CFD Modeling Needs And What Makes A Good Supersonic Combustion Validation Experiment

Richard L. Gaffney, Jr.
NASA Langley Research Center, Hampton, Virginia, 23681

Andrew D. Cutler
The George Washington University, Hampton, Virginia, 23681

Abstract

If a CFD code/model developer is asked what experimental data he wants to validate his code or numerical model, his answer will be: "Everything, everywhere, at all times." Since this is not possible, practical, or even reasonable, the developer must understand what can be measured within the limits imposed by the test article, the test location, the test environment and the available diagnostic equipment. At the same time, it is important for the experimentalist/diagnostician to understand what the CFD developer needs (as opposed to wants) in order to conduct a useful CFD validation experiment. If these needs are not known, it is possible to neglect easily measured quantities at locations needed by the developer, rendering the data set useless for validation purposes. It is also important for the experimentalist/diagnostician to understand what the developer is trying to validate so that the experiment can be designed to isolate (as much as possible) the effects of a particular physical phenomena that is associated with the model to be validated. The probability of a successful validation experiment can be greatly increased if the two groups work together, each understanding the needs and limitations of the other.

Introduction

Compared to other disciplines in the field of aerodynamics, computational fluid dynamics (CFD) is relatively young. Initially the research in this new area focused on algorithm development for simple geometries and simple physics. As solution algorithms improved, some researchers worked on expanding the capability of CFD to compute the flows of complex geometries, while others worked to model more complicated flow physics,[1] such as vibrational and radiation effects and multi-species flows with finite-rate chemical reactions. In both cases, computer limitations in both speed and memory created a trade-off between the number and complexity of the governing equations and the number of points in the grid. The number of points, or to be more precise, the point spacing, is important because the truncation error (error associated with solving the continuous equations on a discrete grid) is proportional to the product of flow gradients and the point spacing:

$$\text{Truncation Error} \propto \frac{\partial \phi}{\partial x} (\triangle x)^p \tag{1}$$

where ϕ represents a flow property, x is a coordinate direction, $\triangle x$ is the point spacing in the x direction and p is the order of accuracy of the numerical scheme. Since computer memory is limited, grids for calculations involving complex models (chemical reaction adds one equation for each chemical species) were often coarse. As a result of this trade-off, the truncation error associated with a coarse grid was often the same order of magnitude or larger than errors associated with the physical models. As the speed and memory of computers has increased, finer grids have become possible (less truncation error) and the limitations of physical models have become more apparent.[2] This has led to a push by CFD customers for more realistic physical models, which in turn has led to a push for experimental data on which to base the models and to validate the models. Unfortunately, experimental data sets used for code validation are usually lacking in some manner. Aeschliman and Oberkampf[3] note that

> "Typically, CFD code validation is accomplished through comparison of computed results to previously published experimental data that were obtained for some other purpose, unrelated to code validation. As a result, it is a near certainty that not all of the information required by the code, particularly the boundary conditions, will be available."

The lack of a complete data set can severely limit the usefulness, or even render the data set useless, for CFD validation purposes.

A major factor in the lack of complete CFD validation data sets is that historically there has not been a close working relationship between CFD researchers and experimentalists. This is somewhat understandable as early CFD research focused on numerical methods as opposed to physical modeling which required validation.[3] However the lack of communication may be partially due to the predictions that CFD would supplant wind tunnels and physical experiments, relegating them to a secondary role behind CFD.[3–5] One article which caused quite a stir in the aerodynamics community in 1975 was titled "Computers vs. Wind Tunnels for Aerodynamic Flow Simulations.[4]" This article not only predicted a "role reversal" of CFD and experiments but predicted it within 10 years of the date of the article. This viewpoint tended to alienate experimentalists,[5,6] which hindered open communication between the two groups.[3] The goal of this paper is to open the lines of communications between the CFD community and the experimentalists/diagnosticians to address some of the needs of CFD model developers and discuss what is needed to obtain complete CFD validation data sets.

Verification vs. Validation

As the capability of CFD increased and it began to be used for design and analysis, there arose a need to quantify errors and uncertainties and to establish formal processes for its usage. This is/was sorely needed as the accuracy of CFD solutions can vary significantly depending on a number of factors including the code, grid and the user. This move to establish definitions and processes produced a plethora of terms (verification, validation, calibration, accreditation, certification), which were often confusing and used inconsistently. Two of the terms which have received a great deal of usage are "Verification" and "Validation." For the purpose of this paper the definitions given in AIAA standard G-077-1998[7] will be used:

Verification: "The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model."

Validation: "The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model."

To restate these in a more generic and casual vernacular:

Verification: Making sure that you have what you think you have.

Validation: Finding out how accurate your assumptions really are.

From a CFD perspective, to verify a code means to make sure that there are no programming errors that significantly affect the accuracy of the solution. (You've coded what you think you coded.) Validation, on the other hand, means to determine the accuracy of the physical models in representing the real world. (For CFD, validation implicitly assumes that the code has been verified and that the solution is spacially, temporally and iteratively converged.) The primary purpose in defining these terms is to clarify their usage in this paper. However, a secondary reason is to implant the idea that experiments used for CFD validation should themselves be verified and validated.

CFD Basics

The goal of an engineer applying CFD is to accurately compute the flow field of interest and to derive from the solution parameters of interest. In order to uniquely specify the flow field he must solve for the three components of velocity, two thermodynamic properties (pressure, temperature etc.), and the chemical composition (for mixing or reacting cases) for each point in the region of interest. The engineer computes these properties by solving the discretized governing equations (which are themselves mathematical models). Often times the governing equations have terms which must also be modeled. The number of equations must equal the number of unknowns in order to mathematically close the system. The flow field solution is computed within a bounded region and boundary conditions must be specified, one for each governing equation on each boundary. Since the boundary conditions drive the solution in the computational domain, they should be physically and mathematically meaningful.

There are a number of mathematical models in a CFD code, many of which are taken for granted, and all of which need to be validated. A list of some of the models is:[8]

- The governing equations (potential, Euler or Navier-Stokes)
- Laminar diffusion models
  - Newtonian stress-strain relationship
  - Fourier's law of conduction
  - Species diffusion models (multicomponent diffusion or Fick's law)
- Thermodynamic models
  - Calorically perfect model
  - Thermal equilibrium (curve fits or tables)
  - Thermal non-equilibrium (additional equations)
- Chemical reaction models
- Turbulence model for:
  - Reynolds stresses
  - Reynolds heat flux
  - Reynolds mass flux
  - Turbulent chemical reaction/species production

As mentioned above, the goal of applying CFD is to accurately compute the flow field of interest and to derive from the solution quantities of interest. Validation is the process of assessing the accuracy of the model by comparison with real world data. Conceptually this is equivalent to characterizing the error in the following equation

$$\text{reality} = \text{model} + \text{error} \tag{2}$$

Strictly, the goal is to estimate the uncertainty of a CFD computed quantity, where the uncertainty is the bounds within which the error is expected to lie for a given (typically 95 %) probability. This is relatively straightforward if there is only a single model that is to be validated. However a CFD code is composed of many models, each with its own error. Assessing the uncertainty is further complicated by the fact that the governing equations are non-linear and the total error is not the sum of each individual model error. As a result, two levels of validation can be defined.

The top level is a validation of the CFD solution for a specific geometry and flow condition. This validation includes the interaction of all of the models acting together. Note that this level of validation is for a specific geometry and flow conditions. The validation is limited because the models have not been tested over the complete range of possible values in all possible combinations (an infinite number). This level of validation is important for understanding uncertainty levels for CFD applications.

The bottom level is the validation of the individual models in the CFD code. This level of validation requires the model to be evaluated independently of all other models in the code. A model can be validated independent of other models if experimental data exists for all of the properties in the model across the applicability range of each property. For example a thermodynamics model can be validated if the energy (or enthalpy) is measured for each combination of measured temperature, pressure and gas composition. Some turbulence models involve terms which are hard or impossible to measure, such as dissipation or pressure-strain, and as such can not be validated independent of other models. This level of validation is of particular interest to CFD model developers who are interested in improving the accuracy of CFD solutions (top level) by validating and improving the individual models (bottom level). Note that even if a model has been validated at the bottom level, it must also be validated at the top level because the effect of its error on the solution is unpredictable due to the non-linearity and complexity of the governing equations and its interaction with other models in the code.

Validation Experiments

There are a number of things that should be considered when conducting an experiment for the purpose of CFD code/model validation. A few things to consider are:

1) Determine the goal of the validation study

The first step to ensuring that an experiment is useful for CFD validation is to set a goal for the validation study. Following the definition of validation, the goal will be to determine the accuracy of the code to compute a particular quantity. This will be done for specific geometries over a limited range of flow conditions. For example the goal of an experiment may be to validate a CFD code's capability to compute the surface heat flux in a combustor operating over a specific range of operating conditions.

Note that validating a code's ability to compute one property (e.g. thrust), does not validate its ability to compute some other property (e.g. combustion efficiency) unless a rigorous relationship between errors in the two properties can be established. (i.e. An x percent error in property X corresponds to a y percent error in property Y.)

2) Design the experiment

Once you know what you want to validate, now determine how best to validate it. The design of the experiment will most likely be an iterative process taking a number of inter-related factors into account.

2a) Understand the constraints

The experimentalist and the CFD developer should work together to understand the constraints on the experiment. Examples of constraints are:

1. Cost
2. Available diagnostic tools
   (a) What can be measured
   (b) The accuracy of what can be measured
   (c) Limits of diagnostic tools (e.g. no hot wires in combusting flows)
3. Physical access of the diagnostic tools to the flow field
   (a) Limited by the geometry of the facility
   (b) Limited by the geometry of the model
   (c) Limited by safety concerns
4. Facility
   (a) Availability
   (b) Type of flow (Mach number, pressure, temperature, gas composition)
5. Time to accomplish task
6. Materials and structural limitations on the model

More than likely, there will be compromises. Given the constraints, the two groups can explore all the options and decide what is really important for the validation effort. This is best accomplished when both groups work together, each understanding what can and can't be done and what is and is not important.

2b) Consider the physical processes

The experiment should be designed to include the physical processes that are pertinent to the model(s) to be validated.[3] In addition, the dependent variables of the experiment (and output of the CFD) should be sensitive to the inputs of the CFD models across the input variable range of interest. For example if a reaction model is being validated for ignition delay or heat release, the experiment should be designed so that the properties to be measured are sensitive to the inputs to the model (e.g. temperature, and species concentrations.)

Similarly, the experiment should be designed to exclude, as much as possible, other physical processes which are not pertinent to the validation effort. Ideally, the dependent variables of the experiment should be insensitive to independent variables which are not inputs to the model. This will serve to simplify the experiment and will reduce uncertainty in the CFD solution introduced from models which are not part of the validation effort.

2c) Determine the sensitivities of the various parameters in the experiment

CFD should be used to determine how sensitive the dependent variables of the experiment are to the independent variables of the experiment. Independent variables may include the geometry, inflow properties and distributions of inflow properties. For example, how sensitive is flameholding (or flame standoff) to the inflow temperature, pressure, contaminant species, geometry, boundary-layer thickness, etc.? The sensitivities of the dependent variables to the CFD boundary conditions (both location and any specified properties) should also be determined. This will give the CFD developer some idea of where to place boundaries and what accuracy is needed in specifying properties on each boundary. The sensitivities will also feed into the design of the experiment as the goal is to design an experiment that is sensitive to the parameters of interest and insensitive to all others (see previous item). Knowing the sensitivities of the dependent variables to the independent variables will also give information on how accurately the independent variables need to be measured (see item 3).

2d) Understand what properties need to be measured and where

The CFD developer needs to work with the experimentalist/diagnostician to explain what properties need to be measured to validate the code/model and where in the flow field they are needed. (Whether or not the property can be measured is considered in the next item.) The measurement needs should be prioritized so that the impact of not achieving the measurement on the validation effort is known and understood by both groups. In all cases, the properties on the boundary of the computational domain which are required as input to the CFD code should be measured. This may include distributions of flow properties such as pressure, temperature, velocity components, turbulence intensity and scales and gas composition. (The properties that are needed depend on the type of boundary, e.g. inflow or outflow, subsonic or supersonic.) On solid surfaces the temperature distribution should be measured. If all of the properties can not be measured (see next item), the sensitivity of the dependent variables on the boundary properties should be determined (see previous item). If the dependent variables are sensitive to unmeasurable boundary properties, then either the experiment needs to be redesigned or the computational domain needs to be extended to a region in which the dependent variables are known or are less sensitive to the boundary conditions. For example instead of specifying a uniform profile at the exit of an injector (or nozzle), it may be necessary to solve the flow inside of the injector from the plenum to the injector exit. In this case, the total pressure and total temperature in the plenum should to be measured as part of the experiment.

The two groups should also determine what properties need to be measured inside of the computational domain. For example, if flameholding is an item of interest, what can be measured that best identifies flame location? They should also determine where measurements should be taken. CFD solutions of the proposed experiment can help locate flow features of interest and help determine measurement locations. The number of locations where measurements can be made may be limited by a number of constraints (see item 2a) so measurement priorities should be worked out in advance.

2e) Understand what properties can be measured and where

The experimentalist/diagnostician needs to work with the CFD developer to explain what can be measured, where the measurements can be made and estimates of expected accuracy. If the needed property can not be measured (or not measured to the needed accuracy) then perhaps it can be inferred (with some assumptions) from other properties which can be measured. In this case, estimates in the uncertainty of the inferred quantity should be made from estimates in the uncertainty in the measured quantities and uncertainty from any assumptions. If it is not possible to measure or infer the desired quantities, the two groups must consider other ways to validate the model. For example one way to validate a model for the turbulent mixing of property ϕ is to simultaneously measure both ϕ and the velocity components at a number of points across a mixing layer. The covariance of velocity and ϕ, which is the CFD term being modeled, can be extracted from the post-processed data and compared to the CFD solution. If these measurements can not be made, an alternative way to validate the model is to measure the mixing layer thickness and/or the growth rate of the mixing layer thickness.

2f) Consider the scale of the experiment

It is also important to consider the physical and temporal scales of the experiment, flow structures and the measurement device. The measurement device/volume should be small enough (compared to the physical geometry and flow structures of the experiment) to provide an acceptable level of spacial resolution. This is particularly true if intrusive diagnostics are used which, by their very nature, affect the flow that they are measuring. Similarly, if the flow is unsteady, the measurement time should be small (compared to the flow time scales) in order to resolve the unsteadiness.

In the case of unsteady flows, the size of the measurement volume depends on whether fluctuations in the property need to be measured or only the mean property. This is because the measurement volume is finite and the measured quantity is actually the spacial average of the flow in the measurement volume. If the measurement volume is small, the properties within the volume are relatively uniform and the measurement is a good representation of a point measurement. This means that a small measurement volume is required in high gradient regions. In a turbulent flow, the instantaneous flow gradients are larger than the mean gradients, thus a smaller measurement volume is required to capture fluctuations. (This is similar to a CFD calculation using large eddy simulation, where subgrid scale properties are a spacial average of the properties within the computational cell volume.)

3) Verify the experiment

The experimental apparatus and diagnostic equipment needs to be verified to make sure that the geometry and set-up are what they are intended to be. CFD calculations should to be done on the "as built" configuration and not the "as designed" configuration. Any assumptions about the flow field should also be verified. For example if the flow assumed to be two-dimensional or axisymmetric, then it should be verified experimentally. Consider also any possible changes to the geometry/device during the experiment, for example surface deflection under pressure loads or thermal growth while under heat loads.

4) Provide estimates of experimental uncertainty

The purpose of the validation effort is to determine the accuracy of the CFD code in simulating the physics of the real world. This must be done by comparing the CFD solution with experimental data. The experimental data must include estimates of uncertainty in order to quantify the difference between the CFD results and the experimental results. Note that the experimental uncertainty should include both the uncertainty in the measured properties and the uncertainty in the location of the measured properties. This is particularly important in regions of high flow gradients.

5) Make sure measurement uncertainty is sufficient to validate the model

The goal of validation is to determine how accurate the model is in simulating the real world. This is done by comparison with real world (experimental) data. If the uncertainty in the experimental data is too large, comparison with the data is useless and the validation goal is not achieved.

The required accuracy of each property being measured has to be determined from CFD code usage. For example an engine designer may require the CFD code to compute surface heat flux to within 5 percent of the true value. Once usage requirements are known, a sensitivity study can be done (item 2c) to determine how sensitive the desired CFD output (surface heat flux) is to the property being measured.

6) Run CFD during the design process to know what to expect

CFD should be an integral part of the design process. Proposed geometries and run conditions should be computed and the flow fields examined carefully. Unexpected flow structure or results (blockage, separated regions, unsteadiness, etc.) should be identified. If problems are identified, the experiment should be redesigned to alleviate the problems.

7) Iterate the CFD and the experiment

As experimental data becomes available, compare the measured data with the pre-test CFD solutions. (If the experimental inflow, outflow or surface temperatures are not the same as the pre-test conditions, recompute the CFD solutions using the experimental values.) If the comparison of the data and the CFD solution is poor, is it possible to determine why? If a problem is found with the CFD or the experiment, correct the problem and re-run either the CFD or experiment, whichever had the problem. This iterative process will help to identify and eliminate problems with both the CFD and the experiment.

Example Validation Experiment

The Test and Evaluation/Science and Technology Program of the Office of the Secretary of Defense is currently sponsoring the Test Media Effects (TME) project to develop tools that can be used to determine/quantify how flameholding is affected by the presence of vitiates in hypersonic airbreathing propulsion ground test facilities.[9] It is known that vitiates affect flameholding[10] and that flameholding is affected by a number of factors including flow properties, physical geometry, type of fuel and turbulence. CFD can be used to study the effects of flameholding, but model improvements are needed for reduced hydrocarbon chemical kinetics and turbulent mixing models. To rectify deficiencies in the currently available models, part of the research work being done under the TME project is to develop and validate improved models for reduced hydrocarbon chemical kinetics and for the turbulent mixing of thermal energy and chemical species. The development of reduced hydrocarbon kinetics models is being done at the University of Virginia[11] while the development of improved turbulent mixing models is being done at North Carolina State University[12,13] and the University of Pittsburgh.[14] Development of the diagnostics and the design of the experiment is being done at NASA Langley Research center in conjunction with George Washington University. For this paper, further discussion of the project will be limited to selected aspects of the validation effort, chosen for illustrative purposes.

The experiment will be conducted in the NASA Langley Direct Connect Supersonic Combustion Test Facility (DCSCTF). This facility has a vitiated heater that is able to heat the test gas to a total temperature between 1600 and 3800° R at total pressures of 115 to 500 psi. Flow rates in the facility can be varied between 1 and 30 lb_m/second. The experiment will require 60 days of test time in the facility with an extra 20 days planned for contingency.

The experiment is a pair of coflowing coaxial jets flowing into quiescent air (see Figure 1). The inner jet is connected to the facility heater and provides either vitiated air or vitiated hydrogen at the desired test total temperature and pressure. Two nozzles will be built, one having a Mach 2 exit flow and the other a sonic exit flow. The exit radius of both nozzles is 1.25 inches. The outer jet is a converging nozzle and will be operated at conditions that vary from subsonic to sonic. The exit of the outer jet extends from a radius of 2.0 inches to 2.25 inches and the centerline of the nozzle is angled 15 degrees toward the inner jet. There is a 0.75 inch, blunt, rearward-facing surface (flameholder) separating the exit of the two jets. Although the facility is a direct connect facility, it will be operated as a free jet for this experiment.

The diagnostics that will be used for the experiment include dual-pump CARS and a velocimetry technique based on Rayleigh scattering. This will enable the instantaneous ($\approx$ 10 ns) measurement of three velocity components, temperature and the mole fractions of either N_2, O_2 and H_2 or possibly N_2 and CO or N_2 and CO_2, at a point in the flow field. The location of the measurement point will be moved through the use of periscopes. Pressures and temperatures will also be measured in the plenna of the two jets as well as the mass flow rates of the supply gases. Planar Laser-Induced Fluorescence (PLIF) of OH will also be used in preliminary flow visualization to locate the flame position. The uncertainty in the mean of each measured property is expected to be less than five percent of the maximum variation in the flow field of the property being measured. The uncertainty in the fluctuating value is expected to be less than ten percent of the maximum fluctuation in the flow field of the property.

Tests to be run will include variations in the total temperature, gas composition and Mach number of the inner jet and different gases and Mach numbers in the outer jet. Table 1 shows the experimental test matrix.

Inner Jet				Outer Jet	
Mach Number	Heater Operation			Mach Number	Gas
1, 2	H_2+O_2+Air vitiated	no unreacted H_2	one $T_\circ$	off	-
1, 2	H_2+O_2+Air vitiated	H_2 rich	various $T_\circ$	off	-
1, 2	H_2+O_2+Air vitiated	H_2 rich	various $T_\circ$	$\leq$1	Air
1, 2	H_2+O_2+Air vitiated	O_2 rich	various $T_\circ$	$\leq$1	CH_4
1, 2	CH_4+O_2+Air vitiated	O_2 rich	various $T_\circ$	$\leq$1	CH_4
1, 2	H_2+O_2+Air vitiated	O_2 rich	various $T_\circ$	$\leq$1	H_2
1, 2	CH_4+O_2+Air vitiated	O_2 rich	various $T_\circ$	$\leq$1	H_2

Table 1 - The experimental test matrix

Each line in Table 1 represents two or more test conditions. In all of the cases two Mach numbers will be run in the inner jet in order to evaluate compressibility effects. The first pair of tests (line 1 in Table 1) are designed to be non-reacting so that the flow is mixing-only. This will allow the turbulence models to be tested on a very simple flow. In the second group of tests (line 2) the inner jet will be run hydrogen rich. This will provide a reacting test case with the same geometry as the non-reacting test case. With the second jet turned off, the flame location is sensitive to the temperature and the turbulence levels. This will be a difficult test case for the CFD models. The outer jet, which acts to anchor the flame, will be turned on for all the remaining test cases. The cases with methane and hydrogen in various combinations of the inner and outer jets will examine the effects of hydrogen/air and methane/air vitiates on hydrogen and methane flames as well as test the reduced kinetics model for methane/oxygen reactions.

Application of the design philosophy

The validation experiment was designed using the design philosophy described in this paper. As mentioned previously the TME validation effort has a clearly defined goal (item 1) of validating turbulent mixing models and reduced hydrocarbon kinetics models. This will be accomplished by measuring the simultaneous and (nearly) instantaneous temperature, velocity components and (several) chemical species in a turbulent mixing flow. The data will then be post-processed to extract the mean properties as well as the variances and covariances of the measured properties. (The covariance of velocity and temperature represent turbulent mixing of thermal energy in a CFD code while the covariance of velocity and species mass fraction represent the turbulent mixing of chemical species.)

The experiment was designed with items 2a-2f in mind. The coaxial jet experiment is physically simple which keeps fabrication cost to a minimum. With various combinations of temperatures and species in the two jets, the experiment isolates the flow physics of interest (i.e. it has the required mixing layers but not other complicating flow structures such as flow curvature or strong shocks and expansions.) Since the jets flow into quiescent air (the test cell), optical access is very good. With the dual-pump CARS and the velocimetry technique, the (nearly) instantaneous temperature, velocities and species will be measured at a sequence of points in the flow field. The instantaneous properties can be post-processed to yield mean properties as well as variances and covariances. The scale of the experiment is large compared to the measurement volume ($1.5x0.2x0.2$ mm^3) giving good spacial resolution for the flow field measurements.

Computational fluid dynamics was used during the design of the experiment in order to determine the sensitivities of the flow field to changes in geometry and nozzle plenum conditions (item 2c). A matrix of 22 cases was run with the Mach 2 nozzle varying

- Total temperature of the inner jet (1000 K, 1100 K, 1355 K)
- Size of blunt rearward-facing surface (0.5 inch and 0.75 inch)
- Outer injector (No jet, 0°, 15°, 30°)
- Turbulent Schmidt number (0.5, 0.9)

The last item in the list was included in order to determine the sensitivity of the CFD solution to the value of the assumed constant turbulent Schmidt number. (Current CFD models for the turbulent mixing of species include a constant turbulent Schmidt number. Typical values for the turbulent Schmidt number range from 0.5 to 0.9, depending on the type of flow. The models being developed for the Test Media Effects project allow the turbulent Schmidt and Prandtl numbers to vary in the flow field as part of the solution.) In all cases the computational domain extends 48 inches downstream and radially outward. In addition, the flow in the nozzles, from the subsonic sections to the nozzle exits, were also included in the computational domain. Note that this matrix of calculations pertains only to a subset of the experimental test matrix. Further CFD cases will be performed to examine flow sensitivities for other aspects of the experiment.

The mass fraction of OH was used to locate the flame and determine flameholding characteristics of the geometry at various flow conditions. Figure 2 shows contours of OH mass fraction at inner jet total temperatures of 1355, 1100 and 1000 K for the geometry with no injection. In the first two cases the flame stands off the rearward-facing surface with the flame farther from the surface as the temperature drops. At 1000 K there is no flame. Figure 3 is similar to Figure 2 but for the 15 degree injector geometry. In this case the flame is attached at total temperatures of 1355 and 1100 K but again blows off at 1000 K. Figure 4 shows OH mass fraction contours for two different base sizes (0.5 and 0.75 inches) with 15 degree injection. The two solutions are very similar but the 0.75 inch base geometry will provide better spacial resolution (since the experiment measurement volume size is fixed - see item 2f). Figure 5 shows OH mass fraction contours for different injection angles but with similar flow conditions. It is clear that the second jet improves the flameholding of the geometry. Figures 6 and 7 show the affect of the turbulent Schmidt number on the flameholding at different temperatures. With the second injector turned off, a turbulent Schmidt number of 0.5 has a flame standing off the rear-ward facing surface at 1100 K while the flame blows off for a turbulent Schmidt number of 0.9. (The turbulent mixing of species is inversely proportional to the turbulent Schmidt number, so a value of 0.9 produces less mixing than a value of 0.5.) With a secondary injection at 15 degrees, the levels of OH are smaller but the flame stays attached at 1355 and 1100 K.

These CFD solutions give some indication of the sensitivity of OH production to the primary parameters of interest, however some additional CFD work is needed to determine the sensitivity of the flame to boundary conditions. Since the jets flow into (nearly) quiescent air which surrounds the jets, the region of influence of the outer boundaries is all of the computational domain. Several CFD solutions need to be done with the boundaries at different distances from main flow to determine the sensitivity of the flow in the flame region to the location of the outer boundaries. In addition, a slight pressure gradient (0.04 psi) was imposed between the subsonic inflow and outflow boundaries in order to improve convergence and to mimic the outer flow entrained by the jets. Several CFD cases need to be run to determine the sensitivity of the flow in the flame region to the imposed pressure gradient. In addition to the outer boundary studies, CFD should also be done to determine the sensitivity of the flame to the inflow boundary of the main jet. In the previously presented solutions, the inflow boundary in the plenum of the main jet was assumed to be post-combustion with low turbulence levels and uniform properties. A recent calculation of a sub-scale combustor for this experiment indicated that the turbulence levels in the dump combustor are very high, the flow is non-uniform and the high levels of turbulence persist through the nozzle.[16] This may impact the solutions since high turbulence levels affect turbulent mixing and flameholding.

This work represents a start on the Test Media Effects validation effort. A sub-scale version of the experiment is currently being built in order to test the diagnostics before moving into the DCSCTF in the 2006, 2007 time frame. Some of the details of where and how many measurements to take at various points (for good statistical values) will be refined in the intervening period based on available time in the facility and priorities set by CFD validation needs.

Summary and Closing Remarks

This paper has discussed items to consider when designing and conducting a CFD validation experiment and has used the Test Media Effects project as an example. Following these ideas will help to ensure that the data taken can be used successfully to validate a CFD code or CFD models. Of the items discussed in the paper, the one that will do the most to determine the success of the validation effort is for the experimentalist and diagnostician to work together with the CFD developer to design the experiment/measurements based on the validation goals. This will require a significant amount of work for all involved parties but is essential to the validation effort.

References

[1] Oberkampf, W. L., "A Proposed Framework for Computational Fluid Dynamics Code Calibration/Validation," AIAA paper no. 94-2540, June, 1994.

[2] Freitas, C. J., "The Issue of Numerical Uncertainty," Second International Conference on CFD in the Minerals and Process Industries, CSIRO, Melbourne, Australia, December 6-8, 1999.

[3] Aeschliman, D. P, and Oberkampf, W. L, "Experimental Methodology for Computational Fluid Dynamics Code Validation," AIAA Journal, Vol. 36, No. 5, pp. 733-741, May, 1998.

[4] Chapman, D. R., Mark, H., and Pirtle, M. W., "Computers vs. Wind Tunnels for Aerodynamic Flow Simulation," *Astronautics and Aeronautics*, pp. 22-35, April 1975.

[5] Daniel, D. C. and Graham, J. R. III, "Integration of Supercomputers with Aerospace Ground Test Facilities," AIAA paper no. 92-0203, January, 1992.

[6] Oberkampf, W. L. and Trucano, T. G., "Verification and validation in computational fluid dynamics," *Progress in AerospaceSciences*, Vol. 38, pp. 209-272, 2002.

[7] American Institute of Aeronautics and Astronautics, "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations," Guide G-077-1998.

[8] Oberkampf, W. L. and Blotter, F. G., "Issues in Computational Fluid Dynamics Code Verification and Validation," AIAA Journal, Vol. 36, No. 5, pp. 687-695, May, 1998.

[9] Montgomery, P. A, Evans, C. and Drummond, J. P., "Efforts to Improve Prediction of Ground Test Media Effects on Flameholding in Scramjet Combustors," JANNAF 40th Combustion, 28th Airbreathing Propulsion, 22nd Propulsion Systems Hazards, 4th Modeling and Simulation Joint Subcommittee Meeting, June, 2005.

[10] Pellett, G. L., Northam, G. B., and Wilson, L. G., "Strain-Induced Extinction of Hydrogen-Air Counterflow Diffusion Flames: Effects of Steam, CO_2, N_2, and O_2 Additives to Air," AIAA paper no. 92-0877, January, 1992.

[11] Chelliah, H. K., Private communication.

[12] Xiao, X, Edwards, J. Hassan, H. A. and Gaffney, R. L., "Role of Turbulent Prandtl Number on Heat Flux at Hypersonic Mach Numbers," AIAA paper no. 2005-1098, January, 2005.

[13] Xiao, X, Edwards, J. Hassan, H. A. and Cutler, A. D., "A Variable Schmidt Number Formulation for Scramjet Application," AIAA paper no. 2005-1099, January, 2005.

[14] Givi, P., "Subgrid Scale Modeling in Turbulent Combustion: A Review," AIAA paper no. 2003-5081, July, 2003.

[15] White, J. A. and Morrison, J. H., "A Pseudo-Temporal Multi-Grid Relaxation Scheme for Solving the Parabolized Navier-Stokes Equations," AIAA paper no. 99-3360, June, 1999.

[16] Baurle, R. A., Private communication, May, 2005.

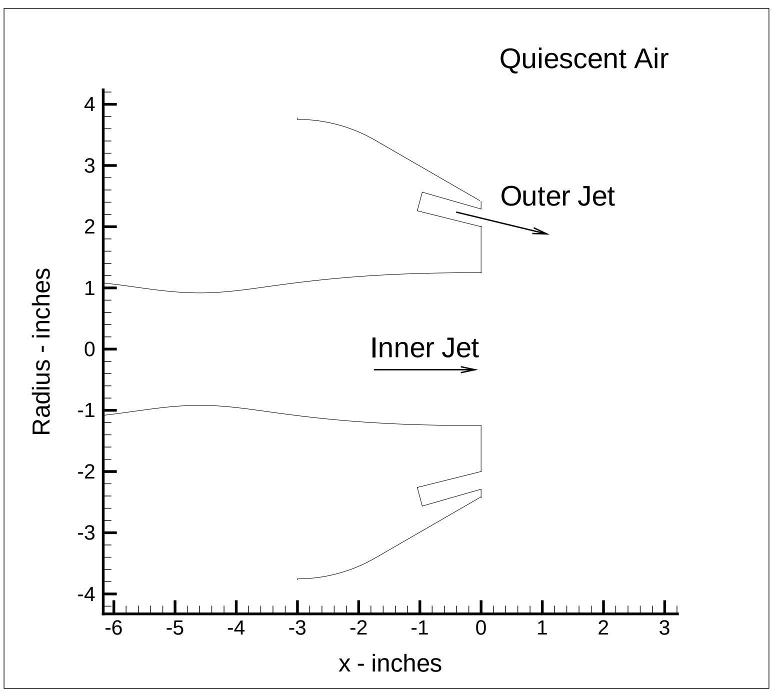
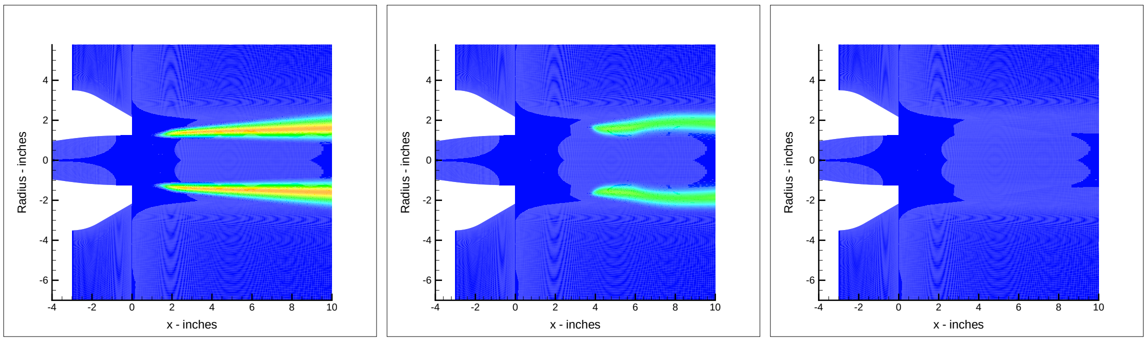
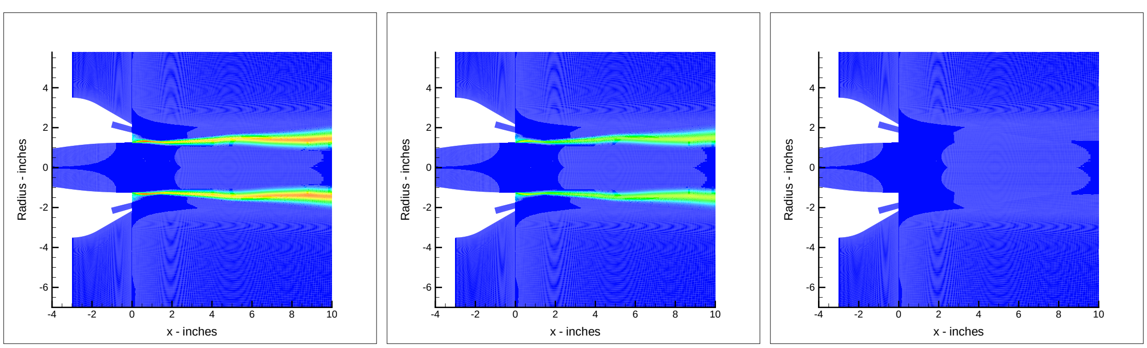


Figure 1: Schematic of the experiment co-axial jets



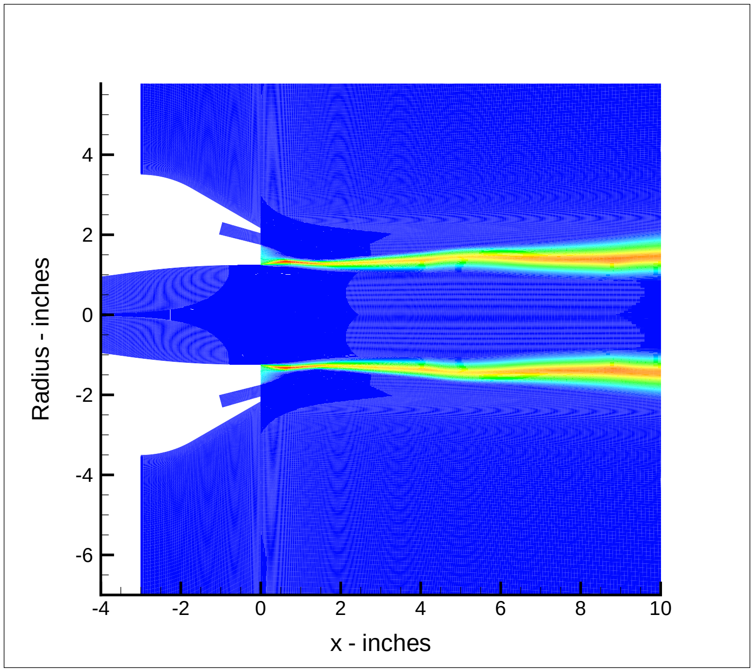
(a) 1355 K (b) 1100 K (c) 1000 K

Figure 2: OH contours showing the effect of temperature variation. No injection, Small base, $Sc_t = 0.5$

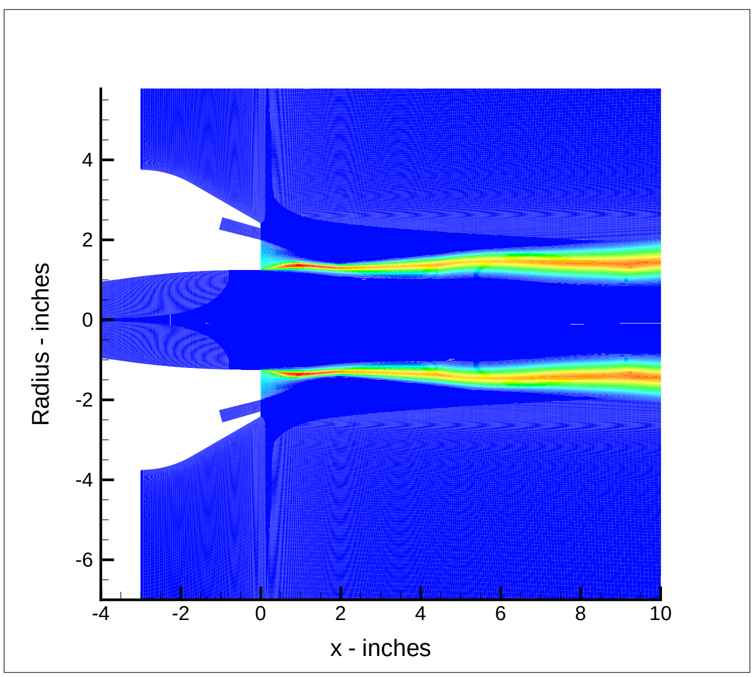


(a) 1355 K (b) 1100 K (c) 1000 K

Figure 3: OH contours showing the effect of temperature variation. 15° injection, Small base, $Sc_t = 0.5$

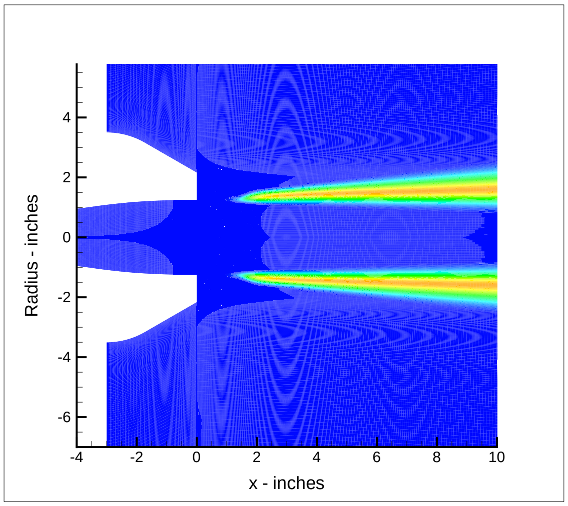


(a) Small Base

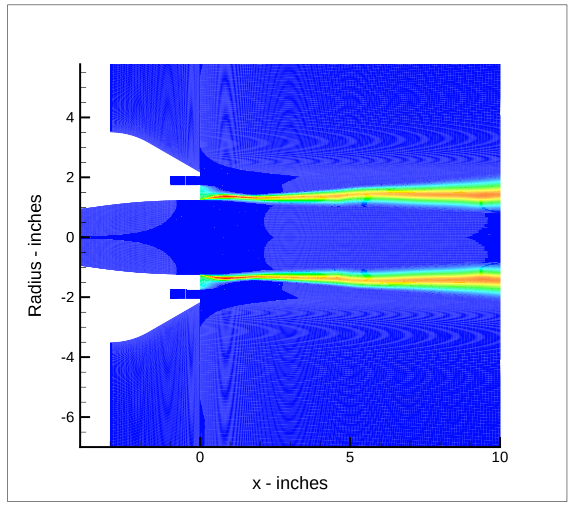


(b) Large Base

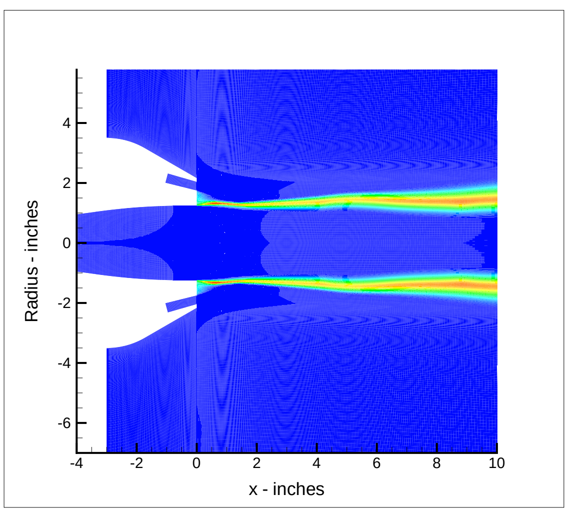
Figure 4: OH contours showing the effect of base size. 15° injection, $T_\circ$ = 1355 K, Sc_t = 0.5



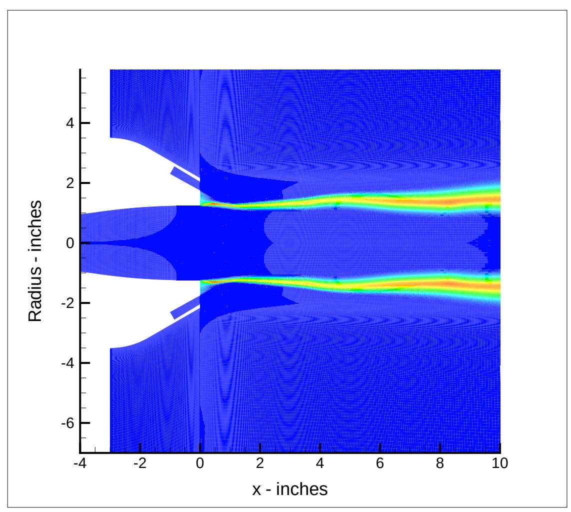
(a) No Injection



(b) 0° Injection

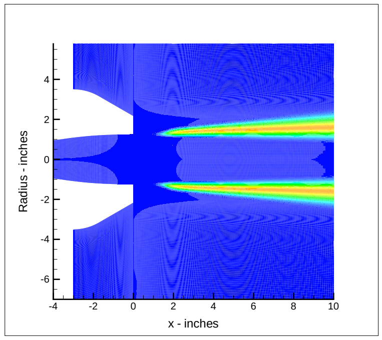


(c) 15° Injection

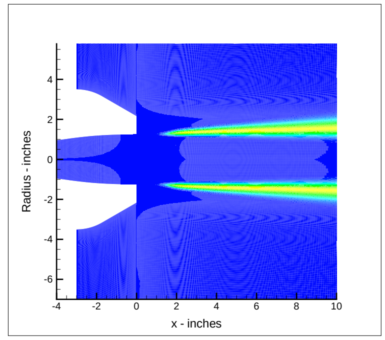


(d) 30° Injection

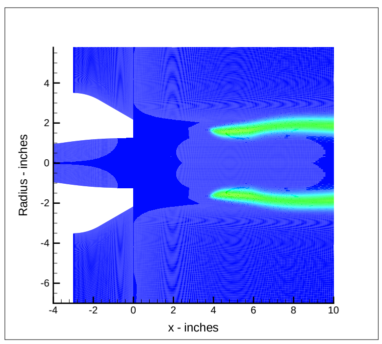
Figure 5: OH contours showing the effect of angle injection. Small base, $T_\circ = 1355$ K, $Sc_t = 0.5$



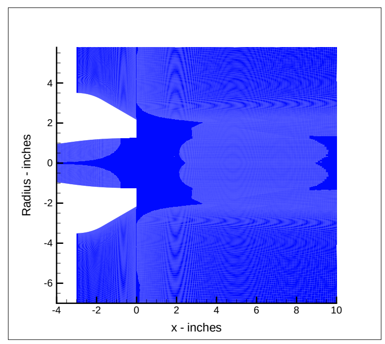
(a) $\mathrm{Sc}_t = 0.5$, $\mathrm{T}_\circ = 1355$ K



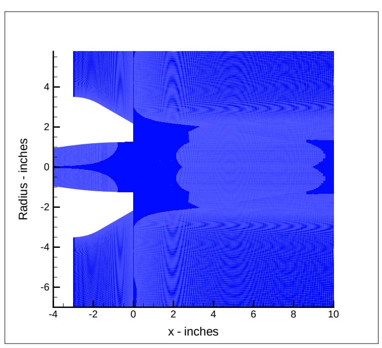
(b) $\mathrm{Sc}_t = 0.9$, $\mathrm{T}_\circ = 1355$ K



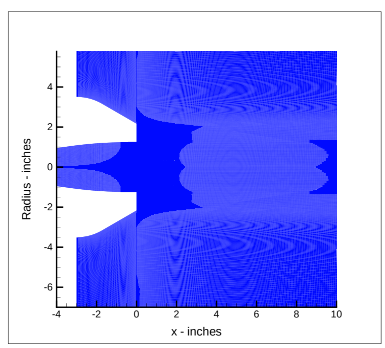
(c) $\mathrm{Sc}_t = 0.5$, $\mathrm{T}_\circ = 1100$ K



(d) $\mathrm{Sc}_t = 0.9$, $\mathrm{T}_\circ = 1100$ K

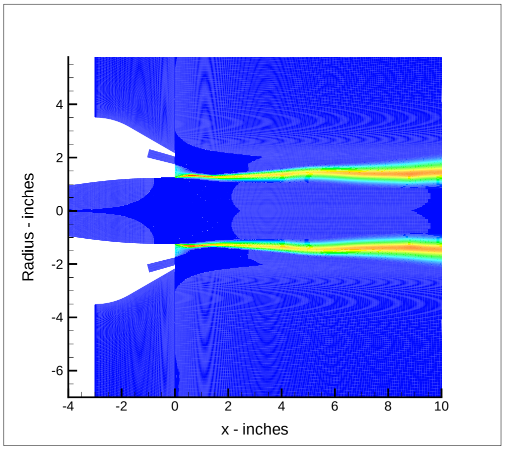


(e) $\mathrm{Sc}_t = 0.5$, $\mathrm{T}_\circ = 1000$ K

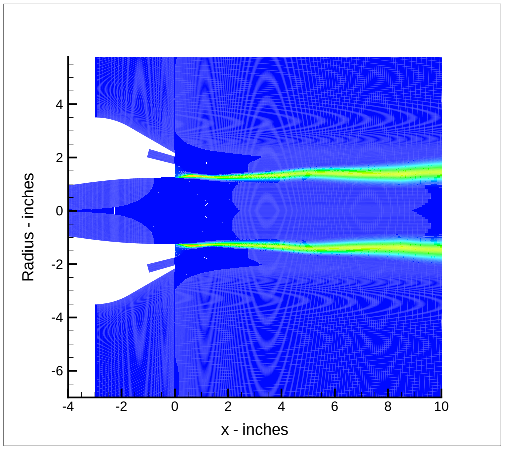


(f) $\mathrm{Sc}_t = 0.9$, $\mathrm{T}_\circ = 1000$ K

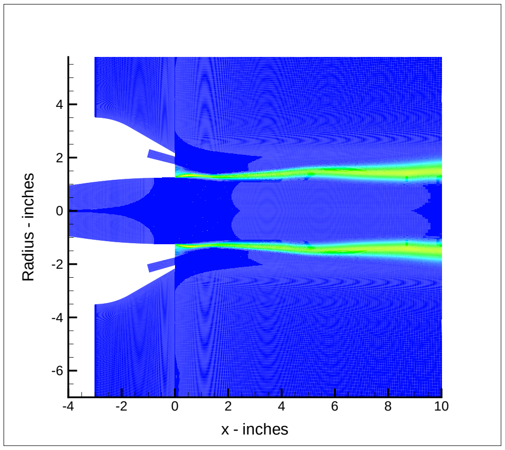
Figure 6: OH contours showing the effect of Sc_t variation at various temperatures. No injection, Small base



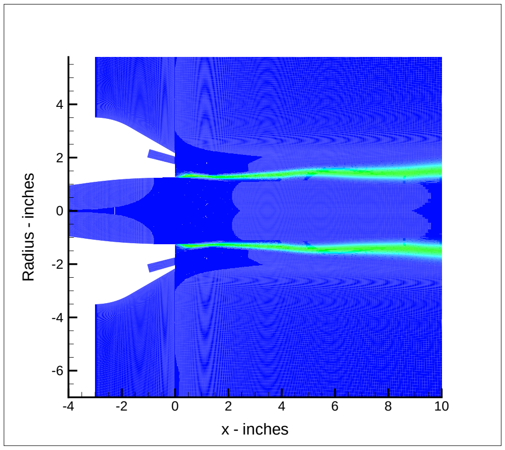
(a) $Sc_t = 0.5$, $T_\circ = 1355$ K



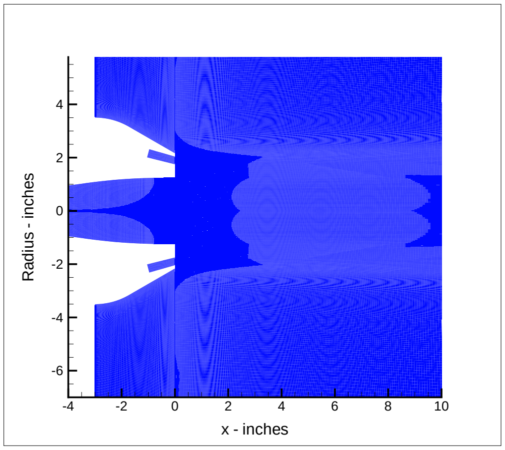
(b) $Sc_t = 0.9$, $T_\circ = 1355$ K



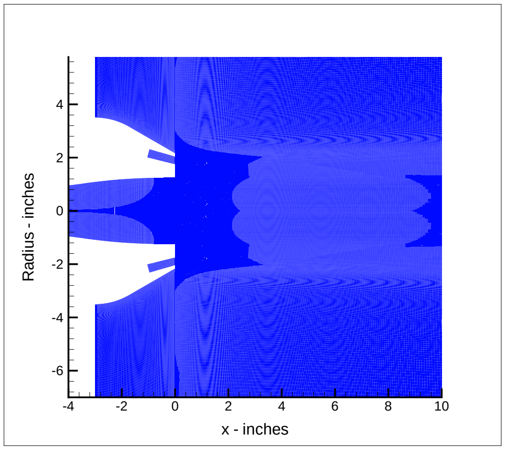
(c) $Sc_t = 0.5$, $T_\circ = 1100$ K



(d) $Sc_t = 0.9$, $T_\circ = 1100$ K



(e) $Sc_t = 0.5$, $T_\circ = 1000$ K



(f) $Sc_t = 0.9$, $T_\circ = 1000$ K

Figure 7: OH contours showing the effect of Sc_t variation at various temperatures. 15° injection, Small base