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and Turbulent Mixing in a Simplified Burner**

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NUMERICAL SIMULATION OF COLD FLOW PATTERNS AND TURBULENT MIXING IN A SIMPLIFIED BURNER

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ABSTRACT

The COYOTE computer program was used to simulate the flow field and turbulent mixing near the fuel and air inlets in a simplified burner. We report the results of four cold flow calculations that illustrate several interesting phenomena in addition to demonstrating the capabilities of the basic hydrodynamics model and the turbulence model. They also demonstrate some interesting facets of the hydrodynamics of burners. We summarize our findings as follows: 1) two different grids gave vastly different answers, underscoring the importance of assuring grid-independence in numerical solutions; 2) cold flow patterns are much different than reactive flow fields, making it unwise to apply conclusions from the former to the latter; 3) the problem is elliptic, and it is necessary to include the whole furnace in the calculations; 4) the flow patterns exhibited weakly unstable, almost metastable, modes that make it difficult to ascertain when steady conditions have been obtained.

I. INTRODUCTION

Numerical simulation of industrial burners is a challenging computational problem. As part of a systematic study of this problem, we report several cold flow solutions produced as part of a screening study of a simplified burner that was proposed for experimental investigation at the University of California at Irvine for the California Institute for Energy Efficiency (CIEE). The long-range goals of this study are to identify parameters that affect the production of NO_x and to discover methods of reducing emissions while maintaining or improving efficiency. Since cold flow calculations are much less expensive than reactive flow simulations, it was hoped to 1) gain understanding of the numerical and physical problems associated with the numerical simulation of burners and 2) investigate the possibility of using cold flow calculations as a starting point for reactive flow calculations.

We used the COYOTE numerical fluid dynamics program [1], which was designed to simulate reacting flows in two-dimensional Cartesian and axisymmetric geometries. The current version of the program has a variety of turbulence models, including the LUVD11 subgrid-scale (SGS) turbulence model [2] and the $k - \epsilon$ model [3-5].

COYOTE is based on the full transient Navier-Stokes equations for a reactive multicomponent gas mixture. Steady-state solutions, when they exist, are found by assuming an arbitrary initial flow and allowing the transient to decay. While this approach is less efficient computationally than a direct steady state approach, it has several advantages. First, it does not make any *ad hoc* assumption that the final flow field is truly steady. That is, it allows the final solution to contain quasi-periodic features such as vortex shedding or flame flickering. If the final flow is truly steady, then that type of solution will evolve naturally. Second, it automatically performs a flame stability study. If, for example, the flame cannot be sustained, it should be extinguished in the calculation (at least to the extent that the gas physics included in the calculation is an accurate representation of the physical system). Third, it allows easy incorporation of complex gas physics,

such as detailed chemical kinetics or radiative heat losses. The main disadvantage is that the computational expense is higher than for a direct steady-state solver. However, in today's world of relatively abundant and inexpensive computational power and high personnel costs, we can afford to trade a certain amount of computational effort (in both algorithmic efficiency and the inclusion of physical detail) for a reduction in the human effort required to obtain solutions.

The experimental burner is axisymmetric, and the apparatus includes a large enclosure to confine the flame. The geometry of the entire furnace is sketched in Fig. 1. The experimental nozzle and flame zone are confined inside a furnace, which is a hexagonal prism approximated by a cylinder 30.48 cm in radius and 93.98 cm tall above the entrance plane of the fuel nozzle. The chamber is 91.44 cm tall above the top of the quarl, and it is topped by a roof with a slope of 45° that necks down to fit a 15.24 cm diameter chimney. The present computational mesh fills this enclosure, so the walls are approximated by a fixed-temperature boundary with a law-of-the-wall boundary layer model along the right boundary and a fixed pressure subsonic outflow boundary at the opening on the top of the grid. Details of the burner are shown in Fig. 2. The swirling air entering the base of the quarl is produced by mixing air from the four tangential jets with air from the axial jet. Swirl number and total air flow are selected by appropriate choices of flow rates in these jets. The detailed geometry of the nozzle used to inject air and natural gas into the enclosure is shown along with a part of the computational mesh in Fig. 3. The vertical and horizontal lines outline the computational zones. Diagonal lines show the locations of solid obstacles. The grid in this figure covers a region 5.08 cm square, and the quarl is chamfered at a 45° angle. Methane is injected through the angled channel at the lower left, and swirling air is injected through the vertical channel next to the fuel injector. All calculations place the bottom of the computational grid at the exit plane of the fuel nozzle. The flow conditions in all calculations are for a heating rate of 29.3 kW (1.0×10^5 Btu/hr).

Section II describes the geometry of the experimental apparatus and the problem setup. Section III describes several cold flow solutions for this burner. Conclusions are presented in Section IV.

II. PROBLEM DESCRIPTION

COYOTE is based on the full Navier-Stokes equations for a mixture of compressible gases. The equations, turbulence model, and numerical algorithms have been described in detail elsewhere [1, 2] and will not be repeated here. Species diffusion is modeled by Fick's law and the heat flux is modeled by Fourier's law plus enthalpy diffusion. The thermal equation of state is the sum of partial pressures for each species treated as an ideal gas. The species internal energies are functions of temperature taken from the JANAF tables [6-8]. The molecular viscosity of the mixture is assumed to be given by

$$\mu = 1.457 \times 10^{-5} T^{3/2} / (110 + T), \quad (1)$$

where T is the absolute temperature. This equation is valid for air and should be adequate for our purposes when methane is included at a mass fraction of no more than a few percent. The thermal conductivity is calculated from the viscosity using a constant Prandtl number with a value of 0.7. The species diffusivities are assumed to be equal and are calculated from the viscosity and a constant Schmidt number, also 0.7.

As discussed in the introduction, the geometry of the experiment is shown in Figs. 1 through 3. The experimental furnace and fuel-air nozzle are axisymmetric, which allows us to make this preliminary study with two-dimensional calculations. Three preliminary solutions have been reported using a 90 by 90 nonuniform mesh covering a region 12.0 cm square in the $r - z$ plane [9]. One conclusion from those simulations is that it is necessary to include a much larger volume of space around the burner to avoid problems associated with the outflow boundary. In particular, recirculation zones can cause inflow through an outflow boundary, which is numerically unstable. Therefore, the present solutions use a much larger computational domain. Two of them include the entire chamber up to the base of the roof, and these two cases use different resolutions. The third and fourth cases use the finer of the first two meshes, and also includes the roof up to the base of the chimney. The last two cases differ in the numerical implementations of the inflow boundary conditions.

The numerical solutions use three different nonuniform finite difference meshes. In all three cases, the bottom of the mesh is along the exit plane of the fuel-swirl air nozzle, as shown in Fig. 3. Obstacles, such as the quarl and the sloped roof, are included by blocking out selected computational zones, as illustrated in Fig. 3 for the quarl. The first mesh is relatively coarse with 45 by 56 zones and extends upward only to the base of the sloped roof. All three meshes extend radially out to the enclosure walls, where a wall function boundary layer model is applied. In the lower left hand corner, the zones are 0.11906 by 0.15875 cm. (Note that we will sometimes give numbers to a larger number of significant digits than is justified by the actual measurements of the experimental apparatus. These are the numbers actually used by the computer program and are given as an aid to anyone who may try to duplicate the present numerical results.) The largest zone, which is in the upper right hand corner, is 4.40453 by 9.15749 cm. The fuel, methane, is allowed to flow in through radial zones numbers 4 and 5 (zone 1 is the fictitious zone at the left side of the mesh), and air flows in through zones 7 through 10. The fuel annulus is from radii of 0.23813 to 0.47625 cm, and the air annulus extends from 0.635 to 1.27 cm in radius.

The second grid covers the same region of space as the first, but with a 125 by 250 grid. It is this grid whose lower left hand corner is shown in Fig. 3. The zones are 0.079375 cm square at the lower left corner, increasing to $\delta x = 0.65252$ cm and $\delta z = 0.59223$ cm at the upper right corner at $z = 93.98$ (the base of the sloped roof). The annular natural gas jet has inner and outer radii of 0.23813 and 0.47625 cm respectively (radial zones 5 through 7), and the annular swirl air jet has inner and outer radii of 0.635 and 1.27 cm respectively (radial zones 10 through 17). Secondary air was not used in these calculations, although a channel was left for it in the obstacles in the fine mesh cases. The top of the grid in both the coarse and fine cases is an outflow boundary with a specified pressure of 1.0×10^6 dynes/cm². In addition, we impose a restriction against inflow along any outflow boundary for reasons discussed in an earlier report [9]. If this restriction is not imposed, a nonphysical inflow tends to occur, and this inflow usually comes to dominate the flow. We use two inflow boundary conditions. One is the type (ii) with specified density and a zero gradient condition on the temperature. The other inflow boundary condition is the same except

that the zero gradient condition is imposed on the pressure.

The third grid is the same as the second, except an extension has been added to the top to include the sloped roof. This grid is 125 by 287 zones. The zone at the upper right corner (at $z = 116.205$ cm, the top of the sloped roof) is 0.65252 by 0.60920 cm. The opening at the top of the roof has a radius of 7.81205 cm and covers zones 2 through 78.

We assume that the inflowing gases are at a temperature of 300 K and a pressure of 1.0×10^6 dynes/cm². The volumetric flow rates are 1.6 scfm for the fuel and 18.2 scfm for the air. The swirl number is defined by, for example [11-13],

$$Sw = \frac{\int_{R_0}^{R_1} \rho v w r^2 dr}{R_1 \int_{R_0}^{R_1} \rho v^2 r dr}, \quad (2)$$

where R_0 and R_1 are the inner and outer radii of the annulus. In this study, we assume that the density ρ , axial velocity v , and angular velocity $\Omega = w/r$ are constant over each opening. With these approximations, the swirl number reduces to

$$Sw = \frac{\Omega (R_1^2 + R_0^2)}{2 v R_1}. \quad (3)$$

The air is assumed to have a swirl number of 0.316 with a constant angular velocity of $\Omega = 900$ s⁻¹. The gravitational acceleration is assumed to be 980 cm/s². The natural gas is modeled as pure methane. The air was assumed to be a mixture of 4 species with mass fractions of 0.23154 O₂, 0.755159 N₂, 0.0133 CO₂, and 1.29109×10^{-6} H₂O. The densities, velocities, and flow rates are summarized in Table 1. The carbon dioxide mass fraction was artificially enhanced by about 0.01 to approximately represent the mass fraction of argon, which has a similar molecular weight.

III. NUMERICAL COLD FLOW SOLUTIONS

The first solution is the coarse-mesh case without the roof. The stream function is plotted in Fig. 4. The contours are equally spaced with a spacing equal to 0.1 of the difference between the minimum and maximum values. This solution was begun using the fine grid solution shown

Table 1.
Mass Inflow Rates

Species	Flow Rate (g/s)	Density (g/cm ³)	<i>u</i> (cm/s)	<i>v</i> (cm/s)	Ω (s ⁻¹)
Total	10.463715				
Fuel	4.844040×10^{-1}	6.41482×10^{-4}	1413.0	1413.0	0.0
Swirl Air	9.979311	1.16181×10^{-3}	0.0	2260.2	900.0
Sec. Air	0.	0.0	0.0	0.0	
CH ₄	4.844040×10^{-1}	6.41482×10^{-4}			
O ₂	2.310607	2.69005×10^{-4}			
N ₂	7.535967	8.77351×10^{-4}			
CO ₂	1.327247×10^{-1}	1.54521×10^{-5}			
H ₂ O	1.288418×10^{-5}	1.50000×10^{-9}			

in Fig. 5, which was mapped onto the coarse grid. After the start of the calculation, the flow pattern appeared to change little over thousands of time steps, the only noticeable change being a very slow rise in the center of vorticity. Given this very weak but monotonic unsteady feature, the calculation was continued. Around 100,000 cycles into the calculation, a new vortex appeared at the bottom of the mesh and pushed the original vortex out the top boundary. This pattern relaxed slowly to the pattern shown in Fig. 4 and finally achieved steady state. The flow pattern shown in Fig. 4 is counterintuitive in that we expect the dominant flow path to be mostly upward along the axis of symmetry. Instead, the swirling flow spreads horizontally along the bottom of the furnace and turns the corner only after it hits the vertical wall. This solution was begun with a free-slip boundary condition along the bottom obstacle, but this flow pattern persisted when this boundary condition was changed to no-slip.

The flow pattern in Fig. 5 is qualitatively different, with the main flow upward along the axis and only a weak recirculation in the outer part of the furnace. This sensitivity of the flow pattern to zoning is due to these flow patterns depending on a delicate balance of large forces. Consequently, a small change in the force arrangement, such as provided by the numerical truncation errors, can produce a huge effect on the overall flow pattern.

The behavior of these two solutions highlights two of the complex questions that arise in using a transient algorithm to find steady or statistically steady solutions. First, how does one insure that a solution is sufficiently relaxed at some point in the calculation? Clearly one does not want to perform unneeded computational cycles. But an inaccurate solution may result if insufficient care is taken to insure convergence. The slow, almost imperceptible, rate of change in the coarse solution leading to a sudden transition is a feature of many nonlinear systems. There is no general procedure for insuring convergence beyond checking as many indicators of steadiness as possible and running a problem beyond what may appear to be a reasonable length of time. We note that requiring a spatially constant axial distribution of radially integrated axial mass flux is an exquisitely sensitive steadiness test, perhaps even too sensitive for routine engineering studies.

The second issue is the question of whether we are using adequate numerical resolution. There is no real alternative to running the same problem on two or more meshes that differ in resolution by at least 50 percent. Given the dramatic qualitative differences between Figs. 4 and 5, it would have been desirable to run additional mesh refinement tests on the present solutions. However, time and computer limitations have precluded such a study for the present.

Figures 6 and 7 show the flow patterns for the fine mesh calculations including the roof on the furnace. The presence of the roof makes a significant difference compared with Fig. 5. The two solutions including the roof differ only in the treatment of the inflow boundaries at the fuel-air nozzle. In Fig. 6, the temperature is allowed to float (that is, a zero gradient condition is imposed) and the pressure in the fictitious cell comes from the equation of state (although it is unused in the present version of the program). In Fig. 7, the pressure is allowed to float, and the temperature is computed from the equation of state. There is little difference between these solutions. The slight difference in the strength of the flows merely reflects the incomplete convergence to steady state. In both cases, the minimum and maximum values are converging slowly without changes in the shapes and locations of the streamlines. However, the presence of the roof has a striking influence on the streamlines in the bulk of the furnace volume. The large vortex in Fig. 5 is much stronger than the two smaller vortices in Fig. 6. It is interesting to note that this sensitivity to seemingly

minor details appeared in the burner experiments as an unexpected dependence of the flame size and shape on small air leaks in the furnace [G. S. Samuelsen, private communication].

Figure 8 shows the velocity vector plot corresponding to Fig. 7. The dominant feature of the flow is the axial jet, which scarcely registers in the streamline plot. This means that the low-speed flow at large radii is fast enough to produce an appreciable mass flow rate, although the velocity is too low to be visible in the velocity vector plot. This difference in the visual impression of the flow pattern produced by the two different representations of the flow field should serve as a warning about the caution that must be exercised in interpreting computational results.

Figure 9 shows the swirl velocity corresponding to Fig. 7. The swirl loses much of its speed near the quarl, although it retains a significant speed all the way up to the chimney. The axial jet thus is a tightly collimated tornado-like vortex that extends the entire height of the furnace.

Figures 10 through 15 zoom in on the solution in the lower left corner of the grid, covering a region approximately 9.8 by 10.8 cm. Figure 10 is the stream function, and Fig. 11 is the velocity vector plot. The velocity vector plot shows only every other zone for the sake of clarity. We see a very small recirculation zone in the wake of the cone annular fuel nozzle, and this recirculation is confined to the quarl. Above the quarl, the axial flow is the dominant feature, and we see the peak velocity is off-axis in the lower part of the furnace.

Figure 12 shows the swirl velocity. Contrary to what one might expect from the centripetal force of the swirling air, the region of highest swirl actually shrinks in radius in the quarl. This appears to be due to the Bernoulli effect, which establishes a radial pressure gradient due to the difference in speed of the fuel, air, and ambient streams of fluid. At larger axial distances above the nozzles, the slip velocity decreases, and the swirling region is able to expand by centripetal force and diffusion (both turbulent and molecular viscosities are included in the calculations).

Figure 13 shows the fuel mass fraction. Much mixing occurs in the quarl, but a very rich (equivalence ratio $\phi > 2$) core persists all the way to the top of the plot.

Figure 14 shows the turbulence kinetic energy density. The largest values are found inside the quarl where the inflowing gases first meet each other and the ambient fluid. These areas have by

far the highest shear rates, and hence the production of turbulence is largest.

Figure 15 shows the sum of the eddy viscosity and molecular kinematic viscosity. The molecular viscosity is essentially $0.16 \text{ cm}^2/\text{s}$ everywhere. Larger values indicate the presence of the eddy viscosity, which is proportional to the zone size and to the square root of the turbulence kinetic energy density. This plot shows that the largest rates of turbulent mixing are inside the quart. The eddy viscosity drops off in the main axial flow, although it is still significant.

The calculations reported here were performed on various models of IBM RS/6000 workstations and SPARCstations. On these machines, single precision (32-bit words) is simply inadequate. Although some researchers apparently have gotten away with using single precision on some fluid dynamics problems, we occasionally have gotten into difficulty with round-off errors when using single precision. Although there is a price to be paid in increased run times, we routinely use double precision and no longer encounter difficulties with rounding errors. The short time steps ($< 8 \mu\text{s}$) and the long integration times required to get reasonably steady solutions ($\gg 0.1 \text{ s}$) require the calculation of many time steps, which requires hundreds of hours for each problem. The long running times are a consequence of the need to use adequate resolution of the fuel-air nozzle and of the philosophy of using a time-marching approach based on the full Navier-Stokes equations. This approach is a step toward our long-term goal of burner simulations based on well-resolved large eddy simulations, which are intrinsically transient and three-dimensional. While the present simulations are running for long times on scalar workstations, massively parallel computers are slowly becoming available that will make the present approach more practical. What is gained in this approach in return for the increase computational expense is more physical detail and fewer modeling uncertainties than can be gained by, for example, using a direct steady-state approach. The additional information gained is a more nearly correct simulation of the interaction between the fluid dynamics (in particular, the turbulence) and the chemistry, automatic stability tests of "steady" solutions, decreasing importance of the subgrid-scale turbulence model as the grid is refined (in sharp contrast to the commonly used $k - \epsilon$ model), and the inclusion of acoustic modes and oscillatory, nearly periodic solutions if present. It is our opinion that this level of detail is

required to study the physics of burners in a reliable, predictive mode.

IV. CONCLUSIONS

The COYOTE hydrodynamics program has been used to simulate cold flows in a simplified experimental burner. An important objective of this study is to demonstrate the ability of the program to simulate real burner geometries. Another objective is to explore the numerical, computational, and physics capabilities required for detailed burner simulations. The absence of experimental cold flow data on this burner and the expense of more finely resolved solutions in the near term make it difficult to assess the accuracy of these calculations, but the fine mesh cases appear to be reasonable. We find no insurmountable difficulties, although the run times are substantial. However, the expenditure of the effort yields a wealth of physical information about the system.

The most important result of these preliminary numerical solutions is the identification of a number of areas that are critical to the accurate simulation of burners:

- 1) The cold flow burner simulations show weakly unstable, almost metastable solutions, which can make it difficult to identify the truly steady solutions. Steady solutions, when they exist, may make discrete transitions at critical values of certain parameters, including Reynolds number and numerical resolution. This behavior also has been observed in flames in the experimental burner, where there can be discrete jumps in the size and shape of the flame as the various flow rates are adjusted.

- 2) The elliptic nature of the computational problem makes it necessary to include the entire furnace in the calculations. The influence of boundary conditions is felt all over the mesh, as shown by the simple addition of the roof in the present study.

- 3) It was discovered early in this study that it is essential to include boundary layer drag and heat transfer. Even in this large furnace, the effects of the boundary layer model propagate all through the grid, emphasizing the elliptic nature of the computational problem.

4) Fuel-air mixing occurs very close to the injector. Turbulence levels are high only near the injector. This result suggests that it would be prudent to include the molecular transport coefficients in burner simulations. Further research is needed to determine just how important this is.

5) The burner simulation problem is both spatially and temporally stiff. That is, there is a wide range of both spatial (3 orders of magnitude) and temporal (7 orders of magnitude) scales. Further grid refinement studies are needed, but this stiffness makes such a project impractical on present scalar and serial computers.

6) It is important to do the outflow boundary "right." Subsonic outflow boundaries should not allow spurious signals to propagate back into the mesh. Good outflow algorithms also may produce faster relaxation, and we recommend investigation of better outflow conditions.

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BURNER TEST STAND

Fig. 1. Schematic diagram of the experimental furnace. Reproduced courtesy of Scott Samuelsen, University of California at Irvine Combustion Laboratory.

Fig. 2. Details of the burner geometry. Reproduced courtesy of Scott Samuelsen, University of California at Irvine Combustion Laboratory.

Fig. 3. Cross section of the nozzle used to inject air and fuel into the combustion chamber. The vertical and horizontal lines outline the computational zones. Diagonal lines show the locations of solid obstacles. Methane is injected through the angled channel at the lower left, and swirling air is injected through the vertical channel next to the fuel injector. The quarl is chamfered at a 45° angle. This grid occupies a region 5.08 cm by 5.08 cm.

MAX = 1.655176D+00 MIN = -4.061824D+00

Fig. 4. Stream function for the coarse mesh solution without the sloped roof.

MAX = 3.070476D+01 MIN = -9.968081D-03

Fig. 5. Stream function for the fine mesh solution without the sloped roof.

MAX = 9.661237D+00 MIN = -3.645800D+00

Fig. 6. Stream function for the fine mesh solution including the sloped roof. This solution uses a floating temperature inflow boundary condition at the nozzle.

MAX = 9.534503D+00 MIN = -3.476722D+00

Fig. 7. Stream function for the fine mesh solution including the sloped roof. This solution uses a floating pressure inflow boundary condition at the nozzle.

VMAX = 2.2607D+03

Fig. 8. Velocity vector plot for the fine mesh solution including the sloped roof. This solution uses a floating pressure inflow boundary condition at the nozzle ($kb = 11$).

MAX = 1.104887D+03 MIN = -7.424086D-05

Fig. 9. Swirl velocity for the fine mesh solution including the sloped roof. This solution uses a floating pressure inflow boundary condition at the nozzle ($kb = 11$).

MAX = 2.564134D+00 MIN = -9.968144D-03

Fig. 10. Lower left hand corner of the stream function plot shown in Fig. 7. The plotted region is approximately 9.8 by 10.8 cm.

VMAX = 2.32380+03

Fig. 11. Lower left hand corner of the velocity vector plot shown in Fig. 8.

MAX = 1.104887D+03 MIN = 0.000000D+00

Fig. 12. Lower left hand corner of the swirl velocity plot shown in Fig. 9.

MAX = 1.000000D+00 MIN = -2.563925D-08

Fig. 13. Lower left hand corner of the fuel mass fraction plot.

MAX = 1.985136D+06 MIN = 1.000000D-60

Fig. 14. Lower left hand corner of the turbulence kinetic energy.

MAX = 4.932541D+01 MIN = 1.588240D-01

Fig. 15. Lower left hand corner of the eddy viscosity plus the molecular kinematic viscosity.