NASA/TM—2006-214417

Turbulent Chemical Interaction Models in NCC: Comparison

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December 2006

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Acknowledgments

The authors wish to thank T.-H. Shih who meshed the grid for the initial one-element case, and also performed a series of calculations using that geometry.

This report contains preliminary findings,
subject to revision as analysis proceeds.

Level of Review: This material has been technically reviewed by technical management.

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Abstract

The performance of a scalar PDF hydrogen-air combustion model in predicting a complex reacting flow is evaluated. In addition the results are compared to those obtained by running the same case with the so-called laminar chemistry model and also a new model based on the concept of mapping partially stirred reactor data onto perfectly stirred reactor data. The results show that the scalar PDF model produces significantly different results from the other two models, and at a significantly higher computational cost.

Introduction

The simulation of turbulent reacting flow by RANS and LES requires the use of many models to solve for various processes. One of the most important, but often most neglected is the model for the interaction between turbulence and the chemistry of combustion. Previous work [1] has shown that the errors in the chemistry source term caused by not using a model can be of several orders of magnitude. However models for this phenomenon are often costly in CPU time and make obtaining a solution very costly. However with advances in computational power, the use of even the most complex of models is now possible for realistic geometries.

In this study, a nine-element hydrogen burner is simulated, using laminar chemistry, a new reactor mapping model and a Scalar PDF model. By comparing the results it is hoped to demonstrate both the capability to perform high-fidelity simulations using these models in NCC, and also compare the results with each other.

Laminar Chemistry

The simplest of turbulent-chemistry interaction models and also the most commonly used is the "Use No Model" technique. In this we assume there is no interaction between the chemistry and turbulence, and as a consequence, simple laminar kinetics are used. This simulation will be the baseline for comparing both the timing and results of the other models.

PDF Model

Almost all codes in use by industry today, are based on solving the mean Navier-Stokes and Species transport equations, with models for the unknown terms such as the k-e model. These codes represent the flow quantities at discrete locations by a single number: the mean. However if one was to take an experiment, and run it many times, obtaining the flow value at some set time, each value would be different. Collecting enough samples this way would give you the distribution of the property, from which one could obtain the PDF (Probability Density Function) of the

property at that location. Clearly the PDF provides far more information about the flow than just the mean value. From the PDF, all other moments can be obtained, such as variance, skewness, flatness etc. And if more than one property is recorded, you have a joint PDF of the properties, from which correlations can be calculated.

PDF methods then, are based on solving the transport equation for the joint PDF of the properties of interest. [2,3] By doing this, a more detailed description of the flow can be obtained. For example, if we were to solve the transport equation for the joint PDF of the three velocity components, U, V and W, we would have the exact value of such correlations as <uv>, <uuu> and <uw> available, and so would not need to calculate separate transport equations for Reynolds stresses. (The angled brackets denoting mean quantities, lower case symbols the fluctuating quantities).

However the real advantage of PDF methods is in turbulent reacting flows. In the source term for the species transport equations, we have the reaction rate of the i'th species, S_{i} as a function of all the species ø_{1..n}, and state properties T, P.

$$S_{i} = S_{i}(ø_{1..n}, ,T, P) \quad - (1)$$

This term has a big effect on the calculations, as it is responsible for large changes in the density and viscosity of the fluid, and so has a large effect on the velocities.

When one solves the equations for a mean Navier-Stokes code, this source term becomes the mean reaction rate: <S_{i}>

$$\langle S_{i} \rangle = \langle S_{i}(ø_{1..n},T, P) \rangle \neq S_{i}(\langle ø_{1..n} \rangle, \langle T \rangle, \langle P \rangle). - (2)$$

The inequality in Eqn. 2. is significant, often of several orders of magnitude, and so the reaction rate term has to be modeled. However, the complexity of the term, as well as the need for a different model for each different species and property combination makes modeling unattractive.

In the PDF approach however, this term does not need to be modeled. The PDF of the species and state variables are known, and so this term is treated exactly. Comparisons between PDF predictions and those calculating the mean reaction rate with Eqn. 2 show errors in temperature of 500K and significant errors in the flow field.

However there are terms that do require modeling in the PDF transport equation. Depending on the properties being solve for, these include the molecular mixing, turbulent diffusion and fluctuating pressure term. Of these, the molecular mixing term is the area of most uncertainty. However the effect of these models on the flow field is secondary to the effect of the reaction rate, which makes the PDF method very attractive in solving turbulent reacting flows.

Reactor Mapping Model

For a finite volume, RANS CFD code, the modeling of the combustion process in a single cell can be thought of as that of a perfectly stirred reactor. There is a mass inflow of certain mean species concentrations, which are mixed instantaneously with the mean gas mixture contained in the cell. The resulting

averaged mixture is then reacted and the resulting mean products are what exit the cell.

Considering the more sophisticated scalar PDF model, one can again liken the process of a single cell to that of a simple reactor: In this case a Partially Stirred Reactor (PaSR). For the PaSR, a distribution of species enters the reactor or cell. There they are mixed via the turbulent process while reacting. And the resulting distribution of products is what exits the reactor, or cell. And in each case, the mean species concentrations and temperatures reflect the physics of the process better than the simple Perfectly Stirred Reactor (PSR) results.

To this end the reactor mapping model (RMM) was developed as a mapping between the PaSR results and the PSR results. PaSR temperature results for a given residence time and turbulence level were mapped onto the temperature results for a PSR using the residence time, R_t, as the mapping variable. Then taking R_t and multiplying by the turbulent frequency, e/k gives a non-dimensional number R for this mapping, and a simple functional relationship between R and the equivalent residence time, R_equiv, provides the mapping function.

The function for the equivalent residence time used in this study was:

$$R\_equiv/R\_t = 0.434 \ln(R) - 0.176 \quad - (3)$$

Similar functions exist for other fuels, and so this model can be applied for most cases.

To apply this model, the time used to compute the change in scalar quantities for a given computational step is adjusted by Equation. 3. That is, while all other processes in a given cell are incremented by a time step R_t, the chemical source term is only integrated over R_equiv. Further details of this model are provided in a separate paper [4].

Simulation

To demonstrate the effect of using a turbulent combustion model in a realistic simulation, the case of the Sandia 9 element hydrogen injector was chosen.

The simulation of the hydrogen burner involved two separate computations. First a simulation of just one nozzle was performed, which included an upstream settling chamber, and a downstream expansion. The size of the settling chamber and expansion chamber was made to provide an identical expansion of area as that of the nine-nozzle case. The two hydrogen jets were provided with plenums, to damp out any possible fluctuations of the inlet conditions. Construction of the grid used 493,015 elements and is shown in Figure. 1.

After the simulation of the single nozzle case had run to convergence, data was taken at a location 5mm. upstream of the expansion region. This location is just downstream of the hydrogen jets, (2.6 mm) and is used as the initial conditions for the nine-nozzle simulation.

The quantities recorded at this location are the profiles of the velocity, turbulence and scalar variables. These fields are then interpolated onto the inlet regions of the nine-element simulation. Each of the nine nozzles had the initial data orientated so the hydrogen jets corresponded to the

experimental location. The grid used contained 282,624 elements and is shown in Fig. 2.

For the scalar PDF simulation, 100 particles were used at each cell to represent the joint scalar PDF. All computations were performed on the NASA Glenn Cortland cluster, using 32 or 64 processors.

For all cases a 9 species, 20 step chemistry model for hydrogen-air combustion was used, as described in Table 1.

Results

Timing results for the simulations are shown below:

Simulation	CPU	Iter.	Time (seconds)	Iteration time for 64 CPUs
Finite Rate	32	5000	10,428	1.04
RMM	32	5000	10,732	1.07
PDF Model	64	5000	153,830	30.76

As can be seen from the table, the difference between the RMM and the baseline Finite Rate model is negligable. However the use of the Scalar PDF model gives an increase of thirtyfold in the required computational resources. Fortunately the code does scale very well for parallel work and so could be run on about 1000 processors to achieve a similar turn around time to the other two simulations.

Looking at the temperature fields shown in Figure 3, it is apparent that there is a significant difference between the scalar PDF results and the other two simulations. The most obvious feature is that the PDF results show a more persistent cool core for all 9 injectors, while at the same time being surrounded by a hotter reacting layer. The laminar chemistry and PSR results show a central core that mixes with the surroundings quicker, and with a hot reacting layer present only about the central core. These temperature fields are also reflected in the major products of combustion data (not shown), which show the same behavior.

Looking at a representative of the minor species fields, OH, shown in Figure 4 shows a similar trend in the data.

The levels of OH reflect the structure of the temperature fields shown in Figure 3. The isolated hot cores of the laminar and RMM results show high levels of OH, while the PDF results show a more distributed amount of OH at lower concentrations. In this data the effect of the RMM can be seen, in that it exhibits a trend toward the PDF results, with a slightly more distributed concentration of OH throughout the burner.

Looking at the velocity fields in Figure 5 also shows the effect of the more complete combustion in the PDF simulation.

The velocity profiles show a significant amount of variability, with the scalar PDF results exhibiting significantly higher velocities and also smaller regions of recirculation. The higher velocities can be attributed to the more complete combustion and resulting expansion of the gasses. This in turn tends to damp out recirculation zones. The laminar and RMM data show very little difference, with the

RMM result having a slightly higher maximum axial velocity.

It should be noted that no experimental data is available so far for this configuration. Hence no quantitative comparision can be made as to which model works best. However the assumed PDF does provide significantly more physics to the combustion model, and the differences between the cases shown here are intriguing.

What can be gained from this study is firstly that the most physically complete model for turbulent chemistry interaction can be used to model realistic problems, though at a significantly greater computational cost than other models. In addition the performance of the RMM is interesting. Overall it showed a similar performance to the laminar chemistry model, however in the ways it did differ, it was in a manner that trended toward the scalar PDF results. As the RMM is very much under development at the moment, there is good reason to suppose that further work might produce a model that provides much of the physics of the scalar PDF model, but without the high computational cost.

Summary

The effect of the interaction between the combustion chemistry and the turbulent flow field is an important phenomena in combustion CFD. Of the models available, the scalar PDF model can be considered the best, as it requires no modeling of the chemistry source term. And with computational resources now available, it is possible to run realistic simulations using the scalar PDF model. In an example run of a 250,000 element simulation, the scalar PDF model showed a very different solution than that of a case with no turbulent-chemistry interaction model or the PSR model. Further development and validation of the Scalar PDF model would seem to be an important goal to enhance the National Combustion Code and NASA computational abilities. In addition the promise shown by the RMM suggests that this might, with further development, provide a simple robust model for turbulent chemistry interactions without the high computational cost associated with the scalar PDF model.

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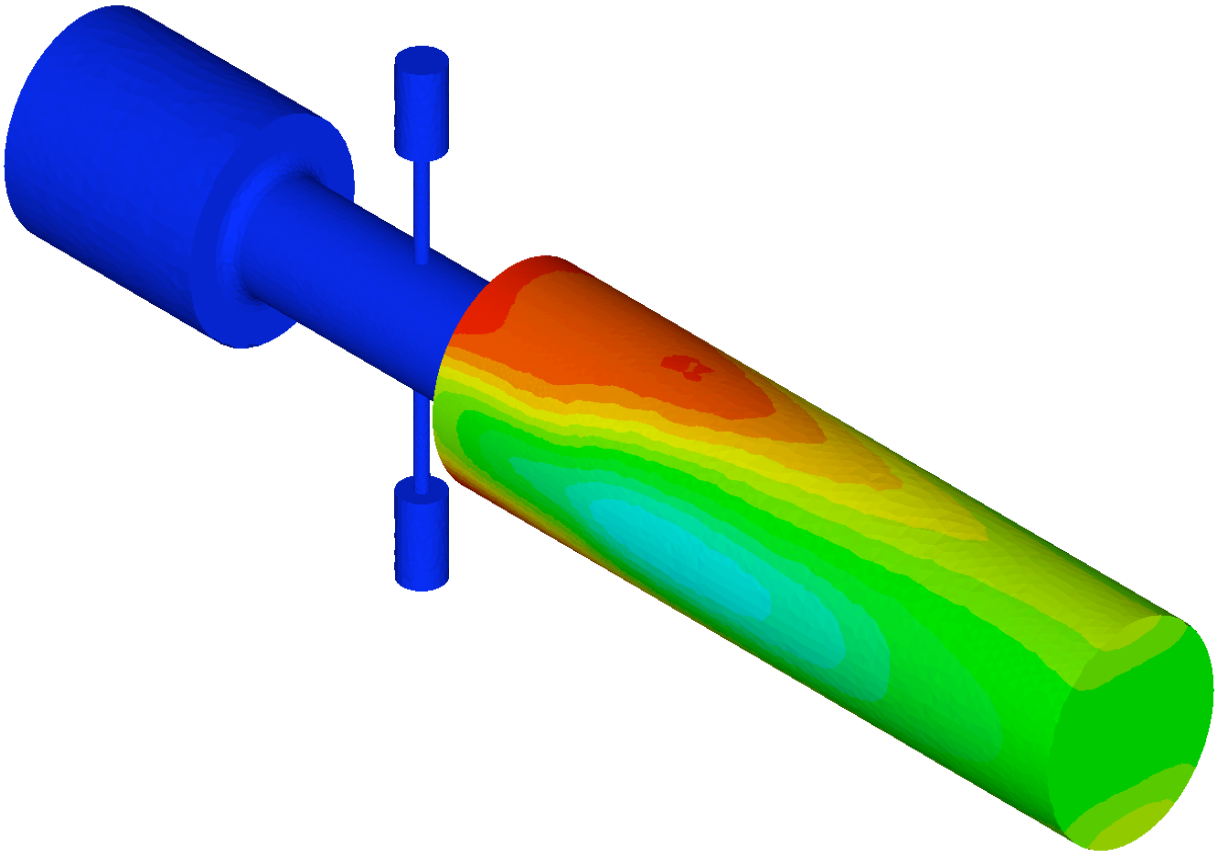

Figure 1. Single-injector geometry, showing upstream chamber to the left, with two fuel ports with plenums and expansion chamber. Contours show temperature for finite-rate simulation with no chemistry-turbulence interaction model.

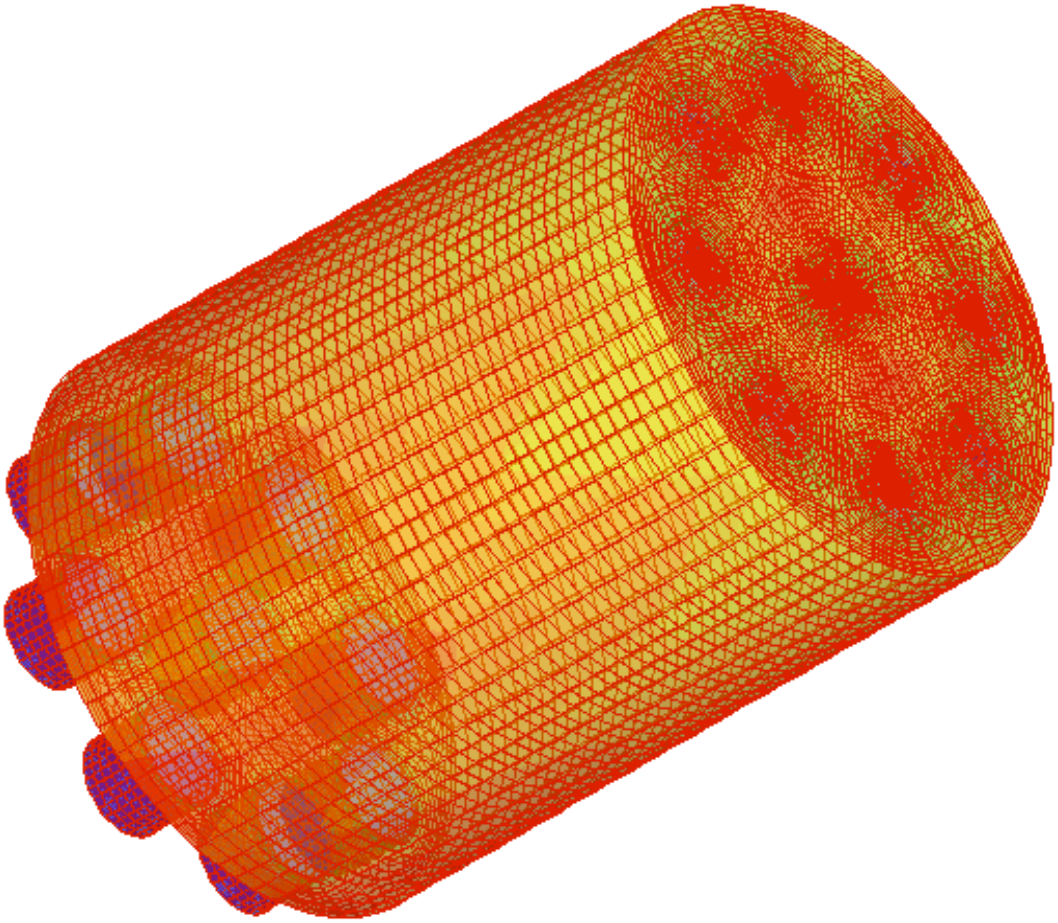

Figure 2. Geometry of Sandia 9-element hydrogen burner. Length is approximately 50mm and diameter is approximately 38mm. Each injector is 7.6mm in diameter, and 5.0mm long. This corresponds to having the inlet located just downstream of the hydrogen injection ports shown in Figure 1.

Reaction	A	n	E
H+O2+M=HO2+M	3.61E17	-0.72	0.
H2O/18.6/ H2/2.86/			
H+H+M=H2+M	1.00E18	-1.0	0.
H+H+H2=H2+H2	9.20E16	-0.6	0.
H+H+H2O=H2+H2O		-1.25	0.
	6.00E19		
H+OH+M=H2O+M	1.60E22	-2.0	0.
H2O/5/			
H+O+M=OH+M		-0.6	0.
H2O/5/	6.20E16		
O+O+M=O2+M	1.89E13	0.0	-1788.
H2O2+M=OH+OH+M		0.0	45500.
	1.30E17		
H2+O2=2OH	1.70E13	0.0	47780.
OH+H2=H2O+H	1.17E9	1.3	3626.
O+OH=O2+H	3.61E14	-0.5	0.
O+H2=OH+H	5.06E4	2.67	6290.
OH+HO2=H2O+O2		0.0	0.0
	7.50E12		
H+HO2=2OH	1.40E14	0.0	1073.
O+HO2=O2+OH	1.40E13	0.0	1073.
2OH=O+H2O	6.00E+8	1.3	0.
H+HO2=H2+O2	1.25E13	0.0	0.
HO2+HO2=H2O2+O2		0.0	0.
	2.00E12		
H2O2+H=HO2+H2	1.60E12	0.0	3800.
H2O2+OH=H2O+HO2		0.0	1800.
	1.00E13		

Table 1: Arrhenius constants for 9 species, 20 step hydrogen-air mechanism used in study.

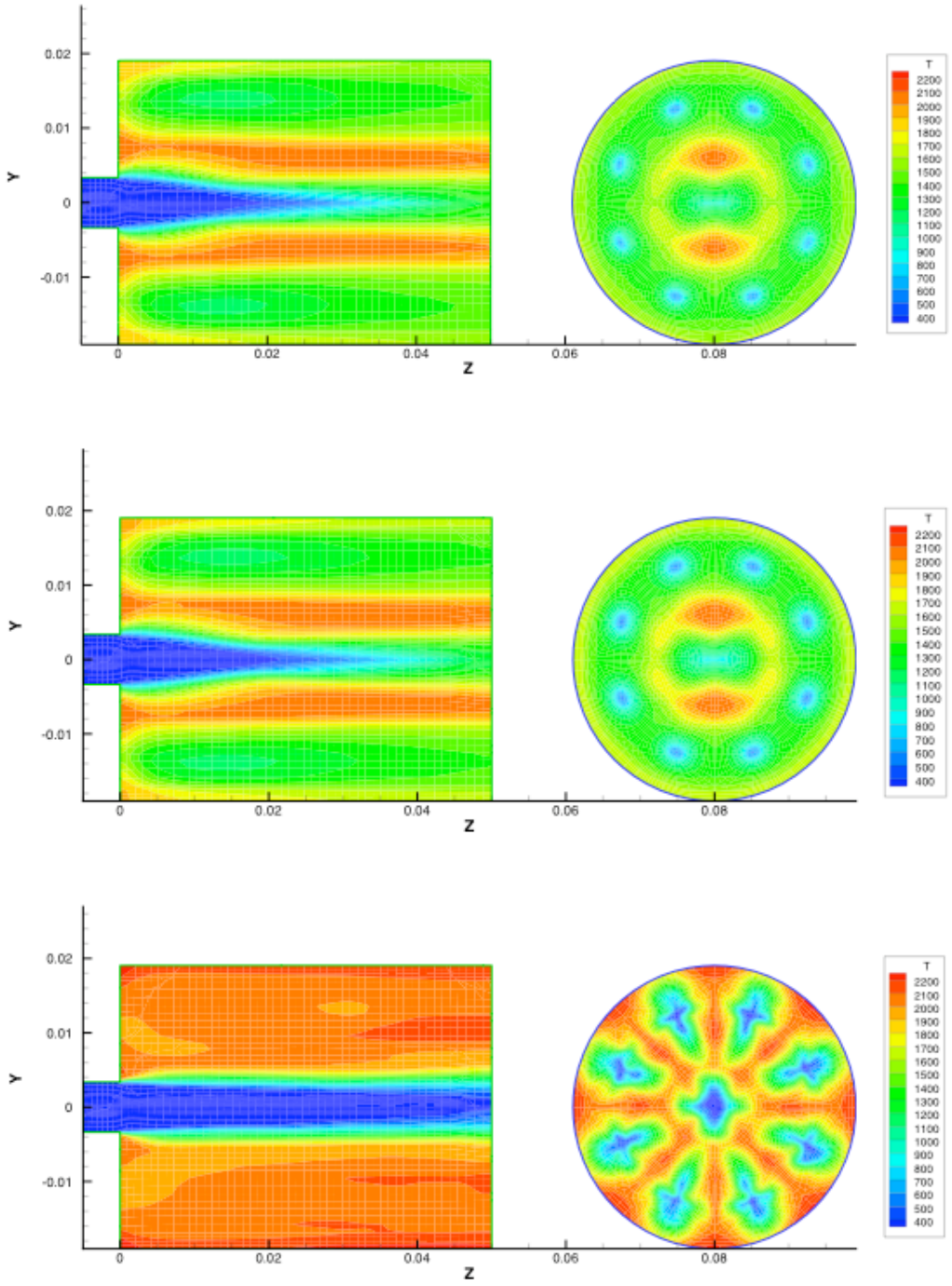

Figure 3. Temperature fields in Kelvins from the top for the laminar chemistry, PSR model and PDF model respectively. Data consists of a slice along the centerline and a cross section at x = 0.04m.

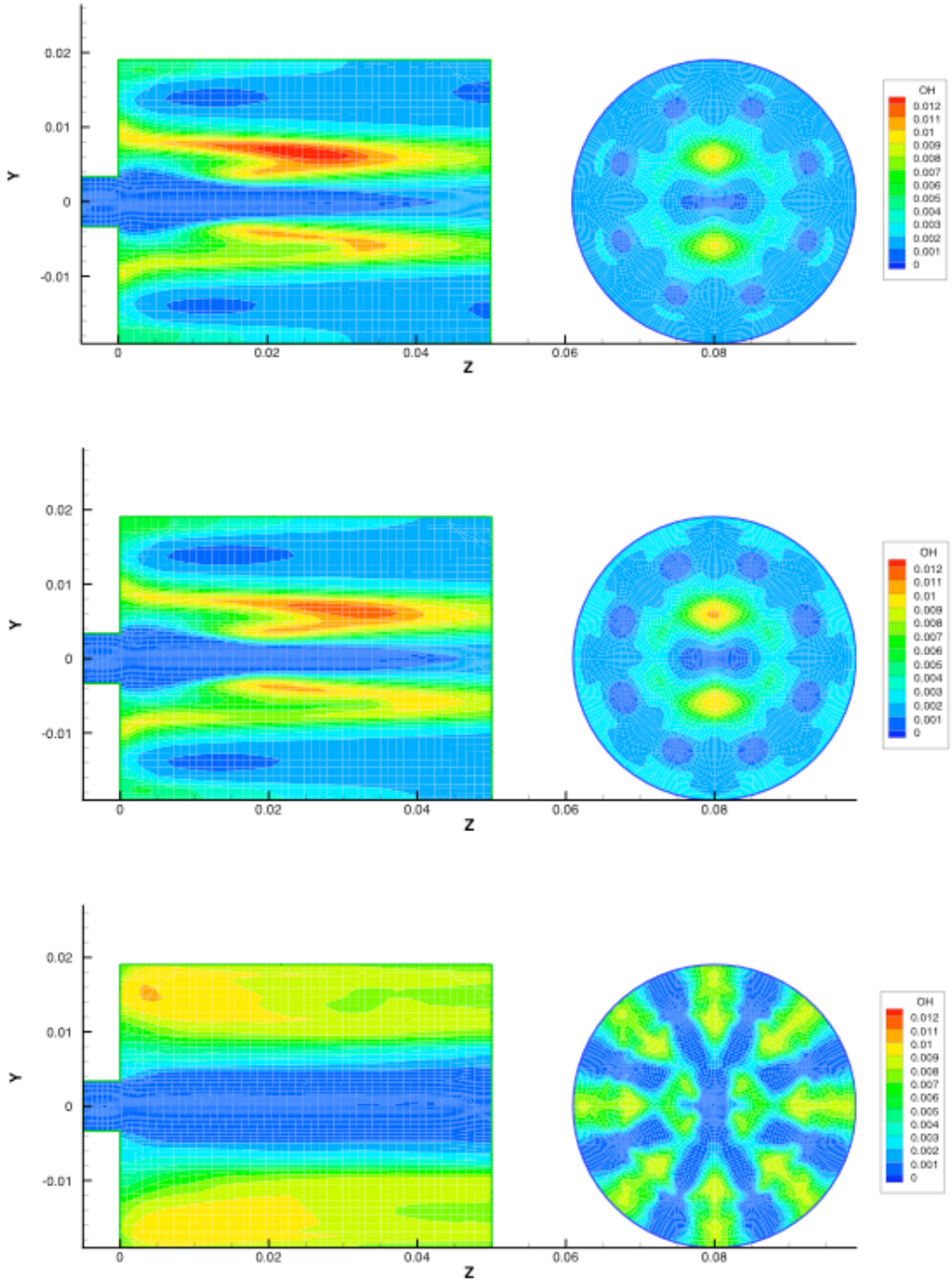

Figure 4. OH mixture fraction fields (from the top) for the laminar chemistry, PSR model and PDF model respectively. Data consists of a slice along the centerline and a cross section at x = 0.04m.

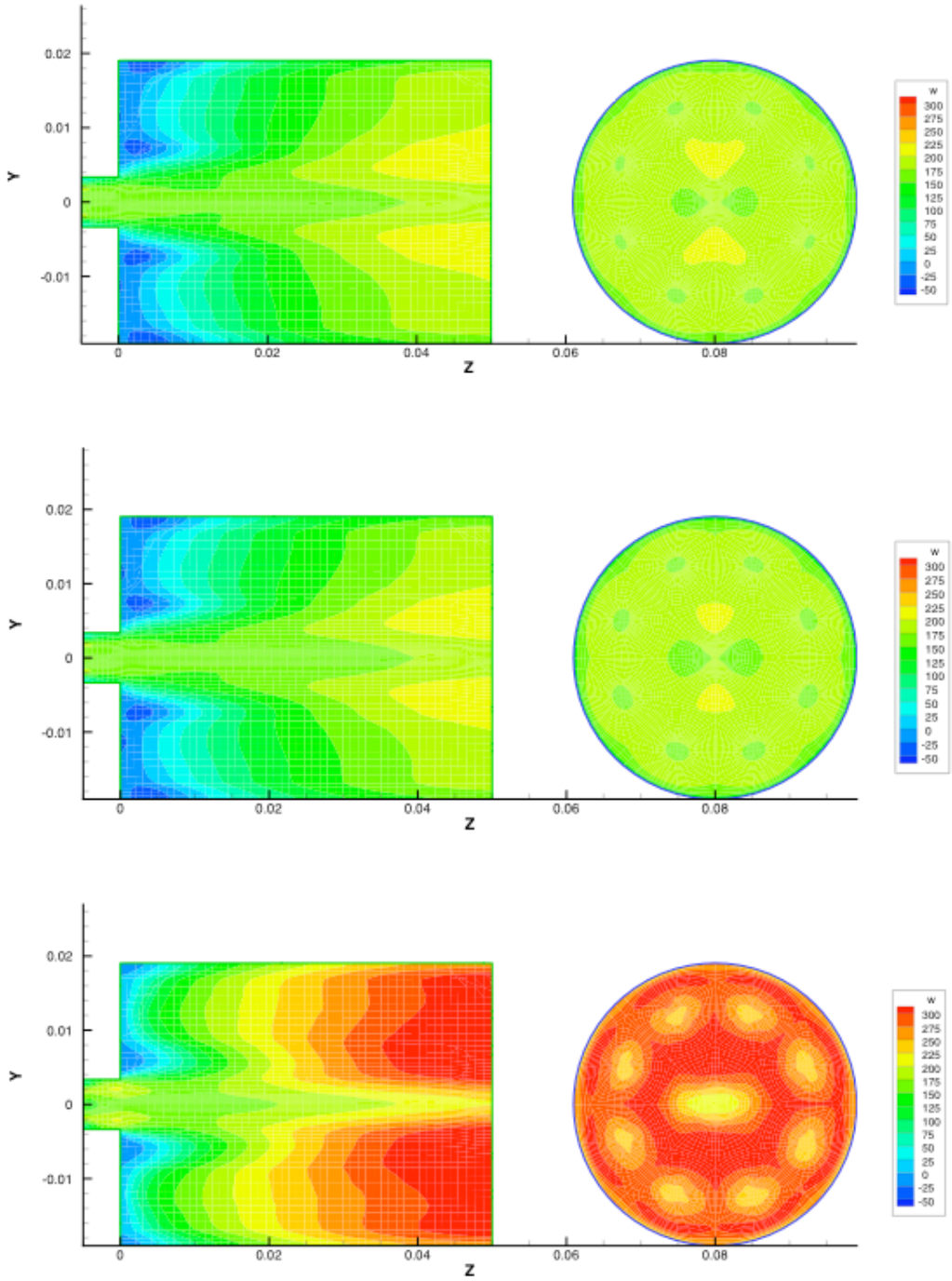

Figure 5. Axial velocity contours, (from the top) for the laminar chemistry, PSR model and PDF model respectively. Data consists of a slice along the centerline and a cross section at x = 0.04m. Units are meter/second.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (*Leave blank*)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	December 2006	Technical Memorandum

4. TITLE AND SUBTITLE

Turbulent Chemical Interaction Models in NCC: Comparison

5. FUNDING NUMBERS

WBS 984754.02.07.03.06.01

6. AUTHOR(S)

Andrew T. Norris and Nan-Suey Liu

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

National Aeronautics and Space Administration
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135–3191

8. PERFORMING ORGANIZATION REPORT NUMBER

E–15697

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

National Aeronautics and Space Administration
Washington, DC 20546–0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

NASA TM—2006-214417

11. SUPPLEMENTARY NOTES

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The performance of a scalar PDF hydrogen-air combustion model in predicting a complex reacting flow is evaluated. In addition the results are compared to those obtained by running the same case with the so-called laminar chemistry model and also a new model based on the concept of mapping partially stirred reactor data onto perfectly stirred reactor data. The results show that the scalar PDF model produces significantly different results from the other two models, and at a significantly higher computational cost.

14. SUBJECT TERMS

Scalar PDF; Hydrogen combustion; Turbulence-chemistry interaction; National combustion code

15. NUMBER OF PAGES

17

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	