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Investigation of Numerically Derived Cellular Structures via the Compressible Reactive Euler Equations with Single-Step Chemical Kinetics

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Premixed gas-phase detonations are supersonic combustion waves that propagate through a homogeneous gaseous mixture, which contains fuel and oxidizer. Under realistic conditions, the detonation wave is unstable with a complex transient multi-dimensional structure. These features are attributed to transverse waves that interact with the leading shock and produce triple-shock configurations. Due to the abrupt pressure variation near the triple points, their trajectories can be experimentally recorded on a soot coated foil, revealing the cellular structure of the detonation front. Previous studies demonstrated that numerical solutions of the multi-dimensional compressible reactive Euler equations can reproduce the experimentally observed cellular structures. Nevertheless, a good agreement between the experimentally measured and the numerically derived cell dimensions is rarely achieved. In the current study, we aim to gain fundamental understanding regarding the influence of different dimensionless groups on numerical solutions of the 2-D compressible reactive Euler equations with single-step Arrhenius chemical kinetics. For this purpose, we carry out an extensive numerical investigation for different values of the three dimensionless groups that govern the detonation cellular structure, namely, effective activation energy, normalized heat release, and ratio of specific heat capacities. A very detailed statistical analysis is conducted for each numerical soot foil using an in-house automated computer-vision-based cell measurement technique. Our analysis results reveal, for the first time, the dependence of the average detonation cell width, length, aspect ratio, and angle as well as the cell irregularity for a wide range of the three governing dimensionless groups. Finally, we compare our results against multi-dimensional numerical simulations with multi-step chemical kinetics and experimental results. We demonstrate that many of the results observed via our simplified numerical simulation approach well agree with more elaborate numerical simulation approaches and realistic experimental findings. Our research results provide new insights to better understand the reasons for current discrepancies between numerically derived and experimentally measured premixed gas-phase detonation cellular structures.