INERT AND REACTING FLOWS WITH A NEW CUBIC EDDY-VISCOSITY MODEL

Bart Merci
Department of Flow, Heat and Combustion Mechanics, Ghent University
Sint-Pietersnieuwstraat 41, B-9000 GENT, Belgium
Bart.Merci@rug.ac.be

Chris De Langhe, Jan Vierendeels and Erik Dick
Department of Flow, Heat and Combustion Mechanics, Ghent University
Chris.DeLanghe@rug.ac.be, Jan.Vierendeels@rug.ac.be, Erik.Dick@rug.ac.be

Dirk Roekaerts
Faculty of Applied Sciences, Delft University of Technology, The Netherlands
dirkr@ws.tn.tudelft.nl

ABSTRACT

A third-order expression of the Reynolds stresses as a function of the local strain rate and vorticity, is developed. Anisotropies in the normal stresses, streamline curvature, rotation of the reference frame, and swirl are accounted for. The relationship is linked to a $k-\varepsilon$ model, with a modified ε-equation. A new low-Reynolds source term is introduced and a model parameter is written in terms of dimensionless strain rate and vorticity. The model is applied to a stationary and rotating fully developed channel and pipe flow, to the flow over a backward-facing step and to a piloted jet diffusion flame. A comparison is made with results from the linear $k-\varepsilon$ model due to Yang and Shih (1993) and Menter's shear stress transport model (Menter, 1994).

INTRODUCTION

Extensive application of linear eddy-viscosity models has revealed a number of deficiencies, as reported by Hanjalic (1999). Firstly, they are insensitive to the anisotropy of normal Reynolds stresses. Secondly, they cannot account for effects from extra strain, such as due to streamline curvature, swirl or rotation. Thirdly, the mathematical concept of realizability is violated under certain circumstances. Finally, there is the limitation of the algebraic stress-strain relationship. Apart from the latter, the mentioned shortcomings can be cured by the use of a non-linear stress-strain relationship ('constitutive law'). The approach of the non-linear eddy-viscosity is followed, as suggested by Pope (1975). Different models can already be found in the literature (e.g. Craft, 1996, Shih et al., 1993). However, they do not properly account for rotation effects, as pointed out by Speziale (1998). A new third order expression is presented, which does have a physically more correct behaviour. The coefficients in the expression are determined on the basis of some basic flows (fully developed stationary and rotating channel and pipe flow).

The application of the non-linear constitutive law requires accurate values for the turbulence quantities. In the presented model, the turbulence kinetic energy k and the dissipation rate ε are used. The transport equation for ε is modified to that purpose. The combination of the non-linear constitutive law with the improved ε equation leads to accurate results, as will be illustrated for the flows mentioned in the abstract.

A more elaborate development of the described turbulence model, as well as a discussion on the realizability of the model, can be found elsewhere (Merci, 2000, Merci, 2001).

DEVELOPMENT OF THE MODEL

Constitutive law

The constitutive law is constructed for the anisotropy tensor a_{ij}:

$$a_{ij} = \frac{\widetilde{v"_i v"_j}}{k} - \frac{2}{3}\delta_{ij} \qquad (1)$$

The Favre averages ($\sim$), used for reacting flows, are replaced by Reynolds averages for inert flows. The averaging symbols are omitted from now on.

The following cubic relationship is proposed:

$$\begin{aligned} a_{ij} &= -2f_\mu c_\mu \tau_t S_{ij} \\ &+ q_1\tau_t^2(S_{ik}S_{kj} - \frac{1}{3}\delta_{ij}S_{lm}S_{ml}) \\ &+ (q_2 + q_1/6)\tau_t^2(\Omega_{ik}S_{kj} - S_{ik}\Omega_{kj}) \\ &+ \tau_t^3(c_1 S_{mn}S_{nm} + c_2\Omega_{mn}\Omega_{nm})S_{ij} \\ &+ c_3\tau_t^3(\Omega_{ik}S_{kl}S_{lj} - S_{ik}S_{kl}\Omega_{lj}) \end{aligned} \quad (2)$$

where S_{ij} and Ω_{ij} are defined in a non-inertial reference frame as:

$$S_{ij} = \left[\frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}) - \frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k}\right] \quad (3)$$

$$\Omega_{ij} = \left[\frac{1}{2}(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}) - C_\Omega \varepsilon_{ijk}\Omega_k\right] \quad (4)$$

In expression (2), τ_t is the turbulence time scale, defined as:

$$\tau_t = \frac{k}{\varepsilon} + \sqrt{\frac{\mu}{\rho\varepsilon}} \quad (5)$$

In (4), ε_{ijk} is the permutation tensor and Ω_k is the rotation speed of the reference frame with respect to the k-direction of an inertial frame. A specific value for C_Ω has been determined by Jongen and Gatski (1998), namely $C_\Omega = 2.25$. Though this value is model dependent, it is appropriate for the presented model, as illustrated in fig. 3.

The coefficients c_μ, q_i and c_i are functions of the dimensionless strain rate

$$S' = \tau_t(2S_{ij}S_{ij})^{1/2} \quad (6)$$

and the dimensionless vorticity

$$\Omega' = \tau_t(2\Omega_{ij}\Omega_{ij})^{1/2} \quad (7)$$

Typically, the maximum is taken:

$$\eta = max(S', \Omega') \quad (8)$$

The coefficient c_μ is based on the expression from Shih *et al.* (1995):

$$c_\mu = \frac{1}{A + \sqrt{3}cos(\phi)\eta} \quad (9)$$

where $\phi = \frac{1}{3}arccos(\sqrt{6}\ W)$, with W defined as:

$$W = 2^{1.5}\tau_t^3\frac{S_{ij}S_{jk}S_{ki}}{S'^3} \quad (10)$$

Expression (9) has been chosen with respect to realizability, since it provides the correct limiting behaviour for both two-dimensional and axisymmetric, purely accelerating flows. Also for the sake of realizability, the coefficients of the higher order terms are such that they become zero for high values of S' and/or Ω'. The value for A is $A = 8$. It has been determined on the basis of DNS data from Kim *et al.* (1987) for a fully developed channel and from Eggels *et al.* (1994) for a fully developed pipe flow.

The coefficients q_1 and q_2 are given by:

$$\begin{cases} q_1 = (7 + 3\eta + 1.2\ 10^{-2}\eta^3)^{-1} \\ q_2 = (21 + 23.2\eta + 4.6\ 10^{-2}\eta^3)^{-1} \end{cases} \quad (11)$$

Note that there is no quadratic vorticity term in expression (2), as it should be, as pointed out by Speziale (1998). Many of the current non-linear eddy-viscosity models violate this restriction.

The coefficients c_1 and c_2 are determined on the basis of the fully developed flow in a rotating channel, studied by means of DNS by Kristoffersen *et al.*(1993). This cubic term accounts for the effect from reference frame rotation or streamline curvature on turbulence. The coefficients are chosen to be equal:

$$c_1 = c_2 \quad (12)$$

Their expression is:

$$\begin{cases} S' \geq \Omega' : c_1 = -600c_\mu^4 \\ S' < \Omega' : c_1 = -min(600c_\mu^4; \frac{4f_\mu c_\mu}{(\Omega'^2 - S'^2)}) \end{cases} \quad (13)$$

The choice of c_μ^4 ensures that the third order term vanishes for S' or $\Omega' \to \infty$. The factor 600 has been chosen from numerical optimisation. The second argument is introduced in (13) when $S' < \Omega'$ in order to avoid a negative eddy-viscosity: closer inspection of eq. (2) reveals that the term premultiplied by c_1 can be lumped into the first order term, yielding an effective eddy-viscosity of

$$\mu_t = \rho(f_\mu c_\mu - c_1(S'^2 - \Omega'^2)/4)k\tau_t \quad (14)$$

The eddy-viscosity can become negative if $S' < \Omega'$, resulting in numerical problems. Therefore, the minimum is taken in (13).

The term premultiplied by c_3 accounts for effects from swirl on turbulence. The coefficient c_3 is determined on the basis of the fully developed flow in a swirling pipe, studied experimentally by Imao *et al.* (1996). The result is:

$$c_3 = -2c_1 \quad (15)$$

Finally, f_μ is a damping function, defined as $f_\mu = 1. - exp(-4.2\ 10^{-2}\sqrt{R_y} - 5.1\ 10^{-4}R_y^{1.5} - 3.65\ 10^{-10}R_y^5)$, with $R_y = \frac{\rho\sqrt{k}y}{\mu}$, y being the normal distance from the nearest solid boundary.

Transport equations

Eq. (2) is used in combination with a $k-\varepsilon$ model in low-Reynolds formulation:

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_k}(\rho k v_k) = \tau_{ik}^T \frac{\partial v_k}{\partial x_i} - \rho\varepsilon \\ \quad + \frac{\partial}{\partial x_k}[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_k}] - \frac{\mu_t}{\rho^2}\frac{\partial \rho}{\partial x_i}\frac{\partial p}{\partial x_i} \\ \frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_k}(\rho\varepsilon v_k) = \\ (c_{\varepsilon 1}\tau_{ik}^T \frac{\partial v_k}{\partial x_i} - c_{\varepsilon 2} f_2 \rho\varepsilon - c_{\varepsilon 3}\frac{\mu_t}{\rho^2}\frac{\partial \rho}{\partial x_i}\frac{\partial p}{\partial x_i})\frac{1}{\tau_t} \\ \quad + \frac{\partial}{\partial x_k}[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_k}] + E \end{array} \right. \quad (16)$$

In (16), τ_{ik}^T is the Reynolds stress $\tau_{ik}^T = -\rho\widetilde{v"_i v"_k}$. The last term in the equation for k and the term premultiplied by $c_{\varepsilon 3} = 1$ account for variable density effects. The other model constants are $c_{\varepsilon 1} = 1.44$, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.3$. The function f_2 is defined as $f_2 = 1 - 0.22exp(-\frac{Re_t^2}{36})$, with $Re_t = \frac{\rho k \tau_t}{\mu}$, as suggested by Hanjalic and Launder (1976). The model parameter $c_{\varepsilon 2}$ is defined as:

$$c_{\varepsilon 2} = 1.83 + \frac{0.075\Omega"}{1 + S'^2} \quad (17)$$

where $\Omega" = (2\Omega"_{ij}\Omega"_{ij})^{1/2}$, with $\Omega"$ the dimensionless absolute vorticity:

$$\Omega"_{ij} = \tau_t \left[\frac{1}{2}(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}) - \varepsilon_{ijk}\Omega_k\right] \quad (18)$$

Thus, the necessary dependence on rotation is brought into the ε-equation correctly, as pointed out by Speziale *et al.* (1998). Many turbulence models do not contain this correct rotation dependence. Moreover, both stationary (Hallbäck *et al.*, 1995) and rotating (Bardina *et al.*, 1985) homogeneous decaying turbulence are adequately described thanks to (17). The denominator in (17) has a damping effect in regions with high rates of strain.

The low-Reynolds source term E is found by transforming the standard $k-\omega$ model by Wilcox (1993) into a $k-\varepsilon$ formulation. The $k-\omega$ model is known to perform well near solid walls and in adverse pressure gradient flows. The transformation is done, using the relation $\varepsilon = c_\mu \omega k$. The result is:

$$E \ = \ -1.8(1 - f_\mu)(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial k}{\partial x_i}\frac{\partial \tau_t^{-1}}{\partial x_i} \quad (19)$$

The factor $(1-f_\mu)$ assures that E is only active near solid boundaries. The factor 1.8 has been chosen by numerical optimisation.

Reacting flows

The 'conserved scalar' is followed, with a pre-assumed β-PDF. The standard transport equations are used for the mean mixture fraction ξ and its variance g:

$$\left\{ \begin{array}{l} \frac{\partial}{\partial x_j}(\rho\xi v_j) = \frac{\partial}{\partial x_j}[(\rho D + \frac{\mu_t}{\sigma_\xi})\frac{\partial \xi}{\partial x_j}] \\ \frac{\partial}{\partial x_j}(\rho g v_j) = \frac{\partial}{\partial x_j}[(\rho D + \frac{\mu_t}{\sigma_g})\frac{\partial g}{\partial x_j}] \\ \quad + 2\frac{\mu_t}{\sigma_\xi}\frac{\partial \xi}{\partial x_j}\frac{\partial \xi}{\partial x_j} - c_g \rho g \frac{1}{\tau_t} \end{array} \right. \quad (20)$$

where g is the mixture fraction variance: $g = \widetilde{\xi"^2}$. The model constants are $\sigma_\xi = \sigma_g = 0.7$ and $c_g = 2$.

The averaged thermochemical quantities are calculated a priori and stored in a table. The tabulation and look-up program FLAME is due to Peeters (1995). Radiation is neglected.

APPLICATIONS

The presented model is referred to as the 'cubic model'. Comparisons are made with results from the linear Yang-Shih model ('YS') and Menter's linear 'SST' model.

Fully developed channel and pipe flow

Fig. 1 shows the mean velocity profile for the fully developed channel flow, studied by Kim *et al.* (1987). The Reynolds number based on the mean velocity and half the channel height is $Re = 7890$. The YS model provides a perfect profile: this model has been tuned for this flow. The SST model is relatively the poorest. The cubic $k-\varepsilon$ model has the correct behaviour (in particular the correct slope in the logarithmic region). There is a slight overprediction (less than 5%).

Fig. 2 shows the mean velocity profile for the fully developed flow in a pipe, studied by Eggels *et al.* (1994). The Reynolds number based on the center line velocity and the pipe diameter is $Re = 6950$. The YS model does not provide a perfect profile any more. With respect to this, the overprediction by the cubic model in fig. 1 is a compromise: the mean velocity for the pipe flow is less underpredicted by the cubic model than by both linear models. Again, the SST model is relatively the worst.

Rotating channel flow

Fig. 3 shows the mean axial velocity for the rotating channel flow, studied with DNS

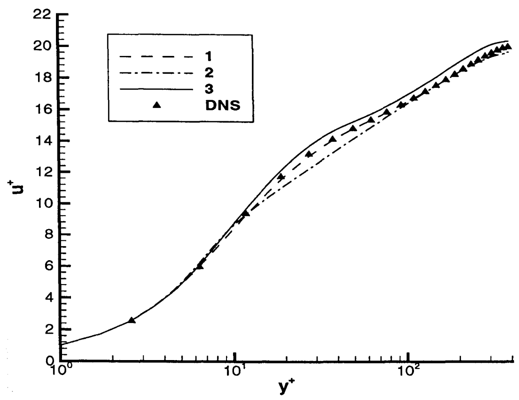

Figure 1: Mean velocity for fully developed channel flow. (1: YS; 2: SST; 3: cubic model)

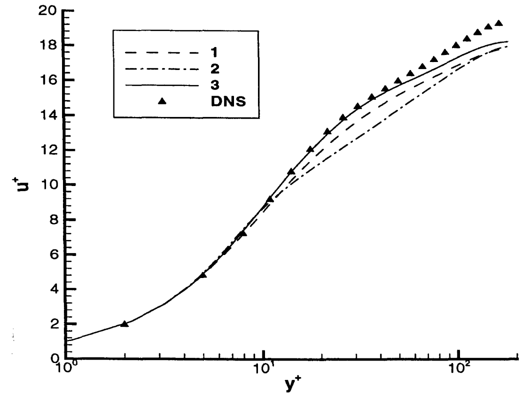

Figure 2: Mean velocity for for fully developed pipe flow. (1-3: see fig. 1)

by Kristoffersen *et al.* (1993). The Reynolds number based on half the channel width h and the bulk velocity U_m is $Re = 2900$. Profiles are shown for $Ro = 2|\Omega|h/U_m = 0$ and $Ro = 0.5$. The linear models are not able to describe the influence from the rotation on the flow field: the same result is produced for both rotation numbers. The cubic model does have the correct tendency: an increase of the mean velocity is observed at the suction side, and a decrease at the pressure side. The slope in the middle region of the channel is in accordance with the DNS data, too.

Rotating pipe flow

Fig. 4 shows the mean tangential velocity component W for the flow in a swirling pipe, studied experimentally by Imao *et al.* (1996). The Reynolds number based on the pipe diameter and the mean velocity U_m is $Re = 20000$.

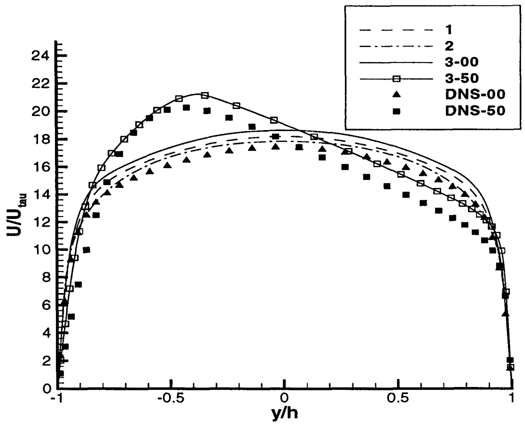

Figure 3: Mean axial velocity for rotating channel flow ($Ro = 0$ and $Ro = 0.50$). (1-3: see fig. 1)

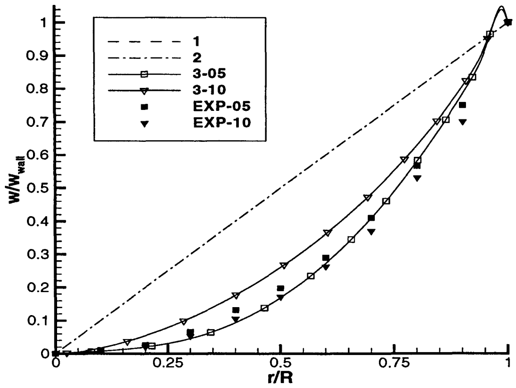

Figure 4: Mean tangential velocity for rotating pipe flow ($N = 0.5$ and $N = 1.0$). (1-3: see fig. 1)

Profiles are shown for $N = W_{wall}/U_m = 0.5$ and $N = 1$. The linear models are unable to capture any swirl effect: the only effect of the pipe rotation is a solid body rotation, superposed on the axial flow. The tangential velocity component increases linearly from the symmetry axis towards the wall. The experiments indicate a more or less parabolic profile, quite well represented by the cubic model.

Backward-facing step flow

Fig. 5 shows the evolution of the friction coefficient c_f for the flow over a backward-facing step, studied by means of DNS by Le *et al.* (1997). The recirculation length l_r is underpredicted by the YS model, while further downstream c_f is overpredicted. Both phenomena are due to an overprediction of the turbulence kinetic energy k. The SST model predicts l_r very well, but underpredicts c_f downstream,

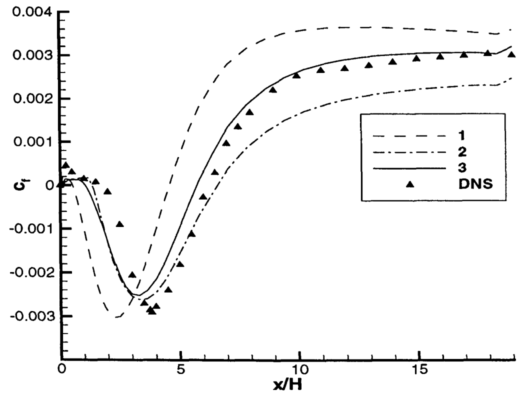

Figure 5: Friction coefficient for the BFS flow. (1-3: see fig. 1)

due to an underprediction of k. Clearly, the cubic model yields the best results. In the recirculation zone, the cubic constitutive law accounts for the stabilization effect of the streamline curvature, while downstream the modified ε-equation yields more accurate values for k.

Jet diffusion flame

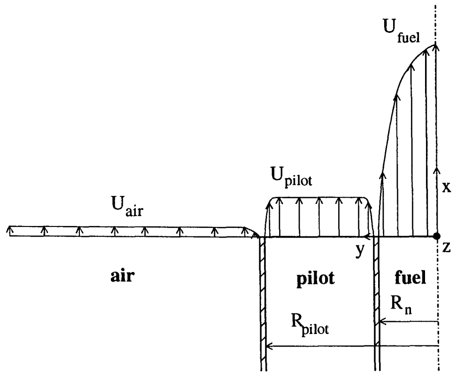

Figure 6: Geometry for the piloted flame.

Figs. 7 and 8 show results for a piloted diffusion flame ('flame D'), studied experimentally by Barlow *et al.* (1998), and numerically in a series of workshops (web, 2000). The geometry is depicted in fig. 6. A simplified version of the constrained equilibrium model by Bilger and Starner (1983) is used as chemistry model.

The profile of the mean mixture fraction ξ on the axis (fig. 7) is best predicted by the cubic model. In particular the position of stoichiometric conditions ($\xi = 0.351$) is predicted correctly. This results in globally better axial profiles, as shown by Merci (2000). Fig. 8, showing the radial profile of the square root of the variance g at $x/D_n = 45$, illustrates the better quality by the cubic model again. Other radial profiles are better for the cubic model, too, as shown by Merci (Merci, 2000).

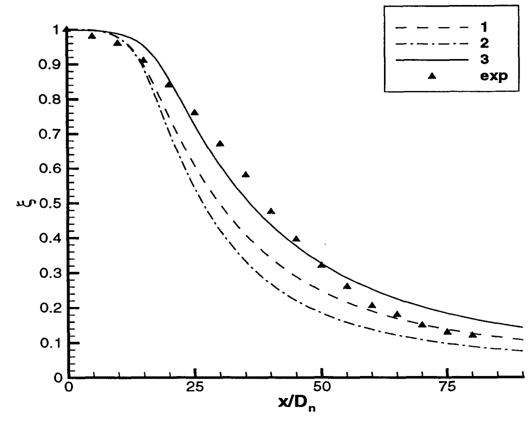

Figure 7: Mean mixture fraction along the symmetry axis for flame D. (1-3: see fig. 1)

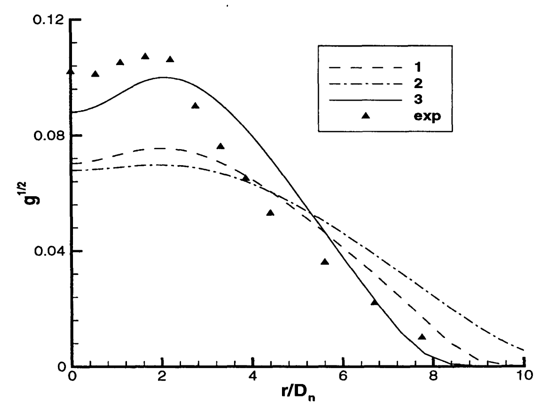

Figure 8: Radial profile ($x/D_n = 45$) of the rms value of the mixture fraction variance for flame D. (1-3: see fig. 1)

CONCLUSIONS

A new eddy-viscosity model has been presented. It combines a cubic constitutive law (2) with a low-Reynolds $k - \varepsilon$ model, in which the ε-equation has been modified (rotation dependence is introduced, together with a new low-Reynolds source term). The model yields accurate results, both for inert and reacting flows, while the computational time and memory requirements remain comparable to linear two-equation models.

ACKNOWLEDGMENTS

The first author works as Research Assistant of the Fund for Scientific Research - Flanders (Belgium) (FWO). The authors thank T.W.J. Peeters (Corus Group, The Netherlands) for his help and the tabulation program FLAME.

REFERENCES

Bardina, J., Ferziger, J.H., and Rogallo, R.S., 1985, "Effect of Rotation on Isotropic Turbulence: Computation and Modelling", *Journal of Fluid Mechanics*, Vol. 154, pp. 321-336.

Barlow, R.S, and Frank, J.H., 1998, "Effects of Turbulence on Species Mass Fractions in Methane/Air Jet Flames," *Proceedings, 27th Symposium (Int.) on Combustion*, The Combustion Institute, ed., Pittsburgh, pp. 1087-1095.

Bilger, R.W., and Starner, S.H., 1983, "A Simple Model for Carbon Monoxide in Laminar and Turbulent Hydrocarbon Diffusion Flames", *Combustion and Flame*, Vol. 51, pp. 155-176.

Craft, T.J., Launder, B.E., and Suga, K., 1996, "Development and Application of a Cubic Eddy-Viscosity Model of Turbulence", *International Journal of Heat and Fluid Flow*, Vol. 17, pp. 108-115.

Eggels, J.G.M., Unger, F., Weiss, M.H., Westerweel, J., Adrian, R.J., Friedrich, R., and Nieuwstadt. F.T.M., 1994, "Fully Developed Turbulent Pipe Flow: a Comparison between Direct Numerical Simulation and Experiment", *Journal of Fluid Mechanics*, Vol. 268, pp. 175-209.

Hallbäck, M., Henningson, D.S., Johansson, A.V., and Alfredsson, P.H., 1995, *Turbulence and Transition Modelling.* Springer-Verlag, Berlin.

Hanjalic, K., and Launder, B.E., 1976, "Contribution towards a Reynolds-Stress Closure for Low-Reynolds-Number Turbulence", *Journal of Fluid Mechanics*, Vol. 74, pp. 593-610.

Hanjalic, K., 1999, "Second-Moment Turbulence Closures for CFD: Needs and Prospects", *Int. Journal for Computational Fluid Dynamics*, Vol. 12, pp. 67-97.

Imao, S., Itoh, M., and Harada, T., 1996, "Turbulent Characteristics of the Flow in an Axially Rotating Pipe", *International Journal of Heat and Fluid Flow*, Vol. 17, pp. 444-451.

Jongen, T., Machiels, L., and Gatski, T.B., 1998, "Predicting Noninertial Effects with Linear and Nonlinear Eddy-Viscosity and Algebraic Stress Models", *Flow, Turbulence and Combustion*, Vol. 60, pp. 215-234.

Kim, J., Moin, P., and Moser, R., 1987, "Turbulence Statistics in Fully Developed Channel Flow at Low Reynolds Number", *Journal of Fluid Mechanics*, Vol. 177, pp. 133-166.

Kristoffersen, R., and Andersson, H.I., 1993, "Direct Simulations of Low-Reynolds-Number Turbulent Flow in a Rotating Channel", *Journal of Fluid Mechanics*, Vol. 256, pp. 163-197.

Le, H., Moin, P., and Kim, J., 1997, "Direct Numerical Simulation of Turbulent Flow over a Backward-Facing Step", *Journal of Fluid Mechanics*, Vol. 330, pp. 349-374.

Menter, F.R., 1994, "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications", *AIAA Journal*, Vol. 32(8), pp.1598-1605.

Merci, B., 2000, *Numerical Simulation and Modelling of Turbulent Combustion.* Ph.D. thesis, Ghent University, Belgium.

Merci, B., De Langhe, C., Vierendeels, J., and Dick, E., 2001, "A Quasi-Realizable Cubic Low-Reynolds Eddy-Viscosity Turbulence Model with a New Dissipation Rate Equation", *Flow, Turbulence and Combustion* (submitted).

Peeters, T., 1995, "Flame: A Fortran Program for Tabulation of Thermochemical Variables using Simplified Chemistry Models", Technical report, TU Delft, The Netherlands.

Pope, S.B., 1975, "A More General Effective-Viscosity Hypothesis", *Journal of Fluid Mechanics*, Vol. 72, pp. 331-340.

Shih, T.H., Zhu, J., and Lumley, J.L., 1993, "A Realizable Reynolds Stress Algebraic Equation Model", Technical Report TM 105993, NASA.

Shih, T.H., Liou, W.W., Shabbir, A., Yang, Z., and Zhu, J., 1995, "A New $k-\varepsilon$ Eddy Viscosity Model for High Reynolds Number Turbulent Flows", *Computers and Fluids*, Vol. 23(3), pp. 227-238.

Speziale, C.G., Younis, B.A., Rubinstein, R., and Zhou, Y., 1998, "On Consistency Conditions for Rotating Turbulent Flows", *Physics of Fluids*, Vol. 10(8), pp. 2108-2110.

Speziale, C.G., 1998, "A Consistency Condition for Non-Linear Algebraic Reynolds Stress Models in Turbulence", *Int. Journal of Non-Linear Mechanics*, Vol. 33(4), pp. 579-584.

web, 2000, www.ca.sandia.gov/tdf/Workshop

Wilcox, D.C., 1993, *Turbulence Modeling for CFD.* Griffin Printing, Glendale, California.

Yang, Z.Y., and Shih, T.H., 1993, "A New Time Scale Based $k-\epsilon$ Model for Near-Wall Turbulence", *AIAA Journal*, Vol. 31(7), pp. 1191-1198.