8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

A Reynolds-Averaged Navier Stokes solver coupled to accurate thermodynamic and transport property models.

*** S. Rebay[1], D. Pasquale[1], J. Harinck[2] and P. Colonna[2]**

[1] Università di Brescia
Dip. di Ingegneria Meccanica
Via Branze, 38, 25123
Brescia, Italy
E-mail rebay@ing.unibs.it

[1]Delft University of Technology
Energy Technology Section
Process and Energy Dept.
Leeghwaterstraat 44
2628 CA Delft
The Netherlands
www.et.3me.tudelft.nl

Key Words: *CFD, transport property model, thermodynamic model, dense-gas.*

ABSTRACT

zFlow is a CFD computer code linked to the FluidProp library, which allows for the accurate evaluation of thermodynamic and transport properties of a large variety of fluids and fluid mixtures. *FluidProp* implements several thermodynamic models, ranging from comparatively simple cubic equation of states (CEOS) to highly-accurate state-of-the-art multiparameter equations of state (MEOS). The code capabilities were recently extended to include the numerical solution of the Reynolds-averaged compressible Navier-Stokes (RANS) equations coupled with a realizable k-ω turbulence model [1]. *zFlow* is therefore suitable for the simulation of flows of dense gases in industrial processes and as such it can be considered a fluid dynamic design tool.

To improve the accuracy and robustness of the code, a non standard implementation of the k-ω model is adopted. First of all, the logarithm of ω is used as independent variable, instead of ω. This improves the accuracy of the simulations, since the variation of $\widetilde{\omega} = \log(\omega)$ across the boundary layer is much smoother than that of ω. In order to improve the robustness of the code, the admissible values of the predicted eddy viscosity are limited so as to fulfill to the realizability constraints. Fur further details, see e.g. Ref. [1].

The equations are discretized in space with a finite-element/finite-volume method suitable for general unstructured hybrid grids [2,3]. The advective terms are discretized with an upwind TVD scheme, generalized to the case of fluids governed by arbitrary equations of state following the approach introduced by Vinokur and Montagné [5]. Both explicit and implicit Runge-Kutta time stepping methods are available. Significant gains in computational efficiency are obtained by adopting implicit time integration schemes in steady state computations, especially for fluids characterized by complex models for the calculation of the thermodynamic and transport properties.

CFD solvers for viscous flows commonly compute the transport properties of the fluid by means of simple models, which are valid only in the dilute-gas region. An example is the Sutherland's law or Power

law for the viscosity. In this case the thermal conductivity is obtained by assuming a constant Prandtl number, which directly relates thermal conductivity to viscosity. Transport property models which are also accurate in the dense gas region are possibly needed in order to accurately simulate flows occurring in this thermodynamic region. Several of such transport models are documented in the literature. The Chung model [6] for viscosity and thermal conductivity is based on kinetic theory. It is an explicit method, valid for nonpolar, polar and associating fluids over a wide range of PVT states, including the dense gas region. The TRAPP model [7] is an implicit method based on the extended corresponding states model and therefore requires a reference fluid. Both models are available in *FluidProp*.

The criteria for selecting a proper transport property model are mainly accuracy and computational cost. For many classes of fluids no experimental data in the vapor phase are available and this prevents from estimating the accuracy of the transport property models in this region. A transport property model with reliable extrapolation behavior is therefore imperative. In that sense, the TRAPP method is not reliable, as it requires many data to fit the parameters of the model. In case limited transport property data are available, the TRAPP method has a poor accuracy and convergence behavior near the critical region. The Chung model on the other hand has good predictive features and its explicit formulation rules out any convergence problem. The Chung model is therefore chosen as the transport property model in the exemplary simulations presented here, in which a siloxane is the working fluid.

To be able to accurately simulate flows also in the dense-gas region, the RANS solver is generalized to density-dependent transport property models. First of all, the evaluation of viscosity and thermal conductivity are uncoupled. Secondly, partial derivatives of viscosity and thermal conductivity with respect to temperature and density are derived and implemented, as they are required in the diffusion term of the generalized version of the RANS equations and in the k-ω turbulence model. The correctness of the implementation is verified by comparing the results of the derived derivatives to the numerically obtained ones.

The correct generalization of the RANS solver and implementation of the Chung model is validated by computing two classical test cases, namely the turbulent boundary layer along the flat plate and the transonic flow around the RAE2822 airfoil. Test cases of flows occurring in the dense gas thermodynamic region are not available, therefore the computations, which rely on real-gas property models employed for ideal-gas conditions, validate the correct implementation. The simulation of the flow through a stator cascade of an organic Rankine cycle turbogenerator is presented as an example of the capabilities of the code.

REFERENCES

[1] F. Bassi, A. Crivellini, S. Rebay, and M. Savini, Discontinuous Galerkin solution of the Reynolds Averaged Navier-Stokes and k-ω turbulence model equations, *Computers & Fluids* **34, 4-5**, 507–540, 2005.

[2] V. Selmin, The node-centered finite volume approach: bridge between finite differences and finite elements, *Comput. Methods Appl. Mech. Eng.*, **102**, 107–138, 1993.

[3] P. Colonna, and S. Rebay, Numerical simulation of dense gas flows on unstructured grids with an implicit high resolution upwind Euler solver, *Int. J. Numer. Meth. Fluids* **46, 7**, 735–765, 2004.

[4] S. Davis, TVD finite difference schemes and artificial viscosity, Technical Report, NASA Langley Research Center, 1984.

[5] M. Vinokur and J.L. Montagné, Generalized Flux-Vector Splitting and Roe Average for an Equilibrium Real Gas, *J. Comput. Phys.*, **89, 2** 276–300, 1990.

[6] T. Chung, M. Ajlan, L.L. Lee, and K.E. Starling, Generalized multiparameter correlation for non-polar and polar fluid transport properties, *Ind. Eng. Chem. Res.*, **27**, 671–679, 1988.

[7] J. Ely and H. Hanley, Prediction of transport properties. 1. Viscosity of fluids and mixtures, *Ind. Eng. Chem. Fund.*, **20**, 323–332, 1981.