Operator splitting in simulation of detonation structure

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1 Abstract

The effect of four splitting procedures; two first order splitting named (i) hydrodynamic-kinetic; *H-K splitting*, (ii) kinetic-hydrodynamic; *K-H splitting* and two second order Strang type splitting, (iii) (*H/2*)(*K*)(*H/2*) and (iiii) (*K/2*)(*H*)(*K/2*) on the cellular structure of detonations are compared. It is found that a minimum grid size of 25 cells per half reaction length (*hrl*) is required to capture a convergent cell structure in all methods. Results indicate that the number of cells that should be refined behind the shock front (NLB), differs in various splitting procedure. 30 cells are required for both first order splitting methods, 10 cells for (*H/2*)(*K*)(*H/2*), and 30 cells for (*K/2*)(*H*)(*K/2*) method. The CPU time required for *K-H* is significantly lower than that of other methods. The Strang splitting (*H/2*)(*K*)(*H/2*) leads to the most CPU time.

2 Introduction

A gaseous detonation wave typically has a cellular structure that involves triple-shock interactions [1]. Oran et al. [2] simulated detonation waves in H_2–O_2–Ar mixture using a detailed chemical reaction mechanism with 1st order splitting. It was found that the coarsest grid led to two more weak triple points than that of fine grid. Singh et al. [3] conducted simulations for both in-viscid and viscous flows with 1st order splitting, with grid sizes varying from 2 to 24 cells in *hrl*. With coarse grids, the numerical diffusion has competed with its physical counterpart, leading to similar solutions for inviscid and viscous flows. Choi [4] by simulation of two-dimensional detonation, with single step reaction model, proposed that a minimum of 5 grid points in *hrl* should be included in the heat release zone to achieve an accurate detonation cell structure. Sabzpooshani [5] with two-dimensional single step Arrhenius reaction model simulated the effect of transverse waves in the propagation of detonation waves, using 1st order *H-K* splitting method, by placing porous wall in the transverse boundary. In their study a minimum of 25 grid points per half reaction zone length was needed to capture the vortex structure of the flow behind the shock font. Dou et. al [6] simulated three-dimensional detonation with Arrhenius kinetic model by WENO scheme. They used 16 and 32 grid points per *hrl* to capture the cellular structure and found no significant difference between two grid resolutions. Most of the studies mentioned above have used first order splitting (*H-K splitting*) in their study, the present work investigates the effect of four different operator splitting on the grid size required for accurate simulation of cell structure is investigated.

3 Governing equations

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The analysis is based on the two-dimensional reactive Euler equations. The reaction rate is expressed with a single step Arrhenus law. The reference length is the half-reaction length (*hrl*). The mixture is characterized by Q/RT_0=50, E_a/RT_0=25, γ=1.2. The set of conservation equations is expressed as:

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=0.0 \tag{1}$$

$$U=[\rho,\rho u,\rho v,\rho E,\rho\beta]^T,\ F(U)=[\rho u,\rho u^2+p,\rho uv,\rho uE+up,\rho u\beta]^T$$

$$G(U)=[\rho v,\rho uv+p,\rho v^2,\rho vE+vp,\rho v\beta]^T,\ S=[0,0,0,0,\rho W]$$

β is the reaction progress variable, E is the specific total energy per unit mass, Q is the heat release per unit mass of reactant and W is the chemical rate which are defined as:

$$E=\frac{p}{\rho(\gamma-1)}+\frac{(u^2+v^2)}{2}+\beta Q \tag{2}$$

$$W=-k\beta\exp(\frac{-E_a}{RT}) \tag{3}$$

The details of the numerical method were discussed in depth in [5].

4 Operator splitting

Equation (1) can be rewritten in the following form $\begin{cases}u_t=A(u)\\u(0)=u_0\end{cases}$. Suppose that the function $A(u)$ splits into two pieces; hydrodynamic term (H) and Kinematic term (K), $A(u)=H(u)+K(u)$. A first order splitting method has the form $u^n=[H(\Delta t)E(\Delta t)]^n u_0$. The local error in this splitting procedure is $O(\Delta t^2)$ and hence the splitting is only first order accurate. A second order splitting may be defined as:. $u^n=[H(\Delta t/2)E(\Delta t)\ H(\Delta t/2)]^n u_0$. This study investigate these two classes of splitting that lead to four splitting procedure; H→K, K→H, H/2→K→H/2, and K/2→H→K/2 [7].

5 Results

The smoke-foil inscription is numerically reproduced based on the peak pressure in the flow field, after a fairly long period that the structure shows a high degree of quasi-steadiness. In the following, NLB is the number of grid cells behind the leading shock that are refined, NR is the adaptive ratio in AMR, XHRL is the initial grid spacing, and L is the channel width.

H-K splitting

Figures (1) and (2) show the effect of utilizing the first order splitting such that the solution of hydrodynamic equation has used as an initial condition for the kinetic equation. The cells have convex curvature tracks in the first half cell and concave tracks in the second half cell. Figure (1-a) shows that for XHRL=0.5, 1 cell formed in the channel width, but the trajectories of triple points do not have adequate luminosity. Figure (1-b) is produced for XHRL=0.2, 1.5 cells formed in the channel width and the cell pattern have adequate luminosity. This is consistent with the result of [8].

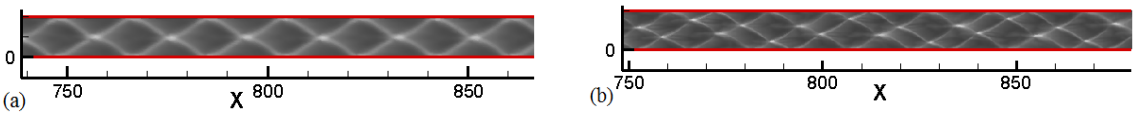

Figure 1. Numerical smoked-foil record; NLB=10, NR=5, L=10, (a) XHRL=0.5, (b) XHRL=0.2

By increasing the NLB to 30, figure (2-a), 1 cell is formed, exhibiting quite regular cells with adequate luminosity. Increasing NLB to 50, figure (2-b) and more, has no effect on the cellular pattern. The calculation was repeated for XHRL=0.16 (not shown here); no noticeable difference with figure (2-b) was observed. So, XHRL=0.2 with NR=5 (25 grids per *hrl*) is the minimum grid resolution to simulate accurately the cellular structure.

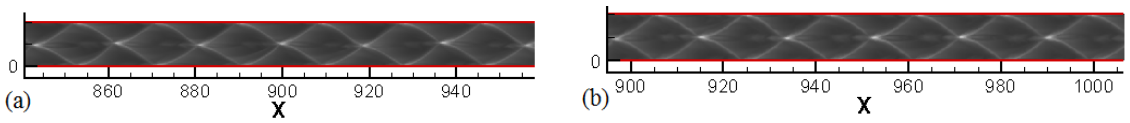

Figure 2. Numerical smoked-foil record; NR=5, L=10, (a) NLB=30, (b) NLB=50

K-H splitting

The result of *K-H* splitting is shown in figure (3). Figure (3-a) shows that 1.5 cells is formed in the channel width for NLB=10, with more regularity than cells formed with *H-K splitting*. Calculation repeated with XHRL=0.5, it is observed that the cells don't have adequate luminosity.

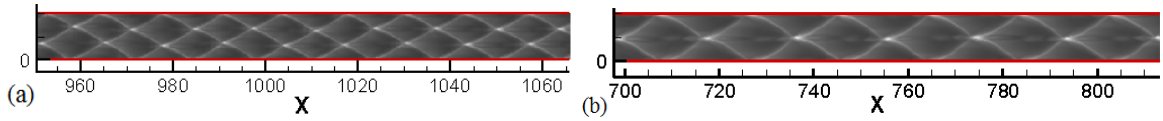

Figure 3. Numerical smoked-foil record (*K-H splitting*); L=10, NR=5, XHRL=0.2,(a) NLB=10, (b) NLB=30

Increasing NLB to 30, 1 cell in the channel width is formed; figure (3-b) with the same quality as figure (2-a). The CPU time is significantly lower than that of *H-K* splitting.

Strang (*H/2*)(*K*) (*H/2*) splitting

Figure (4-a) shows cellular pattern for the Strang splitting. It is observed that for NLB=10, one cell is formed in the channel width. Increasing NLB to 50, no significant difference is observed, figure (4-b).

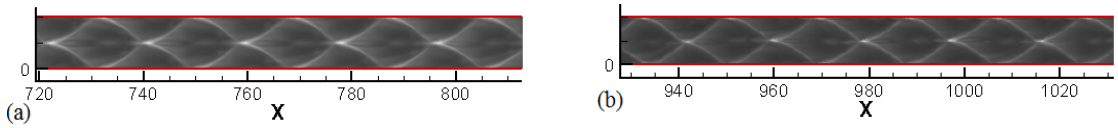

Figure 4. Numerical smoked-foil record (*H/2*)(*K*)(*H/2*); XHRL=0.2 , NR=5, L=10, (a) NLB=10, (b) NLB=50

Strang (*K/2*) (*H*) (*K/2*) splitting

The results of the (*K/2*)(*H*)(*K/2*) method is shown in figure (5). No significant difference, with those of *K-H* splitting, is observed. This method takes much more CPU time than the *K-H* method. The calculation was repeated for NLB=50; no noticeable difference with figure (5-b) was observed.

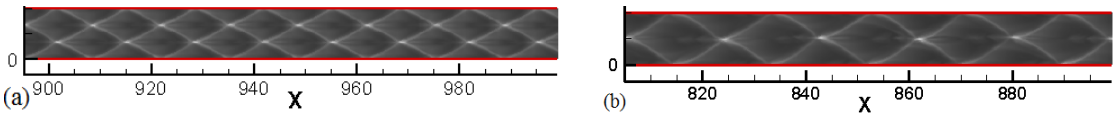

Figure 5. Numerical smoked-foil record (*K/2*)(*H*)(*K/2*); L=10, NR=5, XHRL=0.2, (a) NLB=10, (b) NLB=30

Time required to forms a convergent cellular structure are shown in table 1 for different methods. As the table shows the *K-H* splitting possesses the lower computational time and the Strang splitting (*H/2*)(*K*)(*H/2*) leads to the maximum time.

Table 1: CPU Time for different splitting methods XHRL=0.2, NLB=30, L=10

Method	H-K	K-H	K/2-H-K/2	H/2-K-H/2
Time*10^{-3} (sec)	93.223	89.979	97.903	173.759

Table 2 shows the calculated cell length for different NLB. All method leads to the cell length about 18.6 *hrl*. Except of Strang (*H/2*)(*K*)(*H/2*) method, other methods need at least NLB=30 to give a convergent cellular structure.

Table 2: Calculated cell length for different methods, XHRL=0.2, NR=5, L=10

Method	NLB=10	NLB=30	NLB=50	NLB=70
H-K	-	18.847	18.726	18.621
K-H	-	18.831	18.664	18.632
H/2-K-H/2	18.673	18.652	18.621	18.601
K/2-H-K/2	-	18.876	18.787	18.628

6 Conclusion

The effects of operator splitting and grid size on the cellular structure were examined. The present results indicate that *K-H splitting* converges to a fixed cellular structure in lower CPU time than that of *H-K splitting* and even (*K/2*)(*H*)(*K/2*) second order splitting. (*H/2*)(*K*)(*H/2*) converges to the cellular structure in lower NLB than that of the other methods, by the expense of the most CPU time.

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