'_k = V'_{k,Y} + V'_{k,T} + V'_{k,C} \quad (\text{S5})$$

$V'_{k,Y}$ is the ordinary diffusion velocity given by the mixture-averaged formula [3]:

$$Y_k V'_{k,Y} = -D_{km} \frac{1}{\bar{M}} \frac{\partial(Y_k \bar{M})}{\partial x} , \quad (\text{S6})$$

where D_{km} is the mixture-averaged diffusion coefficient of species k and \bar{M} is the mean molecular weight of the mixture.

$V'_{k,T}$ is the thermal diffusion velocity, which is included only for low molecular weight species (hydrogen atom and hydrogen molecule):

$$Y_k V'_{k,T} = -D_{km} \Theta_k \frac{M_k}{\bar{M} T} \frac{\partial T}{\partial x} , \quad (\text{S7})$$

where Θ_k is the thermal diffusion ratio of species k . **Note that the thermal diffusion was not considered in the present study.**

The correction velocity $V'_{k,C}$ is included to ensure the compatibility of species and mass conservation equations [3]. It is determined by the requirement of

$$\sum_{k=1}^n (Y_k V'_k) = 0 . \quad (\text{S8})$$

In the momentum equation, P is the pressure and the viscous stresses, τ , is

$$\tau = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial u}{\partial x} , \quad (\text{S9})$$

where μ is the dynamic viscosity of the mixture.

In the energy conservation equation, the total energy, E , is defined through

$$E = -P + \rho u^2 / 2 + \rho h , \quad h = \sum_{k=1}^n (Y_k h_k) , \quad h_k = h_{k,0} + \int_{T_0}^T C_{P,k}(T) dT , \quad (\text{S10})$$

where T is the temperature, h_k the enthalpy of species k , $h_{k,0}$ the species enthalpy of formation at the reference temperature T_0 , and $C_{P,k}$ the specific heat of species k at constant pressure. The heat flux is

$$q = \left[\lambda \frac{\partial T}{\partial x} - \rho \sum_{k=1}^n (h_k Y_k V'_k) \right] , \quad (\text{S11})$$

where λ is the thermal conductivity of the mixture. In the energy equation, the viscous dissipation rate is

$$\Phi = \mu \left\{ 2 \left(\frac{\partial u}{\partial x} \right)^2 - \frac{2}{3} \left[\frac{\partial u}{\partial x} \right]^2 \right\} + u \frac{\partial \tau}{\partial x}. \quad (\text{S12})$$

The pressure can be obtained from the density, temperature and mean molecular weight using the equation of state for an ideal gas

$$P = \rho R T / \bar{M}, \quad (\text{S13})$$

where $R=8.314 \text{ J}/(\text{mol}\cdot\text{K})$ is the universal gas constant.

The thermodynamic and transport properties in Eqs. (S6-S13) are evaluated using the CHEMKIN and TRANSPORT packages [2,3] interfaced with A-SURF:

$$\mu = \sum_{k=1}^{NS} \frac{Y_k \mu_k}{M_k \left(\sum_{j=1}^{NS} \frac{Y_j \Phi_{kj}}{M_j} \right)} \quad \text{where} \quad \Phi_{kj} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_k}{M_j} \right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_k}{\mu_j} \right)^{\frac{1}{2}} \left(\frac{M_j}{M_k} \right)^{\frac{1}{4}} \right]^2$$

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k} D_{jk}}, \quad \lambda = \frac{1}{2} \left[\bar{M} \sum_{k=1}^{NS} \frac{Y_k k_k}{M_k} + \left(\bar{M} \sum_{k=1}^{NS} \frac{Y_k}{M_k k_k} \right)^{-1} \right] \quad \text{with} \quad \bar{M} = \left(\sum_{k=1}^{NS} \frac{Y_k}{M_k} \right)^{-1}$$

$$C_{p,k}(T) = \frac{R_0}{M_k} \left(\alpha_{1k} + \alpha_{2k} T + \alpha_{3k} T^2 + \alpha_{4k} T^3 + \alpha_{5k} T^4 \right)$$

$$h_k(T) = \frac{R_0 T}{M_k} \left(\alpha_{1k} + \alpha_{2k} \frac{T}{2} + \alpha_{3k} \frac{T^2}{3} + \alpha_{4k} \frac{T^3}{4} + \alpha_{5k} \frac{T^4}{5} + \frac{\alpha_{6k}}{T} \right)$$

$$s_k(T) = \frac{R_0}{M_k} \left(\alpha_{1k} \ln T + \alpha_{2k} T + \alpha_{3k} \frac{T^2}{2} + \alpha_{4k} \frac{T^3}{3} + \alpha_{5k} \frac{T^4}{4} + \alpha_{7k} \right)$$

$$C_{v,k}(T) = C_{p,k}(T) - \frac{R_0}{M_k}, \quad e_k(T) = h_k(T) - \frac{R_0}{M_k} T$$

$$C_p = \sum_{k=1}^{NS} Y_k C_{p,k}, \quad C_v = \sum_{k=1}^{NS} Y_k C_{v,k}, \quad h = \sum_{k=1}^{NS} Y_k h_k, \quad e = \sum_{k=1}^{NS} Y_k e_k$$

where α_{1k} 、 α_{2k} 、 α_{3k} 、 α_{4k} 、 α_{5k} 、 α_{6k} 、 α_{7k} are coefficients inputted to CHEMKIN packages [3].

References:

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- [2] R.J. Kee, F.M. Rupley, J.A. Miller, in, Sandia National Laboratory Report SAND89-8009B, 1989.
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