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TITLE: **HYDROGEN PROGRAM COMBUSTION RESEARCH: THREE DIMENSIONAL COMPUTATIONAL MODELING**

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HYDROGEN PROGRAM COMBUSTION RESEARCH: THREE DIMENSIONAL COMPUTATIONAL MODELING

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Abstract

In the past year we have significantly increased our computational modeling capability by the addition of a vertical valve model in KIVA-3, a reactive flow code used internationally for engine design. In this report the implementation and application of the valve model is described. The model is shown to reproduce the experimentally verified intake flow problem examined by Hessel. Furthermore, the sensitivity and performance of the model is examined for the geometry and conditions of the hydrogen-fueled Onan engine in development at Sandia National Laboratory. Overall the valve model is shown to have comparable accuracy as the general flow simulation capability in KIVA-3, which has been well validated by past comparisons to experiments. In the exploratory simulations of the Onan engine, the standard use of the single kinetic reaction for hydrogen oxidation was found to be inadequate for modeling the hydrogen combustion because of its inability to describe both the observed laminar flame speed and the absence of autoignition in the Onan engine. We propose a temporary solution that inhibits the autoignition without sacrificing the ability to model spark ignition. In the absence of experimental data on the Onan engine, a computational investigation was undertaken to evaluate the importance of modeling the intake flow on the combustion and NOx emissions. A simulation that began with the compression of a quiescent hydrogen-air mixture was compared to a simulation of the full induction process with resolved opening and closing of the intake valve. Although minor differences were observed in the cylinder-averaged pressure, temperature, bulk-flow kinetic energy and turbulent kinetic energy, large differences where observed in the hydrogen combustion rate and NOx emissions. We conclude that the flow state at combustion is highly heterogeneous and sensitive to the details of the bulk and turbulent flow and that an accurate simulation of the Onan engine must include the modeling of the air-fuel induction.

Introduction

Rapid utilization of hydrogen for stationary power plants and combustion engines for hybrid vehicles requires the development of computational tools to aid in the design of new engines by industry and government laboratories. Our goals are to develop the required computational tools, to validate them by comparison to experimental data, and to demonstrate the utility of the computational approach in a research program to design such internal combustion engines and then to collaborate with industry and government laboratories in their applications of the computer models. Los Alamos has developed a family of computer models that have gained wide acceptance in the automotive industry, as well as the gas turbine, stationary combustion and aerospace industries, primarily for hydrocarbon fuels. Our approach is to refine, modify and utilize computer models embodied in the KIVA-3 and KIVA-F90 computer codes as applied to combustion of both pure hydrogen as a fuel and mixtures of hydrogen and hydrocarbon gases. The work supports collaboration in the DOE Hydrogen Program by developing the knowledge to (1) enable industry to build a stationary hydrogen fueled internal combustion engine to power an electric generator system, and (2) to build an advanced internal combustion engine fueled by hydrogen to meet zero emission requirements. Because of the wide use of the KIVA family of codes in the automotive, diesel and aerospace industries, the capability to use hydrogen fuel in the KIVA family of codes can be quickly utilized by industry.

Los Alamos National Laboratory (LANL) will use the chemistry submodels under development at Lawrence Livermore National Laboratory (LLNL). The hydrogen combustion simulation capability can then be benchmarked with experiments performed by Sandia National Laboratory (SNL) and LLNL and then be used to aid in the support of the development of the optimized test engine and demonstration engine, currently under development by SNL and LLNL.

Earlier investigations, prior to the work described in this report, focused on the hydrodynamics and combustion of a hydrogen jet (Amsden, et al., 1994; Johnson, et al., 1995). From a comparison of detailed experiments performed by SNL, we observed that the KIVA simulations of methane injection modeled accurately the penetration and pressure history, with and without combustion. By contrast, the modeling of the combustion of hydrogen was unsatisfactory using either a single Arrhenius kinetic equation or a 22-reaction model. In particular the simulations prematurely autoignited and required that the combustion be delayed to the experimentally observed value. After the examination of hydrogen injection and combustion, simulations were made of the spark ignited CLR engine being operated at SNL. Preliminary results led us to suspect that simulations without detailed information about the bulk flow and turbulent levels at the onset of spark ignited combustion were deficient. In order to properly simulate the intake flow, the flow through an opening and closing valve was required. We then undertook the implementation of a valve model in KIVA-3.

This report summarizes the new vertical valve capability that has been implemented into KIVA-3, its validation and its application to the spark-ignited, hydrogen-fueled Onan engine being operated by SNL.

Details of the SNL Onan engine can be found in the report by Van Blarigan (1995). The Onan engine is a converted diesel engine with a modified head containing two valves and two spark plugs. Table 1 summarizes the engine specifications. The design of the Onan engine is based on the arguments put forth in the report by Smith and Aceves (1995). The engine design is such that the bulk flow and turbulence are minimized in order to reduce the heat transfer losses, thereby increasing the operating efficiency. The engine operates at low fuel equivalency ratios (0.4–0.5) to reduce the combustion temperature and thereby significantly reduces the NOx emissions. Because of the symmetry of the engine design, the flow and combustion is symmetric through a plane passing through the two valves.

Table 1 Modified Onan Engine Specifications

Bore	82.55 mm
Stroke	92.08 mm
Displacement	493.0 cm^3
Geometric compression ratio	14.82
Rings	4
Valve pocket volume	3.60 cm^3
Spark plug volume	1.30 cm^3
Volume above rings	0.27 cm^3
Volume of depressed gasket	7.52 cm^3
Squish volume	35.65 cm^3

Implementation of the Valve Model in KIVA

The KIVA family of codes, developed at LANL, is a mature, three-dimensional, computational fluid dynamics software for chemically reactive, transient flows with fuel sprays (Amsden et al., 1989). The code features sophisticated sub-models, which simulate the complex flow, thermodynamic and chemical processes accompanying combustion. These models include for applications to combustion engines: turbulence, spray atomization, fuel penetration and vaporization, auto-ignition and combustion. The chemical combustion model can describe complex equilibrium and kinetic reactions, giving it the capability of modeling soot in the presence of carbon and NOx production. The KIVA-3 version (Amsden, 1993) enables complex geometries to be modeled, typical of combustion engines with moving pistons and inlet and exhaust ports. KIVA-3 runs on generic workstations and on supercomputers. A new version of KIVA, KIVA-F90, is written in FORTRAN-90 and will execute on massively parallel machines. For the current application, KIVA-3 is used to model the SNL experiments.

Once the need for a valve model in KIVA was established, the examination of available valve models were considered. It was decided that a valve model that had comparable accuracy as the other fluid flow models in KIVA was desirable, because the experience with the performance of valve models is limited in the engine modeling community. An implementation of the desired valve model was developed in a research version of KIVA-3 by Hessel (1993). This modified version of KIVA-3 was obtained by LANL, and the valve capability was moved to the most recent version of KIVA-3 and made compatible with all existing features. Details of the model can be found in the Ph. D. thesis by Hessel; the highlights of the model as implemented at LANL are summarized below.

The valve model uses an existing capability, the SNAPPER model (Amsden, 1993), in KIVA-3 for modeling pistons in complicated geometries. The SNAPPER model moves the solid surface of the piston (or valve) until the mesh above the piston is reduced in height to a specified value. The squished cells next to the piston are removed from the computational mesh, and their state quantities are added to the expanded cells now above the piston. When the piston is withdrawn, the process is reversed. Consequently, the shape of the piston or valve is resolved to arbitrary degree as determined by the mesh resolution. The implementation, as with the piston model, requires a special mesh generation capability in which the shape of the valve during its entire movement history is included in the fluid portion of the mesh. As a consequence of this restriction on the mesh, parallel with the valve implementation in KIVA-3, the mesh generation capability for valves was also implemented in the companion mesh generator for KIVA-3. In both implementations, additional capabilities and simplification of input were made over the original Hessel implementation. These include, for example, the ability to have an arbitrary number of valves with independent movement histories and automatic reporting of the flow through each valve. Furthermore, some errors in the original implementation were found and corrected. Finally a more efficient sorting routine, which is required after the SNAPPER operates, is used and significantly reduces the execution times.

Because the valve model makes no approximations for the flow through the valve opening, the accuracy of the valve model is comparable to the accuracy of the standard flow solution in the code and dependent upon the mesh resolution in the region of the valve. This is a significant advantage of the model because the accuracy of the valve flow need not be independently validated but can rely on prior comparisons of the performance of KIVA on other flow problems (e.g., Amsden et al., 1992).

To validate the valve model, the intake flow problem examined by Hessel was simulated using the original mesh of 122,000 cells, as shown in Fig. 1. Hessel achieved satisfactory comparisons between the KIVA-3 results and the detailed experimental data for the same flow. The final simulation using the new implementation of the valve model duplicated the results obtained by Hessel to within expected differences associated with the correction of the errors. Due to the improved sorting routine and the elimination of certain errors that had reduced the time step, the simulation time for the new implementation was reduced by about 50%. Based on this comparison, we are confident that the valve model in the current version of KIVA-3 accurately reproduces Hessel's original implementation.

Three-Dimensional Modeling of SNL ONAN Engine

Mesh generation

The development of a three-dimensional mesh for a complex geometry is a significant undertaking. The mesh used to model the modified Onan engine resulted from progressive refinements over a period of several months. The final mesh is shown in Fig. 2. The mesh is generated with a preprocessor that has been written specifically for KIVA-3 without the need for additional modifications. The mesh is generated with 41 pseudo-blocks, resulting in 5 logically hexahedral blocks of mesh with 37,722 cells in the full mesh. As stated in the last section, the setup of the mesh requires the shape of the valves along their path to be included in the initial mesh, as illustrated in Fig. 2. Because the current geometry of the modified Onan engine has a plane of symmetry through the two valves, for the computational results presented here only half of the engine is simulated. The only major simplifications made in the computational mesh were square cross-section of the intake and exhaust manifolds and their reduced length. To reduce the effect of the simplification, the flow area of the simulated and actual manifolds are identical. Because the pressure boundary conditions at the intake and exhaust manifolds were expected to be modified in order to obtain agreement with the breathing performance of the engine, the simplification of the length and cross-section of the manifolds is not considered to be significant. Other simplifications are the omission of the volume associated with the spark plugs (3.5% of the minimum cylinder volume) and the volume above the piston rings (0.7% of the minimum volume). The valve shapes and seating were modeled accurately to within the resolution of the mesh. Other boundary conditions are specified in Table 2.

Table 2. Initial and boundary conditions

Cylinder wall temperature	373 K
Piston temperature	430 K
Head temperature	373 K
Intake valve temperature	373 K
Exhaust valve temperature	585 & 800 K
Exhaust gas temperature	585 & 800 K
Engine speed	1200 & 2400 RPM
Exhaust pressure boundary	0.949 - 1.0 atm
Intake pressure boundary	0.949-1.2 atm
Intake manifold composition	0.4 - 0.41 fuel equivalence ratio in air
Exhaust manifold composition	combustion products of the intake gas
Initial cylinder composition	same as exhaust manifold

Further validation of the valve model

Various validation checks were made to assess the accuracy of the valve model within KIVA-3. For overall flow accuracy, the duplication of the results of the intake flow problem by Hessel summarized in the last section is the primary validation in the absence of detailed experimental data on the Onan engine. Because KIVA-3 has been validated for ported engines (e.g., Amsden et al., 1992), we are confident in the accuracy of the valve model as long as the behavior of the valve flow exhibits no anomalous behavior, because the valve model introduces no new physical or numerical models.

To check for anomalous behavior, the flow through the valve during opening and closing were examined. A simulation was done with the geometry described in the previous section at an RPM of 300, in order to make the primary resistance to flow the valve opening. The velocities in the intake valve gap were measured as a function of time and plotted against the pressure drop across the intake valve at a given time (see Fig. 3). At steady state the velocity through the valve gap should be proportional to the pressure drop across the gap. As can be seen in Fig. 3, most of the points reflect an approximately linear relationship between the velocity and the pressure drop, with the breadth in the plot attributable to unsteady state conditions and the changes in flow area. The only points that lie outside this band of data are when the valve first opens and all the flow is though one cell. This anomalous behavior is attributed to the absence of the law of the wall boundary layer approximation being applied between solid surfaces that have only one cell between them. This treatment allows for a larger flow for a given pressure drop than at other times, and hence, the cause of the outlying points at these times in Fig. 3. Because the mass flow through the valve during these times is small compared to the total mass flow, the effect of this anomaly is considered small. We are investigating alternative treatments that would alleviate this effect. As a result of this analysis we conclude that the valve model within KIVA-3 has been properly implemented and has comparable accuracy to the rest of the code.

The sensitivity of the shape of the valve has on the flow was examined by comparing the flow past an approximate valve shape to the experimental valve shape, as shown in Fig. 4 for identical driving conditions and mesh resolution. The peak velocity during maximum valve opening was observed to be 41% higher (17.3 m/s versus 12.3 m/s) in the resolved shape than in the approximate valve shape. Because turbulence generation is most sensitive to large gradients in velocity and because combustion is sensitive to turbulence levels, we would expect these two geometries to exhibit different combustion and emission behavior. This observed difference in velocity is a significant indication that care must be taken in resolving the geometric details in the neighborhood of the valves.

Exploratory Simulations of the SNL Onan Engine

In the absence of experimental data on the Onan engine for comparison to the KIVA simulation results, a variety of simulations were done to evaluate the performance and sensitivity of the model. The different operating conditions are listed in Table 2. Simulations were initialized at just before intake valve opening (–20 CA BTDC) and carried though the intake cycle, the closing of the intake valve and the compression of the gas, and then stopped just before spark ignition. The state of the calculation was stored at this time so that the simulation could be continued with a variety of spark ignition times and changes in the reactive kinetic models.

The kinetics of hydrogen oxidation were modeled by a single forward kinetic equation, with an Arrhenius temperature dependence. Zeldovich kinetics for the slow NOx production is also included. The effect of turbulence on the combustion rate was included by using a mixing controlled combustion model (a slight variation of the model proposed by Magnussen and Hjertager, 1977) in which the reaction rate is proportional to the ratio of the turbulent kinetic energy divided by the rate of dissipation of turbulence. The inclusion of the mixing controlled model is essential because the flame speed of the hydrogen combustion can be many times the laminar flame speed in the presence of typical turbulent intensities found in engines (Meier et al., 1994), and increases of factors of 25 times the laminar flame speed are observed for propane (Abdel-Gayed and Bradley, 1977). In turn, flame speed is related to combustion temperature and thereby is reflected in NOx emission levels. The present mixing controlled combustion model is applied routinely to hydrocarbon combustion, but has not been applied to hydrogen combustion. Until the model is validated, results using the mixing turbulent combustion model should only be used to examine trends in the simulations. Before reporting detailed simulation results, the following summarizes the early exploratory simulations of the Onan engine.

All the simulations ran without difficulty or unexpected termination. Execution times were about two hours on a Cray YMP to reach the time of spark ignition, or about 360 degrees of crank angle. Combustion simulations from –20 CA to 20 CA required about a hour of computational time. All aspects of the simulations associated with the fluid dynamics were reasonable, and we expect them to be predictive of the Onan engine performance.

The only area of difficulty arose in the simulation of combustion of hydrogen. The primary difficulty that was encountered was the autoignition of the hydrogen during compression, when parameters in the single step oxidation kinetics were used which reproduce the laminar flame speed (Westbrook, 1994). Preliminary experimental results (Van Blarigan, 1995) indicate that for these operating conditions, autoignition does not occur. This deficiency of the hydrogen kinetics was also observed in the KIVA simulations of hydrogen injection and combustion (Johnson et al., 1995) by the absence of an autoignition delay. Our solution to the difficulty is similar: enforce that the hydrogen kinetics reproduce the observed behavior by preventing the hydrogen reaction from proceeding until the cell temperature has exceeded 1000 K. This approach does not require a modification of KIVA, because a cut-off temperature, typically 800 K, is commonly used in which the kinetics will not be calculated if the cell temperature is below this value. The consequence of this approach is to inhibit the reaction as compression of the fuel mixture occurs and enable the reaction at and behind the combustion front, typically at temperatures over 2000 K. We consider this to be a temporary solution until better kinetics are available from the work being done at LLNL. In the absence of the higher cutoff temperature, the hydrogen fuel would autoignite when it reached 800 K, typically about –10 degrees BTDC for an intake manifold pressure of 1.2 atm, independent of the time of spark ignition.

Importance of Modeling Fuel-Air Induction on Combustion and Emissions

In the absence of experimental data to benchmark the performance of KIVA-3 for the Onan engine, we undertook a computational study to evaluate the importance of including the induction of air-fuel into the cylinder prior to combustion. We made two simulations, one with no induction into the cylinder and another with flow through the intake valve and the subsequent generation of bulk flow and turbulence, and then compared the effects on combustion and time histories of flow energies. The simulation with intake flow was accomplished as described in the previous section. The simulation without induction was begun just after intake valve closing and the composition was set to be identical to the simulation with induction at the same crank angle. The bulk flow was specified to be quiescent, and the turbulence kinetic energy per mass was taken to be ten percent of the kinetic energy per mass as obtained from the maximum piston velocity. These are typical starting conditions for a quiescent engine when more detailed information is not known.

Figures 5 and 6 show the cylinder-averaged pressure and temperature during the compression, combustion, and expansion part of the cycle, up until the opening of the exhaust valve at 500 CA (the simulation without induction was only run to 390 CA because after this time the two simulations are similar). Up until the time of combustion these curves are identical for both runs. After combustion at 13.5 CA BTDC (346.5 CA in the simulation), there is significant divergence in the two simulations, a difference of 35 bars in pressure and 400 K in temperature. A plot of the hydrogen mass in the cylinder as a function of crank angle in Fig. 7 shows a further difference in the two simulations: the observed flame speed is about 3.5 times smaller in the non-inducted simulation. The differences in the combustion behavior have a significant impact on the production of NOx emissions. In Fig. 8 the NOx production is 14 times higher in the fast burning combustion, due to the higher temperatures.

The large difference in the combustion and NOx emissions in the two simulations illustrate the importance of modeling the bulk flow and turbulence levels accurately. In Figs. 9 and 10 are plotted the total kinetic energy of the bulk flow and the turbulent kinetic energy as modeled by the k-ε turbulence model. These curves show a significant difference in the initial kinetic energy levels of the two simulations. As the initial high kinetic energy level dissipates in the induction run and as the piston adds kinetic energy during compression, the averaged kinetic energy for both the bulk flow and turbulence are within 10–20 percent of each other just after ignition (350 CA). If the averaged kinetic energy values represented the values near the combustion front, this would result in a comparable increase in the reaction rate, not the factor of 350 percent observed. This is strong evidence that the flow is nonhomogeneous and sensitive to the details of the flow history.

Conclusions and Future Work

A significant extension of the KIVA-3 reactive simulation code was accomplished by the addition of a vertical valve model, which works in concert with all other capabilities of the code. The valve model was validated by comparisons to a experimentally-verified intake flow for a four valve engine. Further test simulations were made to assure that the model has comparable accuracy as the rest of the flow model used in the code and to ascertain the sensitivities of the model, such as the details of the valve-seat geometry. A computational mesh was created of the SNL Onan engine, with an accurate description of the intake and exhaust valves. In the absence of experimental data on the performance of the engine, we focused on observed trends in the simulations. The model of the Onan engine was used to investigate the induction process of fresh air and the subsequent compression and combustion of hydrogen with NOx formation. A major conclusion of the investigation is that the use of a single kinetic reaction for hydrogen oxidation is unable to describe both the observed laminar flame speed and the lack of autoignition in the Onan engine. We also observed that the combustion and emissions are sensitive to the initial flow field at the beginning of combustion. NOx emissions were observed to vary by a factor of 14 with typical choices for the initial conditions of the simulation. We conclude that any modeling of the Onan engine must include the effects of the intake flow on the bulk flow and turbulence levels during combustion.

The KIVA-3 simulations are now at the ideal stage of development to begin the validation process as the experimental data becomes available from SNL. The observed sensitivity of hydrogen combustion on turbulence and bulk flow highlights the need for improved kinetics and then for validation of the kinetics in conjunction with the mixing controlled models. In addition, as experimental data for the Onan engine is available, the simulation conditions can be improved to better model the experiments. For example, the constant pressure boundary conditions can be replaced by time-varying pressure boundary conditions as determined from the experiments. The pressure history and the mass of charge in the engine can then be compared to the experimental results to further validate the performance of the valve model in KIVA-3. Finally, comparison of NOx formation and engine efficiencies will be made. Once the simulations are validated, an analysis of the operation of the engine will be undertaken to better understand the experimental observations of the effect of combustion chamber geometry, turbulence levels, flame speed, and heat transfer on NOx formation and efficiency. The simulations can also be used to suggest modifications to the Onan engine to improve the performance and reproducibility of the engine. For example, the trends in the present report suggest that a reduction in the turbulence levels of the engine through the introduction of shrouds on the valves may improve the NOx emissions of the engine. This is an ideal application of using computer simulations to improve the success of expensive modifications of an experiment.

References

Amsden, A. A., O'Rourke, P. J., Butler, T. D., Meintjes K., and Fansler, T. D., 1992. "Comparisons of Computed and Measured Three-Dimensional Velocity Fields in a Motored Two-Stroke Engine," SAE Paper 920418.

Amsden, A. A. 1993. "KIVA-3: A KIVA Program with Block-Structured Mesh for Complex Geometries," Los Alamos National Laboratory report LA-12503-MS.

Amsden, A. A., Butler, T. D., and O'Rourke, P. J. 1989. "KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays," Los Alamos National Laboratory report LA-11560-MS.

Abdel-Gayed, R. G., and Bradley, D. 1977. "Dependence of Turbulent Burning Velocity on Turbulent Reynolds Number and Ratio of Laminar Burning Velocity to RMS Turbulent Velocity," Sixteenth Symposium on Combustion, The Combustion Institute, pp. 1725.

Hessel, R. P. 1993. "Numerical Simulation of Valved Intake Port and In-Cylinder Flows Using KIVA-3," Ph.D. Thesis, University of Wisconsin, Madison, Prof. C. J. Rutland advisor.

Johnson, N. L., Amsden, A. A., Naber, J. D., and Siebers, D. L. 1995. "Three-Dimensional Computer Modeling of Hydrogen Injection and Combustion," Transaction paper for the '95 High Performance Computing Conference, edited by Adrian Tentner, pp. 61–69. Published by the Society for Computer Simulation.

Magnussen, B. F., and Hjertager, B. H. 1977. Sixteenth Symposium on Combustion, The Combustion Institute, pp. 719–729.

Meier, F., Köhler, J., Stolz, W., Bloss, W. H., and Al-Garni, M. 1994. "Cycle-Resolved Hydrogen Flame Speed Measurements with High Speed Schlieren in a Hydrogen Direct Injection SI Engine," SAE Fuels and Lubricants Meeting and Expositions, #942036.

Smith, J. R., Aceves, S. April 1995. "Hybrid Vehicles Studies and Optimized Engine Design," Lawrence Livermore National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Van Blarigan, P. April 1995. "Hydrogen Hybrid Vehicle Engine Development: Experimental Program, Sandia National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Westbrook, C. K. September 1994. Hydrogen Program Progress Report as submitted to Neil Rossmeissl.

Westbrook, C. K. April 1995. "Chemical Kinetics of Hydrogen," Lawrence Livermore National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Figure Captions

Figure 1. The mesh for the intake flow problem through two valves as examined by Hessel. The two separate valve manifold combine into one large manifold. The two exhaust ports are not modeled.

Figure 2. The mesh for the Onan engine showing the entire perspective view at the top and a cut though the symmetry plane at the bottom. In the lower figure, the inlet valve is on the right, shown at its full open position, and the exhaust valve is on the left, shown closed .

Figure 3. The velocity in the intake valve gap as a function of the pressure drop across the valve.

Figure 4. The velocity vector field when the intake valve is fully open for the Onan engine. The square valve representation is on the left. The peak velocity is 41 percent higher in the more refined valve model on the right.

Figure 5. Pressure histories averaged over the cylinder after intake valve closing.

Figure 6. Temperature histories averaged over the cylinder after intake valve closing.

Figure 7. H_2 mass in the cylinder during combustion.

Figure 8. NO_x production in the cylinder during combustion.

Figure 9. Total bulk-flow kinetic energy averaged over the cylinder.

Figure 10. Total turbulent kinetic energy averaged over the cylinder.