

**Final Report**

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**Modeling Turbulent Combustion for Variable Prandtl**

**And Schmidt Number**

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## Summary

This report consists of two abstracts submitted for possible presentation at the AIAA Aerospace Science Meeting to be held in January 2005. Since the submittal of these abstracts we are continuing refinement of the model coefficients derived for the case of a variable Turbulent Prandtl number. The test cases being investigated are a Mach 9.2 flow over a degree ramp and a Mach 8.2 3-D calculation of crossing shocks.

We have developed an axisymmetric code for treating axisymmetric flows. In addition the variable Schmidt number formulation was incorporated in the code and we are in the process of determining the model constants.

# Role of Turbulent Prandtl Number on Heat Flux at Hypersonic Mach Number

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## I. Introduction

Present simulation of turbulent flows involving shock wave/boundary layer interaction invariably overestimates heat flux by almost a factor of two.<sup>1</sup> One possible reason for such a performance is a result of the fact that the turbulence models employed make use of Morkovin's hypothesis.<sup>2</sup> This hypothesis is valid for non-hypersonic Mach numbers and moderate rates of heat transfer. At hypersonic Mach numbers, high rates of heat transfer exist in regions where shock wave/boundary layer interactions are important. As a result, one should not expect traditional turbulence models to yield accurate results.

The goal of this investigation is to explore the role of a variable Prandtl number formulation in predicting heat flux in flows dominated by strong shock wave/boundary layer interactions. The intended applications involve external flows in the absence of combustion such as those encountered in supersonic inlets. This can be achieved by adding equations for the temperature variance and its dissipation rate. Such equations can be derived from the exact Navier-Stokes equations. Traditionally, modeled equations (see, for example, Ref. 3,4) are based on the low speed energy equation where the pressure gradient term and the term responsible for energy dissipation are ignored. It is clear that such assumptions are not valid for hypersonic flows.

The approach used here is based on the procedure used in deriving the  $k-\epsilon$  model,<sup>5</sup> in which the exact equations that governed  $k$ , the variance of velocity, and  $\epsilon$ , the variance of vorticity, were derived and modeled. For the variable turbulent Prandtl number, the exact equations that govern the temperature variance and its dissipation rate are derived and modeled term by term. The resulting set of equations are free of damping and wall functions and are coordinate-system independent. Moreover, modeled correlations are tensorially consistent and invariant under Galilean transformation. The final set of equations will be given in the paper.

## II. Results and Discussion

Two sets of experiments are used to validate the present approach. The first is the Mach(M) 9.2 experiments of Coleman and Stollery<sup>6</sup> using compression ramps, while the second is the M=8.3 experiments of Kussoy et al.<sup>7</sup> using a double wedge.

Figures 1 and 2 compare the velocity and Mach number profiles over the flat portion of the compression ramp.<sup>6</sup> As is seen from Fig. 1, the variable Prandtl number,  $Pr_t$ , has little influence on the velocity distribution, while Fig. 2 shows improved agreement with experiment when a variable  $Pr_t$  formulation is employed. Figure 3 and 4 compare the pressure and heat flux distribution for the 15 deg ramp. Again,  $Pr_t$  has no effect on the pressure distribution but provides improved comparison with experiment for heat transfer. The ramp 15 case was calculated by Huang and Coakley,<sup>8</sup> in which various modifications were considered for limiting the turbulent length scale.

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The second set of results involve the  $\bullet$  at plate portion of the  $M=8.3$  experiment of Ref. 7. Figures 5 and 6 compare the predictions of the  $k-\epsilon$  model with and without a variable  $Pr_t$  and the SST model of Menter.<sup>9</sup>

The SST model gives better agreement with velocity measurements. However, both SST and the constant  $Pr_t$   $k-\epsilon$  give inadequate agreement compared to the variable  $Pr_t$   $k-\epsilon$  when compared with temperature measurement.

The results shown in Fig. 2, 4 and 6 demonstrate that the variable  $Pr_t$  formulation gives better agreement with experiment. This preliminary result suggests that a variable  $Pr_t$  approach may be the key to better heat  $\bullet$  ux prediction at hypersonic Mach numbers.

The  $\bullet$  nal paper will show comparison with the 34 degree ramp experiment of Ref. 6 and with the 10 and 15 deg crossing shock experiment of Ref. 7.

### III. Acknowledgments

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### References

- <sup>1</sup>Thivet, F., Knight, D. D., Zheltovodov, A. A., and Maksimov, A. I., "Insights in Turbulence Modeling for Crossing-Shock Wave/Boundary-Layer Interactions," *AIAA Journal*, Vol. 39, No. 6, 2001, pp. 985–995.
- <sup>2</sup>Morkovin, M., "Effects of Compressibility on Turbulent Flows," *Mecanique de la Turbulence*, edited by A. Favre, Gordon and Breach, New York, 1964, pp. 367–380.
- <sup>3</sup>Sommer, T. P., So, R. M. C., and Zhang, H. S., "Near-Wall Variable-Prandtl-Number Turbulence Model for Compressible Flows," *AIAA Journal*, Vol. 31, No. 1, 1993, pp. 27–35.
- <sup>4</sup>Abe, K., Kondoh, T., and Nagano, Y., "A New Turbulence Model for Predicting Flow and Heat Transfer in Separating and Reattaching Flows – II. Thermal Field Calculations," *International Journal of Heat and Mass Transfer*, Vol. 38, No. 4, 1995, pp. 1467–1481.
- <sup>5</sup>Robinson, D. F. and Hassan, H. A., "Further Development of the  $k-\epsilon$  (Enstrophy) Turbulence Closure Model," *AIAA Journal*, Vol. 36, No. 10, 1998, pp. 1825–1833.
- <sup>6</sup>Coleman, G. T. and Stollery, J. L., "Heat Transfer from Hypersonic Turbulent Flow at a Wedge Compression Corner," *Journal of Fluid Mechanics*, Vol. 56, No. 4, 1972, pp. 741–752.
- <sup>7</sup>Kussoy, M. I., Horstman, K. C., and Horstman, C. C., "Hypersonic Crossing Shock-Wave/Turbulent Boundary Interactions," *AIAA Journal*, Vol. 31, No. 12, 1993, pp. 2197–2203.
- <sup>8</sup>Huang, P. G. and Coakley, T. J., "Turbulence Modeling for Complex Hypersonic Flows," *AIAA Paper 1993-0200*, January 1993.
- <sup>9</sup>Menter, F. R., "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications," *AIAA Journal*, Vol. 32, No. 8, 1994, pp. 1598–1605.

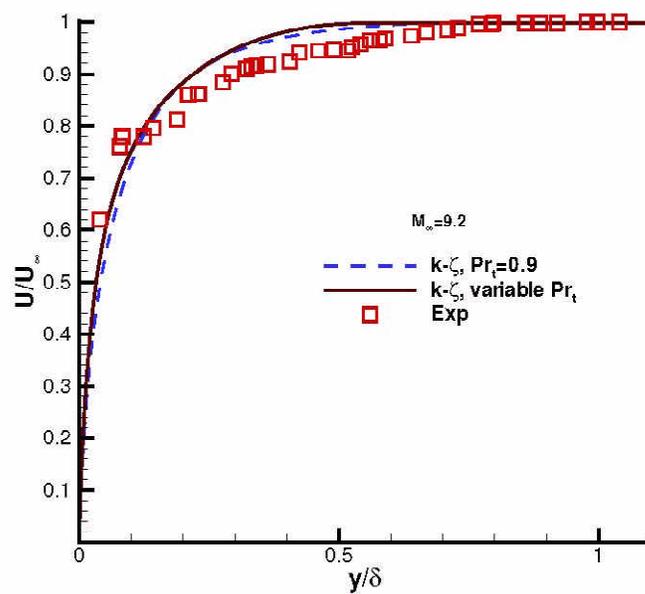


Figure 1. Comparison of Inflow Velocity Profile

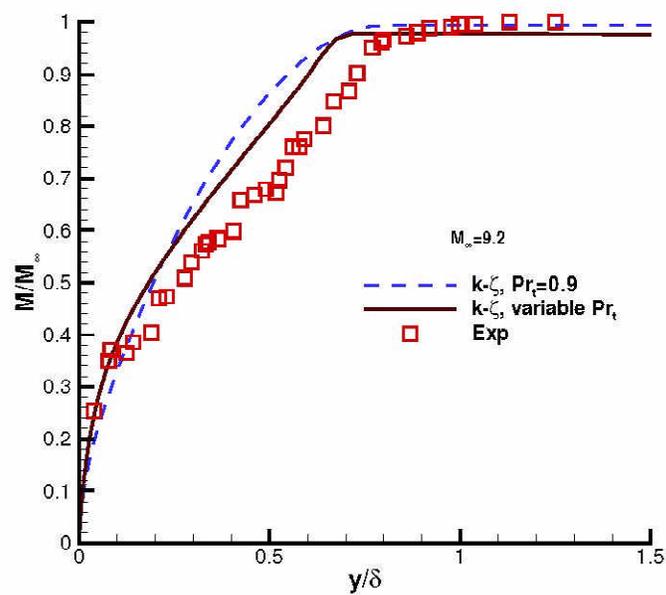


Figure 2. Comparison of Inflow Mach Number

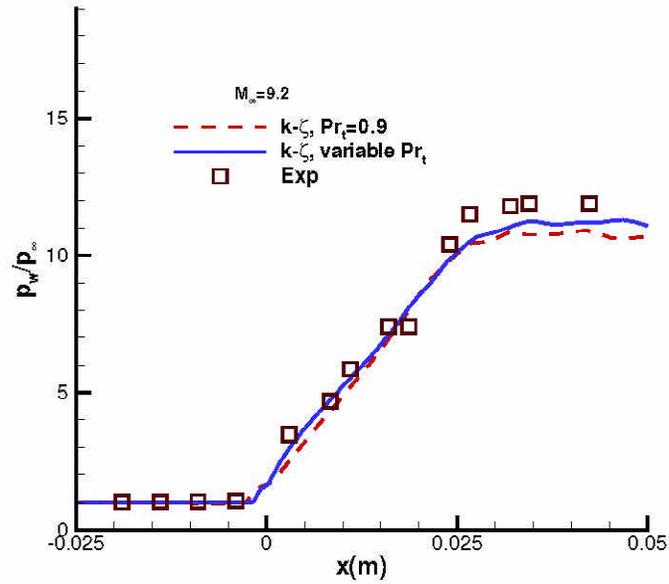


Figure 3. Surface Pressure on a 15 deg Ramp

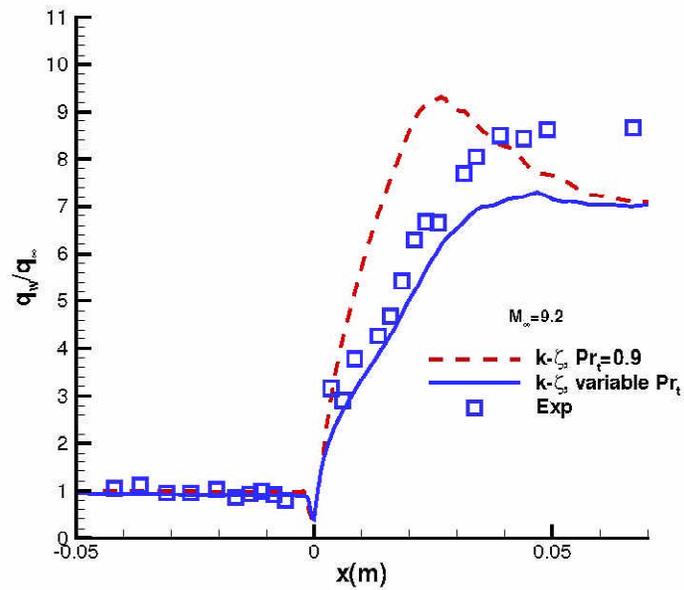


Figure 4. Heat Flux on a 15 deg Ramp

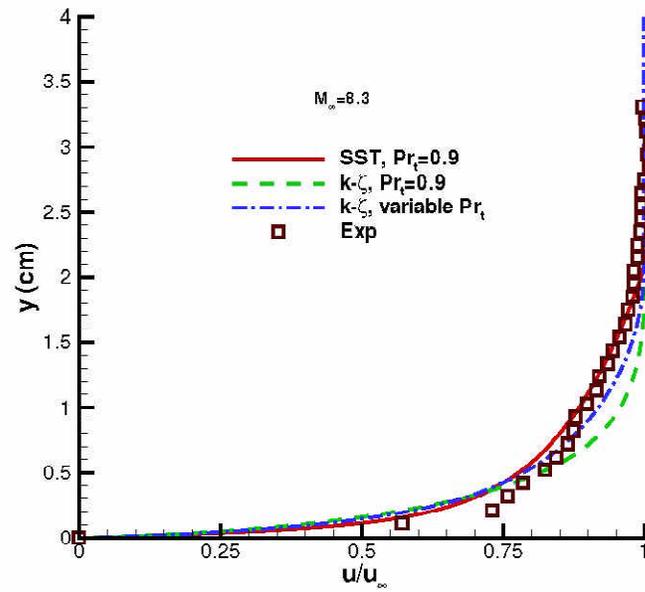


Figure 5. Comparison of Inflow Velocity Profile with Experiment

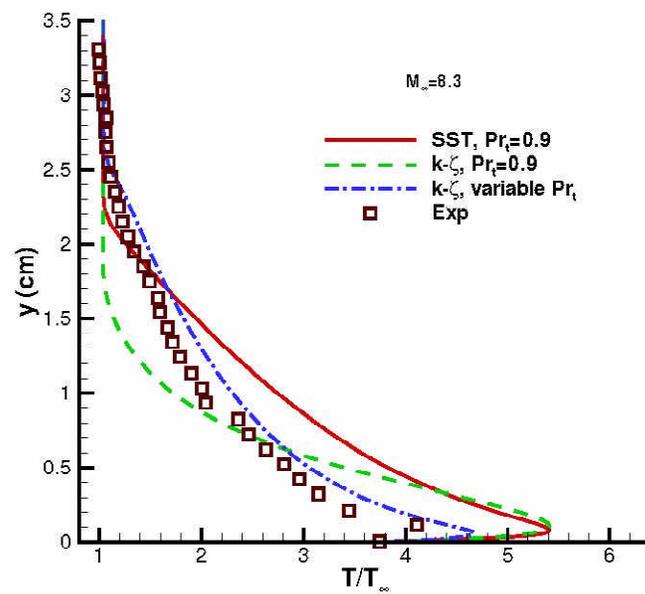


Figure 6. Comparison of Inflow Temperature Profile with Experiment

American Institute of Aeronautics and Astronautics  
**A Variable Turbulent Schmidt Number Formulation for  
 Scramjet Application**

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## I. Introduction

In high speed engines, thorough turbulent mixing of fuel and air is required to obtain high performance and high efficiency. Thus, the ability to predict turbulent mixing is crucial in obtaining accurate numerical simulation of an engine and its performance. Current state of the art in CFD simulation is to assume both turbulent Prandtl number and Schmidt numbers to be constants. However, since the mixing of fuel and air is inversely proportional to the Schmidt number, a value of 0.45 for the Schmidt number will produce twice as much diffusion as that with a value of 0.9. Because of this, current CFD tools and models have not been able to provide the needed guidance required for the efficient design of a scramjet engine.

The goal of this investigation is to develop the framework needed to calculate turbulent Prandtl and Schmidt numbers as part of the solution. This requires four additional equations: two for the temperature variance and its dissipation rate and two for the concentration variance and its dissipation rate. In the current investigation emphasis will be placed on studying mixing without reactions.<sup>1, 2</sup> For such flows, variable Prandtl number does not play a major role in determining the flow. This, however, will have to be addressed when combustion is present.

The approach to be used is similar to that used to develop the  $k-\epsilon$  model.<sup>3</sup> In this approach, relevant equations are derived from the exact Navier-Stokes equations and each individual correlation is modeled. This ensures that relevant physics is incorporated into the model equations. This task has been accomplished. The final set of equations have no wall or damping functions. Moreover, they are tensorially consistent and Galilean invariant. The derivation of the model equations is rather lengthy and thus will not be incorporated into this abstract, but will be included in the final paper.

As a preliminary to formulating the proposed model, the original  $k-\epsilon$  model with constant turbulent Prandtl and Schmidt numbers is used to model the supersonic coaxial jet mixing experiments involving He, O<sub>2</sub> and air of Refs. 1 and 2. This step is important in order to evaluate the underlying turbulence model especially because of some discrepancies noted in comparing theory and experiment in Refs. 1 and 2. Comparisons are made with velocity, concentration, stagnation pressure and temperature at various stations in the jet. The results indicate sensitivity to Schmidt number. Moreover, the discrepancies noted in Ref. 1 and 2 are a result of the underlying  $k-\epsilon$  model used and are absent in the current model.

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## II. Results and Discussion

Comparison are made with the experiments of Refs. 1 and 2. In these experiments, a coaxial nozzle was designed to produce two uniform, coaxial jets at its exit. The center flow consists of 95% He, 5% O<sub>2</sub> and a Mach number  $M = 1.8$ , while the outer flow is that of air at  $M = 1.8$ . Velocity, pitot pressure, composition, and total temperature were measured at various stations.

The grid employed is identical to that used in Refs. 1 and 2. It consists of 188,080 cells and is decomposed into 13 blocks for parallel computing. An axisymmetric finite volume solver is employed to simulate the flow, where a second order ENO(Essentially Non-Oscillating) upwinding method based on the Low Diffusion Flux Splitting scheme of Edwards<sup>2</sup> is used to discretize the inviscid fluxes while central differences are used for the viscous and diffusion terms. Planar relaxation is employed and the code is parallelized using domain decomposition and message passing(MPI) strategies.

As was done in Ref. 1 and 2, the range of  $r$  in the plots is truncated to show more clearly the region of interest. In general, good agreement is indicated beyond the range shown in the figures.

Figures 1–4 compare calculations and measurements for the He-O<sub>2</sub> mass fraction, velocity, pitot pressure and temperature. Calculations were carried out for two sets of turbulent Schmidt numbers. As is seen from the figures, it appears that no single Schmidt number will fit the data thus demonstrating the need for a turbulent Schmidt number formulation. All calculations presented here assume a turbulent Prandtl number( $Pr_t$ ) of 0.89.

Figure 1 compares computed and measured mass fractions at selected stations. As is seen from the figure, a Schmidt number of 0.9 gives better agreement with experiment. In general, calculations underpredict experiment near the axis and slightly overpredict away from the axis. Note also that there is no discontinuity in the slope of the mass fraction for any of the cases considered as was noted in Refs. 1 and 2 using the  $k-\epsilon$  model. As is seen from the figure, calculated results are rather sensitive to the turbulent Schmidt number near the axis; a reduced value of the mass fraction is noted at the lower Schmidt number because of enhanced diffusion.

The mean velocity is shown in Fig. 2. At  $x = 2$  mm, the velocity profile is a result of merging of the coaxial nozzle inner surface boundary layer with the region of separation at the lip and the shock wave emanating from the lip. Downstream, the calculated velocity is in good agreement with the measurements and is not sensitive to the Schmidt number.

The pitot pressure is shown in Fig. 3. As is seen from  $x = 3$  mm station, there is a layer with reduced pitot pressure at the boundary between the center jet and the coaxial flow. Downstream, the center jet spreads with the pressure near the axis falling and then rising in the wake of the nozzle lip. The figure shows that the pitot pressure is somewhat sensitive to the Schmidt number near the axis. This behavior is a result of the behavior of the He-O<sub>2</sub> mass fraction indicated in Fig. 1.

The measured and calculated total temperature is shown in Fig. 4. Measurements<sup>1,2</sup> indicate that the gas supply temperature varied substantially from run to run. Because of this, it was recommended that calculations employ the experimentally measured temperature for that run and not the average temperature over many runs as was done for other parameters. When the probe errors (of the order of 1%) are taken into consideration, it is seen that agreement with experiment is acceptable. However, results are Schmidt number dependent.

## III. Concluding Remarks

The above results demonstrate that the underlying turbulence model does not exhibit the shortcomings of the  $k-\epsilon$  model and indicate the need for a variable Schmidt number formulation. This will be the subject of the final paper. As indicated earlier, all relevant equations and modeling is complete and we are in the process of determining model constants.

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#### IV. Acknowledgment

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#### References

<sup>1</sup>Cutler, A. D., Carty, A. A., Doerner, S. E., Diskin, G. S., and Drummond, J. P., "Fundamental Mixing and Combustion Experiments for Propelled Hypersonic Flight," AIAA Paper AIAA-2002-3879, July 2002.

<sup>2</sup>Cutler, A. D., Diskin, G. S., Danehy, P. M., and Drummond, J. P., "Supersonic Coaxial Jet Experiment for CFD Code Validation," AIAA Paper AIAA-99-3588, July 1999.

<sup>3</sup>Robinson, D. F. and Hassan, H. A., "Further Development of the  $k-\epsilon$  (Enstrophy) Turbulence Closure Model," AIAA Journal, Vol. 36, No. 10, 1998, pp. 1825–1833.

<sup>4</sup>Edwards, J. R., "A Low Diffusion Flux Splitting Scheme for Navier-Stokes Calculations," Computers & Fluids, Vol. 26, No. 6, 1997, pp. 635–659.

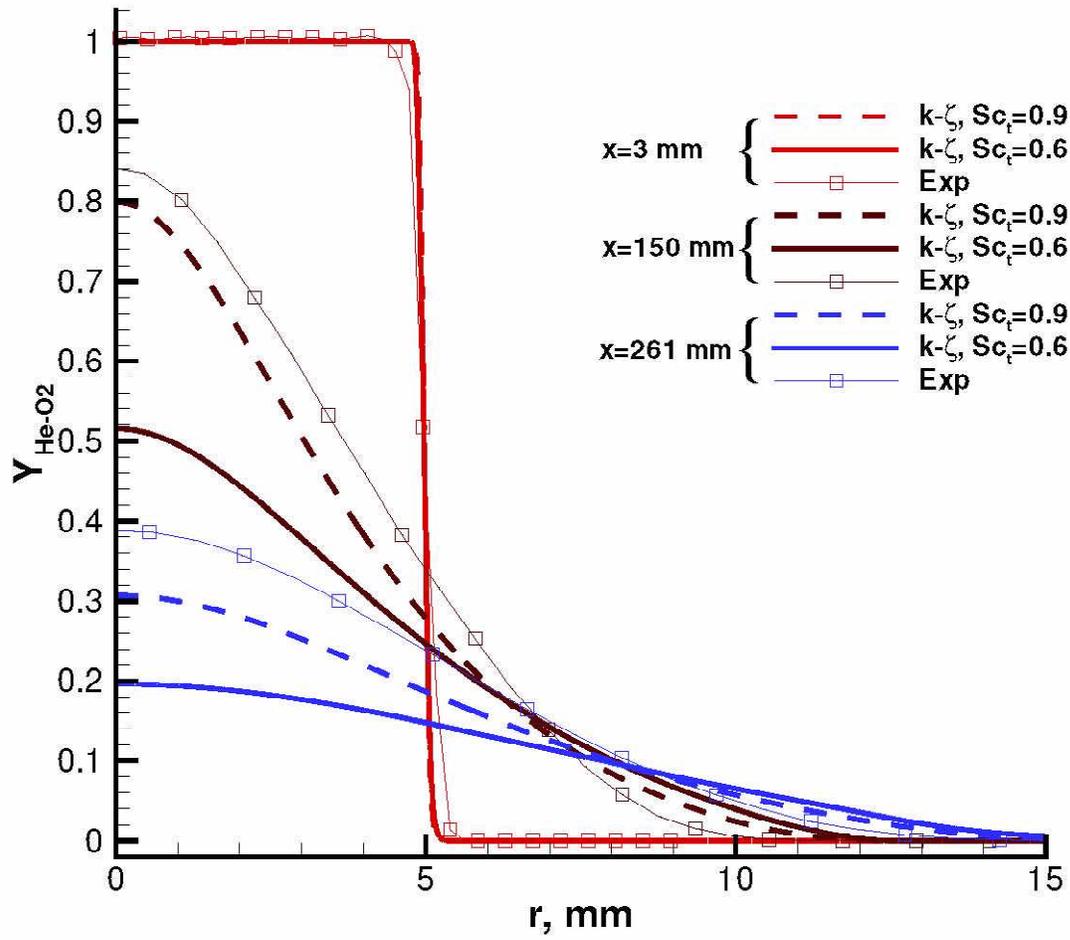


Figure 1. Comparison of mass fraction with experiment

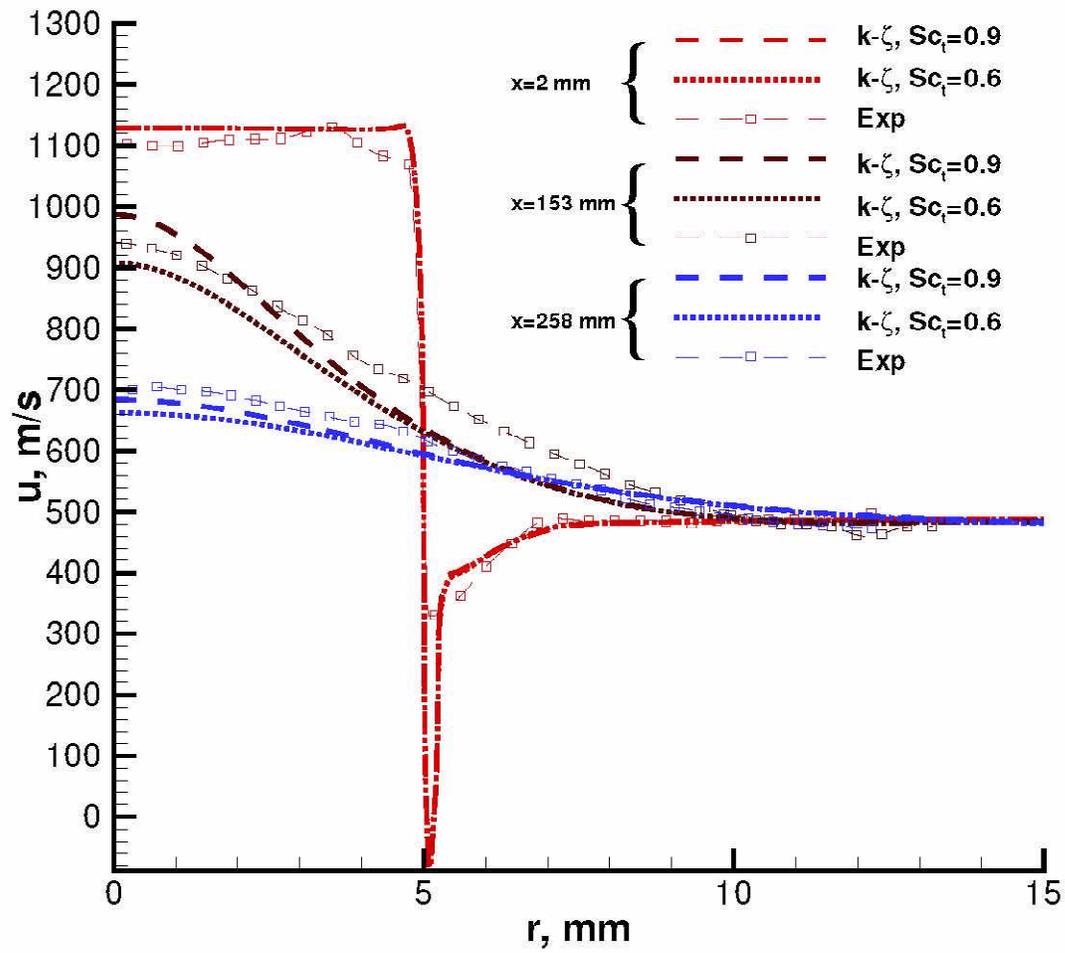


Figure 2. Comparison of mean axial velocity with experiment

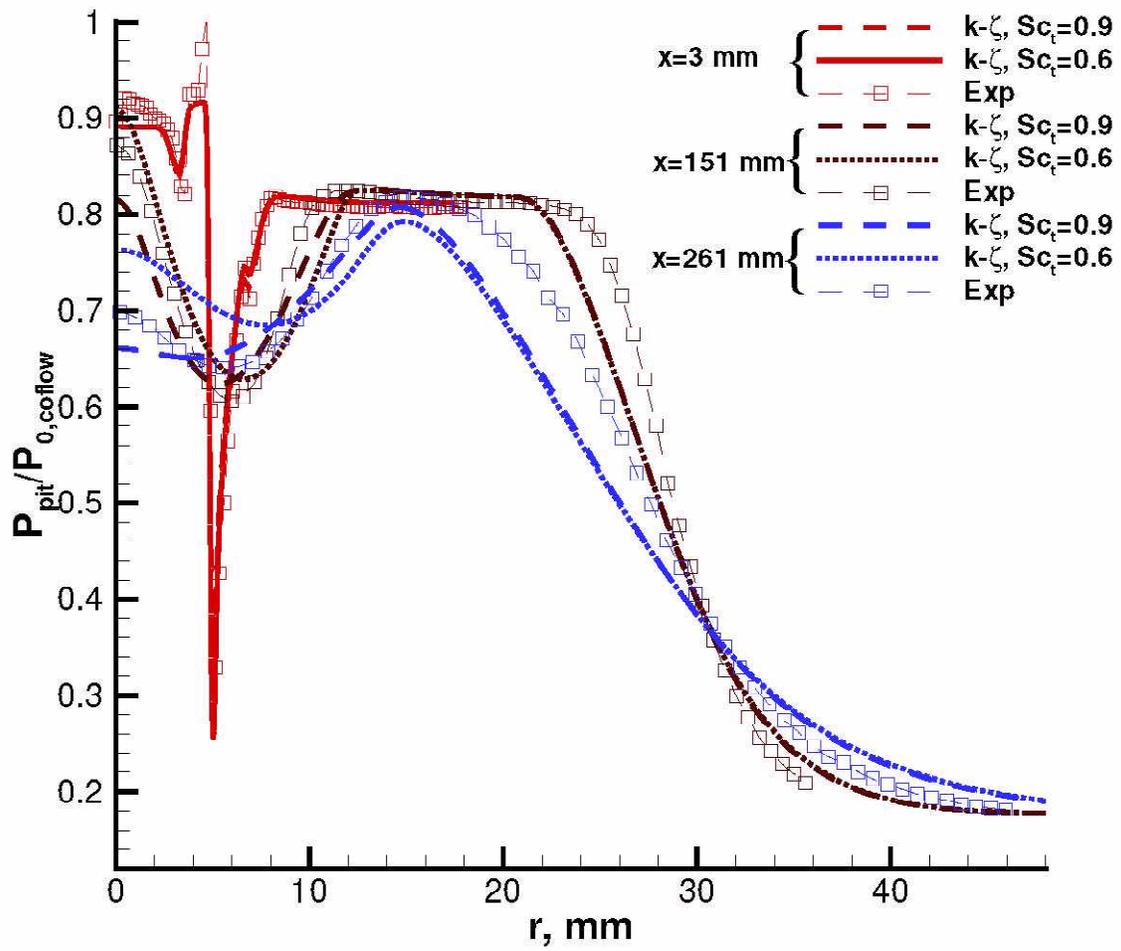
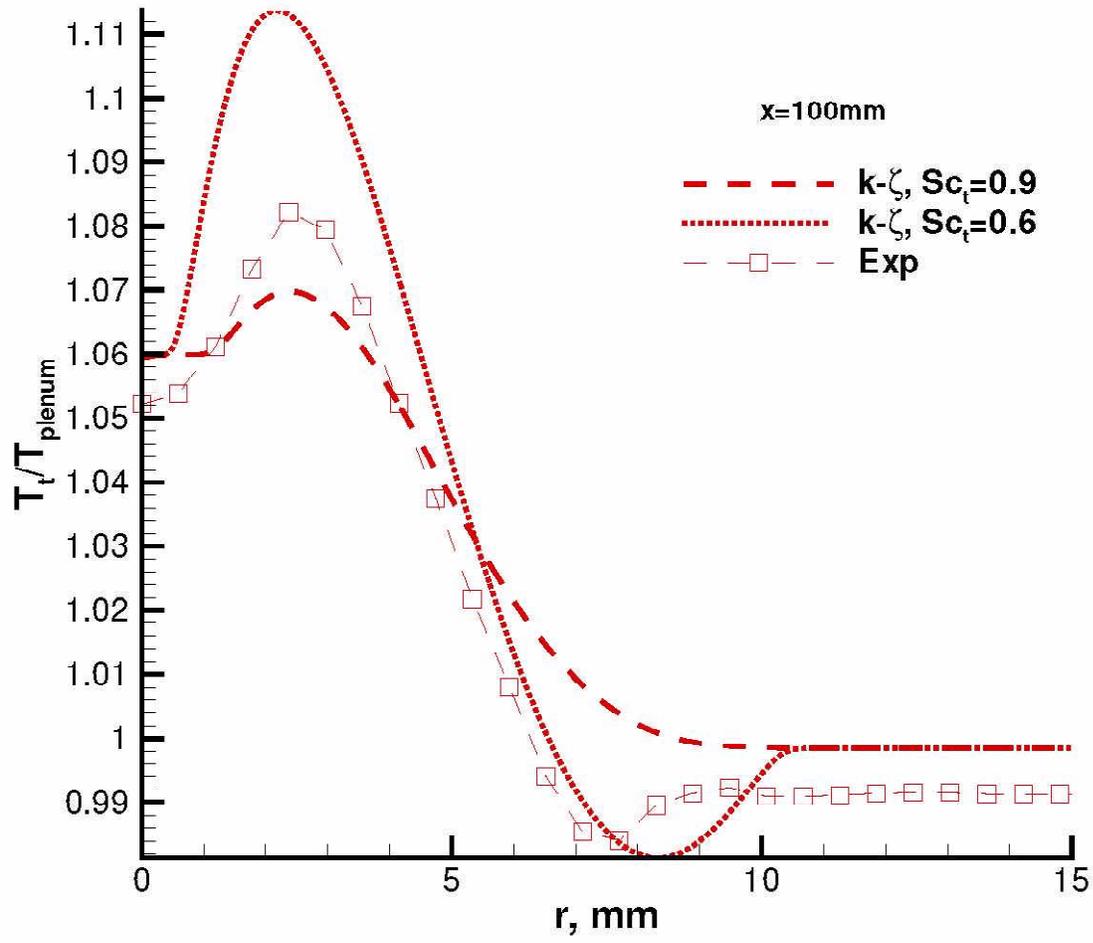


Figure 3. Comparison of pitot pressure with experiment

Figure 4. Comparison of total temperature at  $x=100$  mm with measurements

