Numerical Study of Supersonic Combustors by Multi-Block Grids With Mismatched Interfaces

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Abstract

A three-dimensional, finite-rate chemistry, Navier-Stokes code has been extended to a multi-block code with mismatched interface for practical calculations of supersonic combustors. To ensure global conservation, a conservative algorithm was used for the treatment of mismatched interfaces. The extended code was checked against one test case, i.e., a generic supersonic combustor with transverse fuel injection, examining solution accuracy, convergence, and local mass flux error. After testing, the code was used to simulate the chemically reacting flow fields in a scramjet combustor with parallel fuel injectors (unswept and swept ramps). Computational results were compared with experimental shadowgraph and pressure measurements. Fuel-air mixing characteristics of the unswept and swept ramps were compared and investigated.

Introduction

Interest in chemically reacting flow computation for practical applications has been raised in recent years. One of the goals is simulating three-dimensional chemically reacting flow fields in a supersonic combustor to investigate the fuel-air mixing enhancement. For practical application to a three dimensional complex geometry, such as a scramjet combustor with ramp fuel injectors, the main objective of the present work is to extend a 3D finite-rate chemistry, Navier-Stokes code to a multi-block grid code with mismatched interfaces.

A three-dimensional code, RPLUS3D [1], has been developed for chemically reacting flows at NASA Lewis Research Center. The code uses an implicit finite volume, Lower-Upper (LU) method to solve the Reynolds averaged full Navier-Stokes equations and species transport equations in a fully coupled manner. A chemistry model with nine species and eighteen reaction steps is used to represent the chemical reaction of \( H_2 \) and air which is incorporated with a comprehensive real gas property model.

In the present work, the code has been extended to a multi-block grid code for handling complex three-dimensional geometries. The multi-block grids are allowed to have mismatched grid interfaces at the block juncture plane. The mismatched grid interface produces a great deal of geometric flexibility in grid generation, especially in three-dimensional cases. Since most interest lies in studying mixing mechanisms and chemical reactions in a supersonic combustor, the presence of shock waves in the flow field is inevitable. In order to ensure proper shock-capturing properties, the mismatched grid interface is treated by a conservative algorithm which balances the fluxes at the interface so that global conservation is automatically satisfied. Details of the method will be explained in a later section.

In this study, the modified RPLUS3D code was tested first for validation. A generic supersonic combustor with transverse fuel (hydrogen) injection was considered as a test problem. The computational domain of the combustor was split into two blocks whose interface is set so that the grids mismatch each other. Tests compared result of a two block grid with that of a single block grid, in terms of solution accuracy, convergence rate, conservation requirements, and computational time and memory. The conservation was checked by captured shock definition and local mass flux error. One-to-one comparisons of the two results will be presented in the Results section.

After this testing, a supersonic combustor with parallel ramp fuel injectors was simulated by the present numerical technique. This problem has been extensively investigated experimentally [2,3] and numerically [4,5] at NASA Langley for the mixing enhancement study in a supersonic combustor. Complicated mixing mechanisms were observed due to interactions of various hydrodynamic characteristics and chemical reactions. In the present study, computations with use of the multi-block grid strategy were made for the unswept and swept fuel ramp cases. Wall pressure distributions were compared with the experiment conducted at NASA Langley [3]. Detailed comparisons and analysis will be presented in the Result section.
RPLUS3D Code

The RPLUS3D code solves a strong conservative form of the three-dimensional, compressible, Reynolds-averaged full Navier-Stokes and species transport equations in a fully coupled manner.

The finite-rate chemical reaction of hydrogen and air is modeled with nine species and eighteen step reaction mechanism. The specific heat, thermal conductivity and viscosity of each species are given as fourth-order polynomials of temperature and the coefficients of these polynomials are valid up to a temperature of 6000°K. The specific heat of the gas mixture is obtained by concentration weighting of each species, while the thermal conductivity and viscosity of the gas mixture are calculated from Wilke's mixing rule. The binary mass diffusivity between two species is obtained from the Chapman-Enskog theory in conjunction with the Lennard-Jones intermolecular potential function, and the diffusion of a species in a gas mixture is approximated by Fick's law [6,7].

Once the thermodynamic properties, chemical reaction rates, and diffusion coefficients have been computed, the governing equations are solved by an implicit, finite-volume, LU(Lower-Upper) scheme [8]. Here source terms in the species equations are treated implicitly, to suppress the stiffness problem. Also the LU scheme in the left hand side is formulated in such a way that only scalar diagonal inversion is required for the flow equations and diagonal block inversion for the species equations. The spatial differencing uses the central differencing with the second and fourth order artificial dissipation terms.

Multi-Block Grids and Mismatched Interfaces

For enhanced application of CFD to practical, complex three-dimensional applications, multi-block grids are necessary unless unstructured grids are used. A single block structured grid encounters not only difficulties in grid generation but also issues in grid quality such as skewness or clustering in unnecessary regions. The RPLUS3D code is presently written as a single structured grid solver, and therefore extension of the code to a multi-block grid (three dimensional patched grid) with mismatched interfaces has been pursued. For minimal complication, a main program module was developed for multi-block data storage, management and communication, and interfaces with the single block solver with chemistry.

In the present work, multi-block grids are allowed to have a mismatched interface at the block juncture plane. The mismatched grid interface produces more geometric flexibility in grid generation, especially in three-dimensional problems. Since current interest lies in supersonic combustor computations, the presence of shock waves in the flow field is inevitable. In order to ensure proper shock-capturing properties, the mismatched grid interface must be treated by a conservative approach. The basic principle is based on balancing of the spatial fluxes at the interface so that global conservation is automatically satisfied. However in the present work an alternative approach was taken, i.e., balancing the time fluxes at the interface. The shock capturing capability of this approach was demonstrated for two and three dimensional patched grids [9,10] and also for two dimensional overlaid grids [11].

At a juncture plane, the time flux balance is written as

\[
\int \int Q^{(1)} d\xi d\eta d\zeta \equiv \int \int Q^{(2)} d\xi d\eta d\zeta \quad (1)
\]

By assuming equal spacing in the \(\xi\)-direction across the interface, Eq. (1) is reduced to a two dimensional form as

\[
\int \int Q^{(1)} d\eta d\zeta \equiv \int \int Q^{(2)} d\eta d\zeta \quad (2)
\]

Eq. (2) requires the partial areas of overlap between mismatched cells, which are used for weighting coefficients in the interpolation process. With the above approach, one more step of generalization was taken for handling mixed block boundaries, that is, a cell of block 1 faces with partial cells of block 2 and with a physical boundary such as a wall. In this case, the block 1 cell interpolates with area-based coefficients from the block 2 cells and from the block 1 cell itself to which the no-slip wall condition applied. This mixed boundary update procedure was required for the parallel fuel ramp combustor calculations in the region along the ramp edge.

Data between multi-blocks communicate at each iteration through boundary interface treatment. This procedure updates the boundary condition at each interface after interior cells of each block are solved.

Results and Discussion

Test Case

As a validation test, a generic supersonic combustor with transverse fuel injection was considered. Incoming air is at Mach 4, 1 atm, and 1300 °K. A sonic hydrogen jet is transversely injected at 8 atm and 700
A scramjet combustor with parallel fuel injection ramps has been studied experimentally [2,3] and numerically [4,5]. The main purpose of this investigation was to explore techniques to enhance the relatively slow mixing associated with parallel injection which may be useful due to a thrust contribution by the momentum of the fuel at high speeds. This particular problem was chosen as a suitable application to test the present multi-block/mismatched interface, chemically reacting code.

The perspective view of the unswept and swept injector ramps is shown in figure 7(a), with a schematic geometry description shown in figure 7(b). Nominal test conditions for the Mach 2 high temperature vitiated incoming air at the leading edge of the ramps are

\[ P = 102000 \, (N/m^2) \]
\[ T = 1024 \, ^oK \]
\[ M = 2 \]
\[ \alpha_{H_2} \, = \, 0 \]
\[ \alpha_{H_2O} \, = \, 0.182 \]
\[ \alpha_{O_2} \, = \, 0.256 \]
\[ \alpha_N \, = \, 0.562 \]

and at the hydrogen jet at the injector port are

\[ P = 325200 \, (N/m^2) \]
\[ T = 187 \, ^oK \]
\[ M = 1.7 \]
\[ \Phi \, = \, 1.2 \]

where \( \Phi \) is fuel equivalence ratio.

The detailed informations for this experiment can be found in reference [2].

In the present study, the computational domain was limited to the region between centerplanes of the injector port and the duct. For both the unswept and swept cases, three blocks of grid were used (see figure 8(a,b)). Notice that block 1 and 2 occupy different regions of space around the ramp in the unswept and swept cases. The geometry of the unswept ramp is simpler than that of the swept ramp which has a connecting bridge at the leading edge with the mated one. The unswept ramp consists of meshes, 44x20x30, 44x30x44, and 44x40x44 for the block 1, 2, and 3, respectively, while the swept ramp meshes are 44x40x30, 44x30x30, and 44x40x44. The meshes of each block for both cases are shown in figure 9(a,b). In the computations, walls are considered adiabatic and flow is assumed laminar. Also the top wall was considered as a symmetry plane (inviscid wall) to reduce grid points. At the mismatched block interfaces, boundary conditions are updated by the procedure explained in the previous section.

Ramps
Approximately 20 megawords of memory were required for the unswept and swept cases where a total of 0.162 and 0.17 million mesh points were used, respectively. The CPU times were 19 sec/iteration on CRAY Y-MP and took approximately 25.3 hours of computation for 4800 iterations in each case. The convergence history for both cases is shown in figure 10, where solid and dotted lines represent the unswept and swept cases, respectively. The residual for the unswept case drops approximately three order of magnitude, while even slower convergence was observed in the swept case due to more unsteadiness of the flow characteristics. Local mass flux errors for both cases are shown in figure 11 (downstream of the jet injection). The local maximum of the mass flux error is below 1%. Contour plots of density at the jet centerplane for both unswept and swept cases are compared with an experimental shadowgraph (swept case) in figure 12 (a-c). Most flow features such as the ramp shock, fuel jet plume, shear layers, and expansion fan at the end of the ramp can be seen in both cases. Simply due to a difference in ramp shape (sweep), two things can be clearly noticed. First, the swept ramp generates a stronger ramp shock and a more persisting reflected shock from the top wall, because its geometry is two dimensional at the leading edge. Second, the fuel jet at the downstream exit is more lifted off from the ground due to the interaction with strongly-induced vortical flow generated along the edge of the swept ramp side wall. Figure 13 (a,b) show contours of axial component of vorticity (only in clockwise rotation) generated along the ramp side wall edge for the unswept and swept cases. The vortices of the unswept case are bound closely to the side wall of the ramp, while stronger and more coherent structures of vortices are exhibited in the swept case due to the sweep of the ramp itself.

Some pressure distributions of computational results are compared in figure 14 and 15 with experimental data [3]. Figure 14 (a,b) show wall pressure distributions at the jet centerplane for both cases. Despite the fact that the measured flow condition was turbulent and a limited number of grid points was used, good agreement was obtained for the unswept ramp case. However, for the swept case, some discrepancies are evident at the leading edge of the ramp and downstream of the jet injection. According to reference [8], the swept ramp has a small forward facing step in the test section caused by model misalignment, possibly resulting in a higher pressure at the leading edge. In addition the swept ramp case showed a distinct side wall effect [3] which was not dramatically discernable in the unswept case, and in consequence mixing and combustion downstream of the jet injection was directed toward the centerplane between two swept ramps. This might explain disagreement of the data point at the downstream of the injection, since the present computation assumed perfect symmetry at the centerplane of the jet injection. Figure 15 (a,b) shows wall pressure distributions of both cases at the centerplane between the two ramps. Agreement with experiment seems reasonable for the unswept ramp case, considering the coarseness of the grid at the centerplane. However, the swept case shows a considerable disagreement at the two middle points, while disagreement at the first two points can be similarly noticed in the unswept case and at the last data point due to the movement of the jet direction explained earlier. These two points are located at and upstream of the fuel injection port. A high pressure rise might be caused by a flame holding effect due to the hydrogen penetration in the upstream direction [3]. Unfortunately the present calculations did not pick up this effect. As pointed out by C. McClinton and D. Capriotti [12], two possible contributors may be a laminar flow assumption, and uniform inflow condition started at a very short distance upstream of the ramp leading edge, so that the boundary layer was not fully established when entering the ramp.

Figures 16(a-f) shows cross flow velocity vectors at six different locations downstream of the fuel jet injection for the swept ramp. Mixing of the fuel jet develops in an interaction with the strong vortical flow generated by the swept ramp. Figures 16 (b,c) show merging of a ramp vortex into the jet and formation of a single vortex (figure 16(d)). Figures 16 (e,f) show further development of the vortex and also a growing counter-rotating secondary vortex at the lower corner, indicating jet lift-off from the ground.

Figures 17 (a,b) and 18 (a,b) show contours of $H_2$ and $H_2O$ mass fraction at five different downstream locations of both unswept and swept cases, exhibiting mixing and combustion characteristics of the parallel fuel injection. Downstream development of the jet structure deformation can be well observed. Deformation of the fuel jet has already begun at the second location for the swept case, and at the third location the jet is off the wall. Finally the jet core region is detached from the centerplane and mixed with air, while in the unswept ramp case the core is deformed but remains at the centerplane. Similarly, better mixing and combustion for the swept ramp case can be observed by development of $H_2O$ formation.

Conclusions

The extended three-dimensional, finite-rate chemistry, Navier-Stokes code for a multi-block grid with
mismatched interfaces has been tested for a generic supersonic combustor with transverse fuel injection. The solution of a two block grid was compared with that of a single block grid. Accuracy was not affected by the mismatched interface treatment, while the convergence was slightly slowed. Also local mass flux errors are within 0.2%, indicating that conservation was maintained.

The code was then used for simulating chemically reacting flow fields of parallel fuel injectors in a scramjet combustor. The combustor with unswept and swept ramps was filled by approximately 0.17 million mesh points in three blocks of grid with mismatched interfaces. Computation required approximately 20 megawords of memory and 25 hours of CPU time on CRAY Y-MP for 4800 iterations (three order of magnitude drop in residual). Density contour plots at the ramp centerplane favorably compare with the experimental shadowgraph. The wall pressure distribution agrees well with experiments for the unswept case. However some discrepancies were observed for the swept ramp case, due to model misalignment in the experiment and computationally neglecting side wall effects. Also the assumption of laminar flow may possibly contribute to missing upstream combustion. Finally, mixing and combustion enhancement was distinctively demonstrated for the swept ramp case, due to the interaction of the fuel jet with more strongly induced vortical flow generated at the swept ramp side edge.

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References


Figure 1. Configuration of supersonic combustor with transverse fuel injection

Figure 2(a). Two block meshes:
- block 1 (50x40x44)
- block 2 (13x40x44)

Figure 2(b). Detailed view of mismatched interface

Figure 3. Convergence comparison

Figure 4. Local mass flux error (%)
Mismatched Interface

Figure 5(a). Density contours (1 block)

Figure 6(a). Density contours (2 blocks)

Figure 5(b). H₂O mass fraction (1 block)

Figure 6(b). H₂O mass fraction (2 blocks)

Figure 5(c). H₂ mass fraction (1 block)

Figure 6(c). H₂ mass fraction (2 blocks)
RAMP INJECTOR BLOCKS

Figure 7(a). Perspective view of ramp injector blocks

Figure 7(b). Schematics of geometry (swept ramp)

Figure 8(a). Multi-block strategy: (3 blocks for unswept ramp)

Figure 8(b). Multi-block strategy: (3 blocks for swept ramp)

Figure 9(a). 3 block meshes (unswept), (44x20x30, 44x30x44, 44x40x44)

Figure 9(b). 3 block meshes (swept), (44x40x30, 44x30x30, 44x40x44)
Figure 10. Convergence comparison

Figure 11. Local mass flux errors (%)

Figure 12(a). Density contours at jet centerplane (unswept)

Figure 12(b). Experimental Shadowgraph (swept)

Figure 12(c). Density contours at jet centerplane (swept)
Figure 13(a). Vorticity contours (unswept)

Figure 13(b). Vorticity contours (swept)

Figure 14(a). Wall pressure at jet centerplane (unswept)

Figure 14(b). Wall pressure at jet centerplane (swept)

Figure 15(a). Wall pressure at centerplane between ramps (unswept)

Figure 15(b). Wall pressure at centerplane between ramps (swept)
Figure 16(a-f). Cross flow velocity vector at six different locations downstream of the fuel jet injection (swept)
Figure 17(a). H₂ mass fraction (unswept)

Figure 17(b). H₂ mass fraction (swept)

Figure 18(a). H₂O mass fraction (unswept)

Figure 18(b). H₂O mass fraction (swept)
A three-dimensional, finite-rate chemistry, Navier-Stokes code has been extended to a multi-block code with mismatched interface for practical calculations of supersonic combustors. To ensure global conservation, a conservative algorithm was used for the treatment of mismatched interfaces. The extended code was checked against one test case, i.e., a generic supersonic combustor with transverse fuel injection, examining solution accuracy, convergence, and local mass flux error. After testing, the code was used to simulate the chemically reacting flow fields in a scramjet combustor with parallel fuel injectors (unswept and swept ramps). Computational results were compared with experimental shadowgraph and pressure measurements. Fuel-air mixing characteristics of the unswept and swept ramps were compared and investigated.