Interaction between Grid and Design Space Refinement for Bluff Body-Facilitated Mixing

Tushar Goel*, Yolanda Mack†, Raphael T. Haftka‡, Wei Shyy§
Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL 32611

and

Nestor V. Queipo†
Applied Computing Institute, Faculty of Engineering, University of Zulia, Venezuela

The interaction between grid refinement and features in design space is investigated for time dependent Navier-Stokes flows over a bluff body. A mixing measure and total pressure loss are calculated for a range of geometries and several grid refinements. In particular, 52 geometries are analyzed and a response surface surrogate-based outlier analysis revealed that as the grid is refined, three of these configurations stand out with off-trend mixing indices. Both grid refinement and multiple surrogate modeling exercises reveal that very high mixing indices are found in a very small island in design space. This important design region manifests itself only when the grid resolution is adequate. The high value of the mixing index is due to interaction between viscous flows and abrupt geometric variations of the bluff body.

1. Introduction

Accuracy of CFD simulations depends on the proper selection of grid. For Navier-Stokes computations, the convective and viscous effects result in multiple length scales. In practical computations, a grid refinement exercise is often necessary to identify adequate resolution. For time-dependent flow computations, the effort is more demanding because the scale variations change in time.

Recently, there is a growing interest in using CFD to facilitate design optimization. For flow problems with strong convective effects, which are frequently encountered, the grid resolution requirement implies substantial cost in obtaining accurate CFD solutions, making it a challenge to generate sufficient data to meet the need for optimization. Surrogate modeling is a valuable tool to generate additional design data based on selected number of original CFD solutions.

In addition to offering a low-cost alternative for evaluating designs, surrogate models also offer advantages associated with the fact that they require a large number of designs to be evaluated together. Besides obvious advantages in terms of parallel computation, this can also reveal cases with significantly different behavior than others. Histogram and outlier analysis can identify and examine designs exhibiting unusual departure from the overall trend. The outliers can occur due to incomplete convergence or high errors due to inappropriate computational set-up such as grid distributions or boundary conditions. In that case, outlier analysis helps find and possibly correct these problems. However, outlier may also represent designs where the physical behavior changes significantly.

In this study, the mixing problem associated with bluff body flows is investigated. Mixing is a process with many practical applications, including propulsion and power generation, homogenization of multiple...
materials and/or species, and various heat exchange and geophysical processes. In man-made devices, while achieving high rate of mixing is often a desirable goal, it is also important to minimize the penalty associated with the total pressure loss of the fluid flow so that the system does not suffer from low efficiency. In the present effort, the mixing is promoted by high streamline curvatures and flow recirculation resulting from a trapezoidal bluff body.

An earlier investigation of mixing facilitated by a trapezoidal bluff body was conducted by Burman et al.\textsuperscript{7}. They employed iteratively re-weighted response surface approximation to optimize the time-dependent Navier-Stokes flow over the bluff body. The optimization objectives were to minimize the drag coefficient and to maximize a measure of mixing, which was the time-averaged maximum negative velocity. This measure of mixing does not account for the interactions of the velocity components which are significant at higher Reynolds numbers. These conflicting objectives were combined by constructing a desirability function. Multiple trade-off solutions were obtained by varying the desirability of each objective. At the designated Reynolds number Re, which is 120 based on the free stream velocity and the frontal bluff body height, the response surface was found to be very smooth and offered little variation in the response as design variables were changed.

Flows over trapezoidal shaped bluff body with Re < 200 were experimentally studied by Goujon-Dourand et al.\textsuperscript{12}. Kahawita and Wang\textsuperscript{13} conducted numerical simulations of the flows over trapezoidal shape bodies. The focus of their study was flows with Re < 200. Here, the Reynolds number based on the inlet flow speed and frontal bluff body height is 250, resulting in time-dependent flow structures. The current investigation adds insight into the fluid physics and design issues for flows with Re = 250.

To assess the interplay between numerical accuracy and grid resolution, multiple grid systems with different number and distributions are employed. Polynomial-based response surface approximations (RSAs) have been adopted to construct surrogate models for the two primary objectives: mixing effectiveness, which is to be maximized and total pressure loss, which is to be minimized. Specifically, the scope of this paper is to (i) study the effect of grid resolution on the flow over a bluff body and highlight the requirement of grid resolutions for adequate construction of surrogate models, and (ii) demonstrate the effectiveness of outlier analysis as a tool to identify cases with significantly different behavior.

The time-dependent nature of flow with non-linear governing equations makes the optimization task more computationally demanding. To date, there has been insufficient effort in addressing the design optimization problem for time-dependent problems. In a companion paper by Mack et al.\textsuperscript{14}, the high fidelity CFD simulation data obtained here is used to construct different surrogate models and solve the multi-objective optimization problem. They also conducted global sensitivity analysis to identify the importance of different variables.

II. Problem Description

The total pressure loss and mixing efficiency are the two measures of performance of the configuration of a bluff body. The total pressure loss is defined as the sum of pressure and shear forces on the body resisting the flow. The total pressure loss coefficient $C_D$ is the ratio of the total pressure loss and the dynamic pressure force based on the inlet velocity. For time-dependent flow, $C_D$ is averaged over the fluctuation time period, $T$:

$$C_D = \frac{1}{T} \int_{t'}^{t''} \frac{1}{\nu_2 \rho U_0^2 d S} \int \left( p n_x - \tau_{xy} n_y \right) dS \, dt$$

(1)

where $\rho$ is the fluid density, $p$ is the pressure and $\tau_{xy}$ is the viscous stress tensor. The pressure term in Equation (1) is the time-dependent pressure over the body and the viscous stress term is the time-dependent shear stress. Time $t'$ is selected such that the initial transients are eliminated.

A measure of mixing effectiveness, defined as mixing index (M.I.) is obtained by time and space averaging of the sum of the time-averaged shear stress and unsteady stress as follows:

$$M.I. = \frac{1}{T} \int_{t'}^{t''} \int \left( \frac{1}{V} \int \left( \frac{\mu}{\nu_2} \frac{\partial U}{\partial y} - \rho \left[ \vec{u} \cdot \vec{v} \right] \right) dV \right) \, dt$$

(2)
where \( \mu \) is the dynamic viscosity of fluid, \( U \) is the time-averaged velocity and \( u' \) and \( v' \) are the fluctuation velocities \( (u' = u - U, \ v' = v - V) \). The first term in Equation (2) denotes the time-averaged shear stress and second term denotes the unsteady stress component. The absolute value was used to consider only the magnitude of the mixing index. For non-periodic flows, the time-averaged quantities were computed by averaging the quantities for a sufficient amount of time.

A. Geometric Description and Computational Domain

A typical bluff body shape is shown in Figure 1. Dimensions of the bluff body and computational domain are based on the study by Burman et al. The frontal height of the bluff body \( D \) is unity. Variables of interest \( B, b \) and \( h \) are shown in Figure 1. Variations in these design variables change the slant angles of the upper and lower faces of the body. Area of the body \( A \) is kept unity by introducing the constraint

\[
H = \frac{[2A + h(b - D)]}{(D + B)}
\]  

Following Burman et al.\(^7\) other constraints are introduced as follows:

\[
\begin{align*}
B + b & \leq 1 \\
0.5 & \leq B \leq 1.0 \\
0.0 & \leq b \leq 0.5 \\
0.0 & \leq h \leq 0.5
\end{align*}
\]  

The first inequality constraint in Equation (4) ensures constant frontal height and hence constant Reynolds number for all geometries. Side constraints define the design domain and are chosen to avoid grid generation difficulties. Side constraints also maintain the convexity of the geometry. The computational domain of the body is shown in Figure 2. The flow domain is 37 units long and 14 units wide. The body is placed symmetrically along y-axis at a distance of 5 units from the left boundary. The computational domain and the bluff body had a unit width in direction perpendicular to the paper.

B. Computational Set-up

A multi-block, body fitted, structured, non-uniform grid was used to discretize the computational domain. The computational domain was divided in eight blocks. ICEM-CFD\(^8\) was used for grid generation. A typical grid distribution is shown in Figure 3. Grid density near the body was increased using an exponential meshing law for placing nodes. Multiple grid refinements were investigated to identify the adequate resolution for this problem. The number of grid points in different grids is given in Table 1. While the difference in the total number of grid points between Grid 1 and Grid 2 is not large, the grid density in the near field and wake region for Grid 2 is higher than Grid 1. In Grid 3 and Grid 4, both the near field grid density and far field grid density are high, making them more refined. Overall, Grid 1 has the poorest resolution and Grid 4 has the best resolution.

The north, south, top and bottom faces were modeled as slip boundaries. No slip boundary condition was imposed on the flow over the solid walls. The west boundary was modeled as inlet with a fixed inflow velocity \( u = U_{in}, v = 0 \) and east boundary was modeled as outlet with constant mean pressure \( P_{mean} = Const \).

The fluid was assumed to possess constant density and viscosity. The flow behind the combustion devices is turbulent in nature. To simplify the analysis, an effective viscosity is often estimated based on engineering turbulence closures. The effective Reynolds number is therefore considerably lower than the nominal Reynolds number. In this study, the flow is modeled as an idealized case of laminar flow using a Reynolds number in the range of the effective Reynolds number which is \( O(10^3) \). The Reynolds number based on frontal bluff body height and inlet velocity was selected as:
\[ Re = \frac{U \Delta x}{\nu} = 250 \] (5)

In this effort, a finite volume code, called STREAM\(^{16}\), was used to solve the flow problem numerically. Time-dependent calculations were solved using the PISO (Pressure Implicit with Splitting of Operators) algorithm\(^{17}\). Convective terms were discretized using second-order upwind scheme and all other terms were discretized using second order central difference scheme. Time step was selected to maintain the CFL number based on inlet velocity and smallest grid size less than one.

\[ \frac{U \Delta t}{\Delta x} \leq 1 \] (6)

The resulting dimensionless time step for each grid is shown in Table 1. The flow was simulated for a sufficient time to eliminate the transient behavior. The actual number of time steps varied for each case. The computational time required for the simulations increased with refinement in grid. Numerical simulations for Grid 4 for a typical case required a few days of computational time on a 1.3GHz Itanium processor SGI machine with 16GB shared RAM. Grids 1 and 2 were used for detailed analysis of the designs due to relatively smaller computation times where as grids 3 and 4 were used for selected cases to verify the results. The individual cases used for simulations using grids 3 and 4 are given in Table 1.

Large variations in the total pressure loss coefficient and mixing index at early stages indicate the initial transient region before the low variation recurring flow evolved. Time averaging of the total pressure loss coefficient and mixing index was initialized after the transients were subdued and recurring behavior was established for both total pressure loss coefficient and mixing index.

C. Design of Experiments

One objective of this study was to develop suitable surrogate models based on direct CFD simulations. Polynomial response surface models were used as the low cost alternative to evaluate the designs. The design of experiments (DOE), used to select the location of the data points to fit polynomial response surface consisted of 27-design points modified face-centered composite design (FCCD) as shown in Figure 4. The FCCD uses corners and center faces of a cube for point selection but in this case the upper half of the cube will violate the constraints. Points were added on the interior of the cube to compensate for the missing points. Another 25 design points to fill the space were generated using Latin Hypercube sampling (LHS). A total of 52 designs were used to approximate the response surface are given in Table 2.

III. Results

Numerical simulations using the grids 1 and 2 were conducted for all 52 design points. The total pressure loss coefficient and mixing index for all cases on both grids are given in Table 2. Some general observations from the flow field are as follows:

1. The pressure in front of the body was high. Low pressure was observed near the sides and rear of the body and in the vortex regions.
2. Vortex shedding was observed on the edges of the bluff body. The angle and length of the upper and lower sides of the body dictate the strength and direction of vortex.
3. Far from the body (three times the frontal bluff body height) in the y-direction, the effect of body was not felt.
4. Streamlines with time-averaged velocity components (mean \( U \) and mean \( V \)) showed that the body was enveloped in a recirculating flow but far from the body the time-averaged flow was uniform.
5. Transients in \( C_D \) diminished more quickly than that for mixing index.
6. The effect of viscous stress component on the total pressure loss coefficient was much smaller than the effect of the pressure component.
7. The unsteady stress was more important than the time-averaged shear stress in determining the mixing index.
A. Impact of Grid Resolution

The total pressure loss coefficient and mixing index values from Grid 1 and Grid 2 were different. Differences in the mixing indices from the two grids were larger than the differences in the total pressure loss coefficient. Differences in pressure field with improved grid resolutions are small compared to the differences in velocity fields with grid refinement, so the total pressure loss coefficient has lesser impact of grid refinement than the mixing index. The effect of grid resolution on the total pressure loss coefficient and mixing index is analyzed by studying the results for all simulations and individual cases:

1. Comparison of Results for 52 designs

Histogram analysis was used to compare and contrast the results from two grids. The total pressure loss coefficient and mixing index for all 52 cases from Grid 1 and Grid 2 were plotted in histograms with 6 bins in Figure 5–Figure 6. Figure 5(a) shows the histogram of $C_D$ for Grid 1 and Grid 2. The total pressure loss coefficient values for Grid 2 results had wider range and more uniform distribution compared to the total pressure loss coefficient values for Grid 1. The total pressure loss coefficient values for Grid 1 were concentrated in the central region. The histogram charts had substantial overlap. Mean values of $C_D$ for Grid 1 and Grid 2 were 2.00 and 2.03 respectively and standard deviations of $C_D$ for Grid 1 and Grid 2 were 0.06 and 0.11 respectively. Higher standard deviation of $C_D$ from Grid 2 correlated with the wider spread of the data. Figure 5(b) shows the histogram plot of differences in $C_D$ values from the two grids. The difference histogram was continuous and took both negative and positive values. The interplay between better resolution and more accurate estimation of the actual loss of the pressure in fluid flow and lower numerical viscosity-induced loss results in substantial overlap in the total pressure loss coefficient histograms from two grids.

Figure 6(a) showed mixing index histogram for two grids. The mixing indices for Grid 2 results had wider range than the mixing indices for Grid 1, but most of the data was concentrated towards the left. The overlap between the mixing indices for results from the two grids was small. Also the histogram pattern for both grids was similar. Mean values of the mixing index for Grid 1 and Grid 2 results were 474 and 617 respectively and standard deviations of the mixing index were 33 and 66 respectively. Higher standard deviation for results on Grid 2 was obtained primarily due to the presence of a few designs with very high mixing index. Figure 6(b) shows the difference in the mixing indices for results from two grids. It was observed that the results on Grid 1 consistently underestimated the mixing index. With the refinement of the grid, better resolution was attained, resulting in improved capturing of smaller length scales and reduced impact of numerical viscosity. Consequently, higher mixing indices were obtained. In particular, histogram analysis revealed that three cases had much higher mixing and slower grid convergence resolution than other cases.

2. Comparison of Individual Flow Fields

Next the flow fields were analyzed for the individual cases. As observed in the histogram plots for most cases, the differences in the mixing indices between grids were in the range of 100-150, but for three cases the differences were larger than 300. Case 7 ($B=0.5$, $b=0.25$, $h=0.25$), a representative case of most results and Case 1 ($B=0.5$, $b=0.0$, $h=0.0$), a representative case for high differences between two grids, are presented in detail here. The total pressure loss coefficient, mixing index and the standard deviations of the time histories of total pressure loss coefficient and mixing index for two cases are given in Table 3. The changes between the grids in the total pressure loss coefficient for both cases were modest but the changes in the mixing index were large indicating the lack of convergence in terms of grid resolution. Note that motion and time histories are not strictly periodic and there are multiple frequencies. Finding the amplitude of the motion is cumbersome, for example the amplitude of the mixing index of Case 7 for Grid 2 ignoring amplitude of small peaks is approximately 45 units. In such cases, variations in the quantities are easily represented by the standard deviation, for example in the above mentioned case the standard deviation of the time history of the mixing index is approximately 30 units which gives a good representation of the variation.

Figure 7 and Figure 8 show the time-averaged flow field for two grids for Case 7 and Case 1, respectively. Figure 7a-Figure 8a show the results for Grid 1 and Figure 7b-Figure 8b show the results for Grid 2. For both cases, the body is enveloped by the recirculation zones and the flow far from the body is uniform and the same. For both cases, differences in the time-averaged flow for two grids were observed near the body. The region of influence of the body for Grid 2 was more than that for Grid 1. Differences in

American Institute of Aeronautics and Astronautics