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Application of Quadratic Constitutive Relation to One-Equation k-kL Turbulence Model

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This paper analyzes the accuracy of the recently developed one-equation k-kL turbulence model with Quadratic Constitutive Relation (QCR) compared to the linear Boussinesq relation and Algebraic Reynolds Stress Model (ARSM). The computational results in several benchmark cases from NASA TMR are compared to other widely used one equation turbulence models with QCR, such as Spalart-Allmaras model (SA), Wray-Agarwal model (WA) and SST *k-ω* model. In particular, one-equation k-kL-QCR model shows good accuracy with experimental data for supersonic flow in a square duct where the effect of QCR is clearly visible in capturing the secondary flow vortices which is not feasible with the any standard model without QCR. In addition, both one-equation k-kL and one-equation k-kL-QCR models show better accuracy for subsonic separated flow in 3D NASA Glenn S-duct compared to other one-equation models. Other test cases show little difference in the results obtained without and with QCR.

Nomenclature

C_f	=	skin friction coefficient
C_p	=	pressure coefficient
P	=	production of turbulent kinetic energy
L_{vk}	=	von Kármán length scale
Re	=	Reynolds number
Re_τ	=	friction Reynolds number
S	=	mean strain rate magnitude
W	=	vorticity magnitude
d	=	distance normal to the nearest wall
k	=	turbulent kinetic energy
kL	=	turbulent kinetic energy x length scale
t	=	time
y	=	Cartesian coordinate
κ	=	Karman constant
ν	=	kinematic viscosity
μ_t	=	turbulent eddy viscosity
ρ	=	density

I. Introduction

Solving the Reynolds Averaged Navier-Stokes (RANS) equations with a turbulence model is still the standard practice in industry for prediction of turbulent flows. Considering with both the cost and accuracy of simulations, one-equation and two-equation turbulence models are most frequently used. The wide application of Spalart-Allmaras model (SA) found in most commercial CFD codes has illustrated the potential of one-equation models for

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computing wide variety of flows in many industries. Among the one-equation models, the recently proposed Wray-Agarwal model has shown some improvement over the SA model in large number of applications with mildly separated wall bounded flows, flows with rotation and curvature and high temperature effects [1]. Recently proposed one-equation k-kL model [2] is based on the two-equation k-kL model [3] following the method of derivation for one-equation k-ε model from Menter et al [4]. Shuai and Agarwal [2] have shown that one-equation k-kL model has the ability to predict the separation and reattachment charateristcs of flow over a backward-facing step and flow past a 2D NASA hump, but did not verify its ability in computing 3D flows with small regions of separation.

When applying linear eddy viscosity models with Boussineq assumption, these models appears to lack capability for prediction of vortical flows and wall bounded flows with mild separation. To improve on some shortcomings of linear Boussineq relation, the use of nonlinear Quadratic Constitutive Relation for turbulent eddy viscosity [5] and Explicit Algebraic Reynolds Stress Modeling (ARSM) have been proposed [6]. Nagapetyan et al. have implemented QCR with WA model and has shown that WA-QCR can accurately compute the supersonic flow in a square duct which is not feasible without QCR [7]. Following the development of two–equation k-kL-ARSM model by Abdol-Hamid [8], Wen and Agarwal [9] proposed the one-equation k-kL-ARSM model and showed that the inclusion of higher order Reynolds stress terms can improve the for prediction of many wall bounded flows in several cases except for supersonic flow in a square duct.

In this paper, the influence of QCR is investigated by implementing it in one-equation k-kL model. The one-equation k-kL-QCR, one-equation k-kL-ARSM and one-equation k-kL model are employed to compute supersonic flow in a square duct. The computed results from one-equation k-kL-QCR, one-equation k-kL-ARSM and one-equation k-kL model are compared with the experimental data from from the paper of Davis and Gessner [10]. In addition, the results from one-equation k-kL-QCR are also compared with results from other one-equation QCR models namely the WA-QCR and SA-QCR models. The computations show that the application of QCR in one-equation k-kL model accurately predicts the supersonic flow in square duct and improves the accuracy of results compared to the results from one-equation k-kL and other one-equation and two-equation models without QCR. One equation k-kL-QCR does produce results of comparable accuracy as SA-QCR and WA-QCR. In addition in this paper one-equation k-kL and one-equation k-kL-QCR models are implemented to predict the flow in 3D NASA Glenn S-Duct and the results are compared with the experimental data from Ref. [12] and computations using other models namely the WA, SA and SST *k-ω* models. The results for S-Duct flow field show that both one-equation k-kL and one-equation k-kL-QCR model have the best agreement with experimental data compared to all other models except WA model. Also, one equation k-kL QCR shows slightly better improvement in prediction of S-Duct flow field compared to one equation k-kL model. Several other benchmark test cases from NASA TMR [11] e.g. flow over a hump, flow in an asymmetric diffuser and flow over a backward facing steps were also calculated but they showed little difference between reults without and with QCR.

II. One-Equation k-kL Turbulence Model

The one-equation k-kL turbulence model was recently proposed by Shuai and Agarwal [4]. This model has basic underlying characteristics of two-equation k-kL model but has been shown to be more accurate than SA model and at least as accurate as the two-equation k-kL model and SST k-ω model for many bemchmark test cases from NASA TMR [11]. Details of the derivation of one-equation k-kL model are given by Shuai and Agarwal [4]. It results into the following equation for kinematic turbulent eddy viscosity:

$$\frac{D\nu_t}{Dt} = a_1\left(C_{\phi 1} - \frac{1}{2}\right)\frac{P}{S} + \left(\frac{1}{2}a_1 - \frac{C_{\phi 2}}{\sqrt{a_1}}\right)\nu_t S + \frac{\nu\nu_t(1-6f_\phi)}{d^2} + \frac{\sigma}{2}\frac{\nu_t}{S}\frac{\partial \nu_t}{\partial x_i}\frac{\partial S}{\partial x_i} + \frac{3\sigma}{4}\frac{\partial \nu_t}{\partial x_i}\frac{\partial \nu_t}{\partial x_i} - \frac{\sigma}{4}\frac{\partial S}{\partial x_i}\frac{\partial S}{\partial x_i}\frac{{\nu_t}^2}{S^2} + \frac{\partial}{\partial x_i}\left((\sigma\nu_t + \nu)\frac{\partial \nu_t}{\partial x_i}\right) \quad (1)$$

$$P = \frac{\tau_{ij}}{\rho}\frac{\partial u_i}{\partial y}$$

$$\tau_{ij} = \mu_t\left(2S_{ij} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\rho\delta_{ij}$$

$$S_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial y} + \frac{\partial u_j}{\partial x})$$

$$C_{\phi 1} = (\zeta_1 - \zeta_2 \left(\frac{\sqrt{\nu_t}}{L_{vk}\sqrt{S}}\right)^2)$$

$$C_{\phi 2} = \zeta_3$$

$$L_{vk} = \kappa \left|\frac{U'}{U''}\right|$$

$$U' = \sqrt{2S_{ij}S_{ij}}$$

$$U'' = \sqrt{(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2})^2 + (\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2})^2 + (\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2})^2}$$

$$f_\phi = \frac{1 + C_{d1}\varepsilon}{1 + \varepsilon^4}$$

$$\varepsilon = \frac{d\sqrt{0.3\,\frac{\nu_t S}{a_1}}}{20\nu}$$

$$\zeta_2 = \zeta_1 - \frac{\zeta_3}{C_\mu^{\frac{3}{4}}} + \frac{\kappa^2\sigma}{C_\mu^{\frac{1}{2}}}$$

To avoid very large or small values of the von Karman length scale, the following limiter on L_{vk} is employed:

$$L_{vk,min} \leq L_{vk} \leq L_{vk,max} \tag{2}$$

$$L_{vk,max} = C_{12}\kappa d f_p$$

$$f_p = min[max\left(\frac{P}{\rho\nu_t S^2}, 0.5\right), 1.0]$$

$$L_{vk,min} = \frac{\sqrt{\nu_t}}{C_{11}\sqrt{S}}$$

The constants in the model are obtained as:

$$\zeta_1 = 1.5 \qquad \zeta_2 = 0.95 \qquad \zeta_3 = 0.16 \qquad \kappa = 0.41 \qquad a_1 = \sqrt{C_\mu} = 0.3$$
$$C_{11} = 10.0 \qquad C_{12} = 1.3 \qquad C_{d1} = 4.7 \qquad \sigma = 0.6$$

III. Quadratic Constitutive Relation (QCR)

The Quadratic Constitutive Relation (QCR) has been proposed by Spalart et al[5] to introduce nonlinear turbulent stress/strain relation in existing turbulence models.. The QCR relation employed in this paper has no effect on how one-equation k-kL turbulence model solves for the turbulent eddy viscosity, but alters the way turbulent stresses are calculated in the model. The traditional linear Boussinesq relation between stress and strain tensor is given by:

$$\tau_{ij} = 2\mu_t \left(S_{ij} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \right) - \frac{2}{3}\rho k \delta_{ij} \tag{3}$$

The QCR2000 version modifies Eq.(3) to the following nonlinear form:

$$\tau_{ijQCR} = \tau_{ij} - C_{cr1}\left[O_{ik}\tau_{jk} + O_{jk}\tau_{ik} \right] \tag{4}$$

$$O_{ik} = 2\, W_{ik} \Big/ \sqrt{\frac{\partial u_m}{\partial x_n}\frac{\partial u_m}{\partial x_n}}$$

$$W_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} - \frac{\partial u_k}{\partial x_i} \right)$$

where constant $C_{cr1} = 0.3$.

IV. Test Cases and Results

To verify the improved accuracy of the one-equation k-kL-QCR model compared to one-equation k-kL model , several benchmark cases from NASA TMR are computed. They are flow over a hump, flow over a backward facing step, flow inside an asymmetric plane diffuser , and supersonic flow in a square duct. It turns out that there is very small difference in computed results with and without QCR except in case of supersonic flow in a square duct where the details of the secondary flow vortices in the corners cannot be captured by any one and two equation turbulence model without QCR. For the supersonic flow in square duct, the predictions of one equation k-kL-QCR model are not only compared with one-equation k-kL model, one-equation k-kL-ARSM model [9] and experimental data [11] but are also compared with other QCR turbulence models, namely the WA-QCR model and SA-QCR model from Ref. [7]. In addition, one-equation k-kL and one-equation k-kL-QCR models are implemented to predict the flow in 3D NASA Glenn S-Duct and the results are compared with the experimental data from Ref. [12] and computations using other models namely the WA, SA and SST *k-ω* models. The results for S-Duct flow field show that both one-equation k-kL and one-equation k-kL-QCR model have the best agreement with experimental data compared to all other models except WA model. Also, one equation k-kL QCR model shows slightly better improvement in prediction of S-Duct flow field compared to one equation k-kL model. The results for other test cases will be presented in the complete paper to be presented at the conference. The open source CFD software OpenFOAM was used for flow simulations.

A. 3D Flow in a Supersonic Square Duct

The numerical simulation for this case was run to match the experiment of Davis and Gessner from NASA TMR [11]. The square duct has a width and height of D = 25.4 mm and a length x/D = 50. The Reynolds number, Re_D, based on channel height or width is 508,000, and the Mach number upstream of the duct is 3.9 with a reference temperature T = 520 R. In this case, the dimensionless velocity profile is compared at two different cuts of duct cross-section (diagonal and vertical) at x/D =40. Figure 1 shows the geometry and boundary conditions of the square duct and two different cuts of duct cross section.

Figure 2 shows the comparions of computed dimensionless velocity profiles, u/u_{CL} (where u_{CL} is the centerline velocity) at cross section x/D = 40 using the one-equation k-kL model, one-equation k-kL-ARSM model and one-equation k-kL-QCR model with experimental data along the diagonal cut and the vertical cut. It is clear that the one equation k-kL-QCR model has the best predition with the experimental data. Figure 3 shows the comparison of computaions using the one-equation k-kL-QCR, WA-QCR, SA-QCR and one-equation k-kL-ARSM model with experimental data along the diagonal cut and vertical cut. All models show good match with the experimental data except the k-kL-ARSM model along the diagonal cut; however none of the models agree well with experimental data except WA-QCR.

Figure 4 shows the contour plots of secondary flow at x/D = 50 using the one-equation k-kL [4]. One-equation k-kL-ARSM [9], and one-equation k-kL-QCR model; it is clear that both one-equation k-kL and k-kL-ARSM models cannot capture the secondary flow while one-equation k-kL QCR can. Figure 5 shows the contour plots of secondary flow at x/D = 50 using the one-euqation WA-QCR and one-euqation SA-QCR model; it is clear that both WA-QCR and SA-QCR can capture the secondary flow. Secondary flow plots in Fig. 4 and Fig. 5 were created using the following equation:

$$\sqrt{v^2 + w^2}/u_{CL} \tag{5}$$

where v is the y-component of velocity and w is the z-component of velocity. For linear eddy viscosity turbulence models, it is known that they cannot capture the corner vortices in the duct, however the QCR correction to the models can calculate the flow field with good accuracy. This test case is one of the few test cases where the usefulness of the QCR correction is clearly demonstrated.

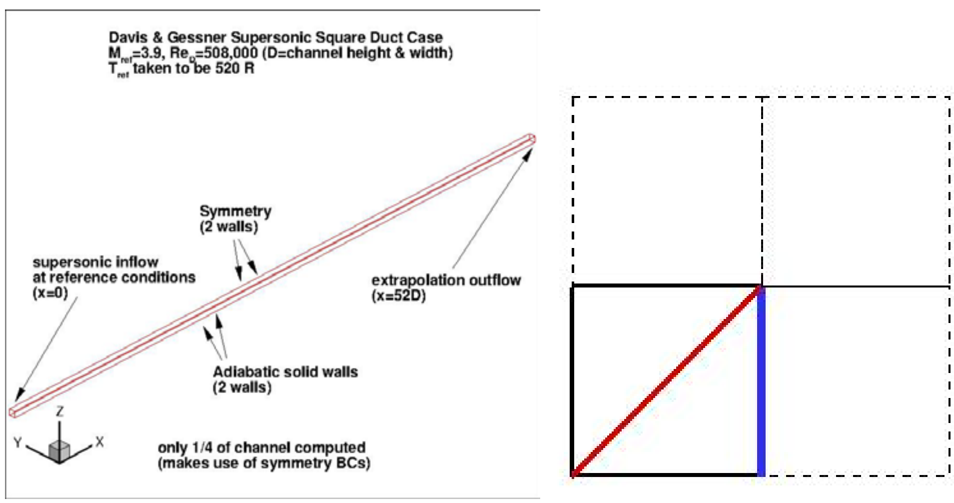

Fig. 1: Geometry and boundary conditions of the square duct (left) and diagonal/vertical cuts (right) [10].

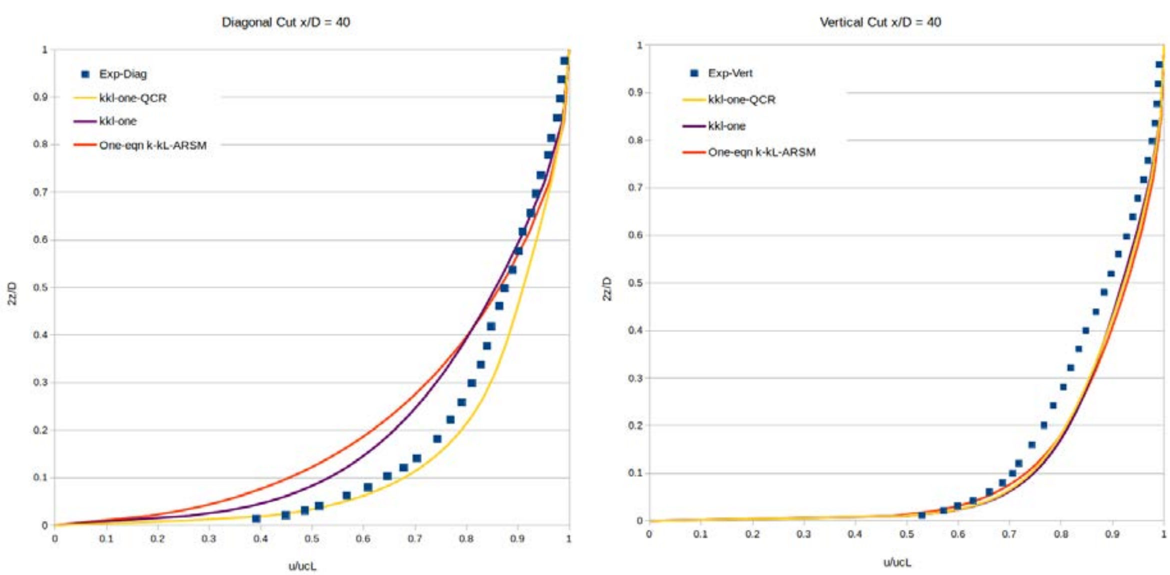

Fig. 2: Comparison of dimensionless velocity profiles on diagonal cut (left) and vertical cut (right) at x/D = 40 computed with one-equation k-kL, one-equation k-kL-ARSM and one-equation k-kL-QCR models with the experimental data.

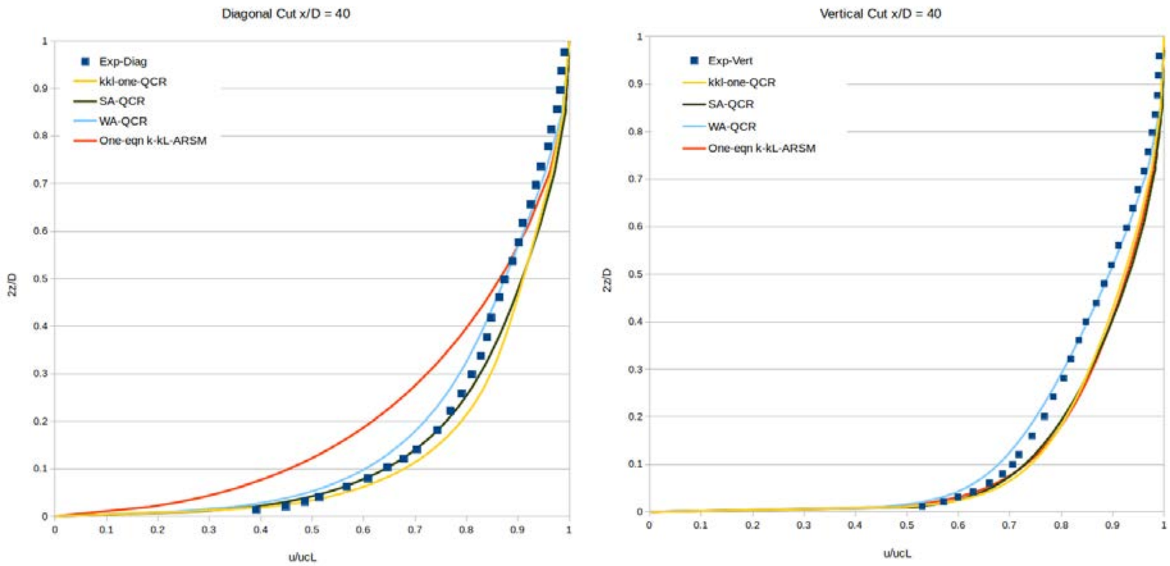

Fig. 3: Comparison of dimensionless velocity profiles on diagonal cut (left) and vertical cut (right) at x/D = 40 computed with one-equation k-kL-QCR, SA-QCR, WA-QCR and one-equation k-kL-ARSM with the experimental data.

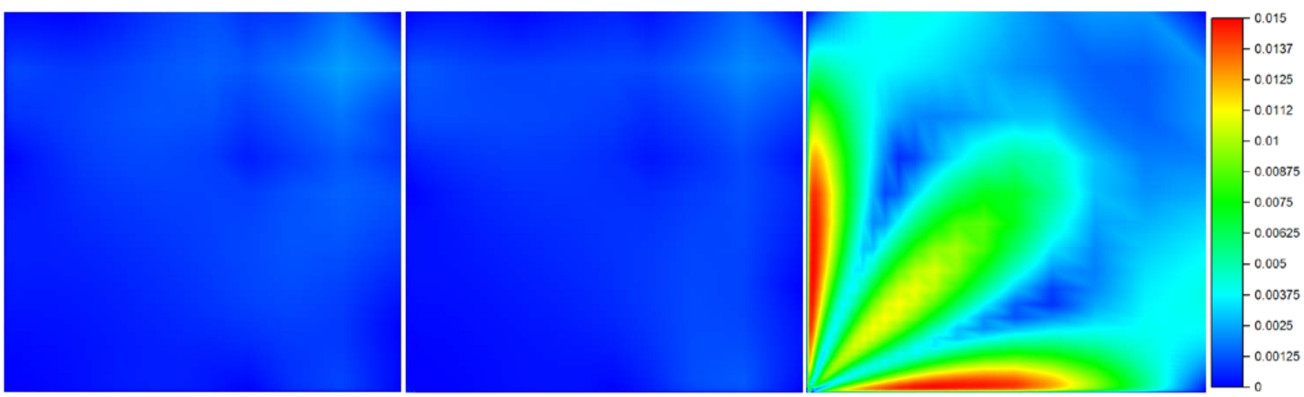

Fig. 4: Contour plots of secondary flow at x/D = 50 using one-equation k-kL (left), one-equation k-kL-ARSM (middle) and one-equation k-kL-QCR (right) models.

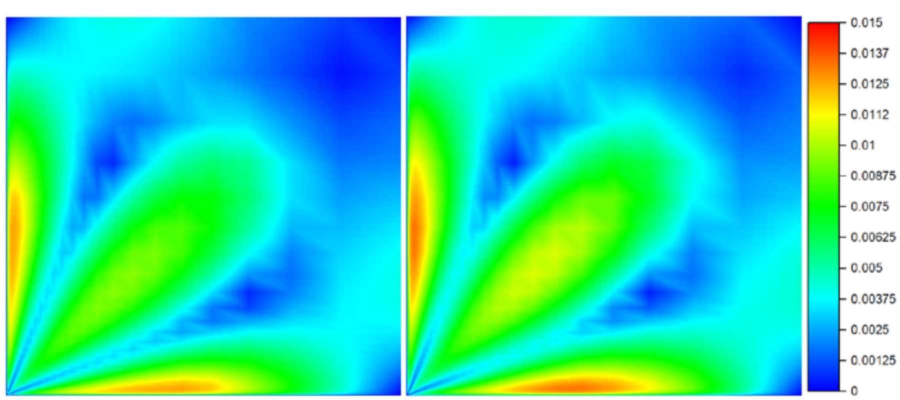

Fig. 5: Contour plots of secondary flow at x/D = 50 using SA-QCR (left) and WA-QCR (right) models.

B. Flow in 3D NASA Glenn S-Duct

The subsonic flow in NASA S-duct is a complex three-dimensional flow consisting of small region of boundary layer separation and secondary flow; it is also sometimes used to test the accuracy of RANS turbulence models. The centerline of S-duct was created by the union of two identical circular arcs, both of the same radius R = 1.02m and located in the same plane as shown in Fig. 6. The area ratio of S-duct (ratio between the outlet and inlet sections) is equal to 1.52. The inlet diameter D_1 is 0.2042m and the outlet diameter D_2 is 0.2514m. The offset of the intake resulting from the centerline curvature is 1.34 times the inlet diameter.

Inflow conditions in the computation are matched using the NASA Glenn's experimental conditions [12]. Figure 6 shows the NASA Glenn's S-Duct with planes of interests in analyzing the flow field. Figure 7 shows the S duct computational domain as well as the cross-section including the grid structure [13]. In order to compare the experimental and computational results, the non-dimensional ratio of centerline curve length to inlet diameter (s/D_1) is used. The 'reference inlet' flow conditions in the experiment are the centerline Mach number M = 0.6 and Reynolds number Re = 2.6 million at the position s/D_1 = -0.5 (Plane A in Fig. 6). At the reference inlet plane, the flow is considered turbulent and fully developed since it has not reached the curved portion of the duct yet. The outlet of the duct is at s/D_1 = 5.23.

Figures 8-11 show the comparison of the calculated coefficient of pressure along the duct walls at three different circumferential angles (ϕ = 10^o, 90^o, and 170^o). The results of one-equation k-kL and one-equation k-kL-QCR models are compared for each angle, which are also compared with the reults using WA, SA, and SST k-ω models and their QCR extensions from Ref. [14]. These figures indicate that there is little difference with the application of QCR compared to standard models. The one-equation k-kL and one-equation k-kL-QCR results show the closest agreement with the experimental results, which demonstrate the strong potential of bolth one-equation k-kL and k-kL-QCR models; WA and WA-QCR results are the second closest. The SA-QCR model seems to show the most improvement over the SA model.

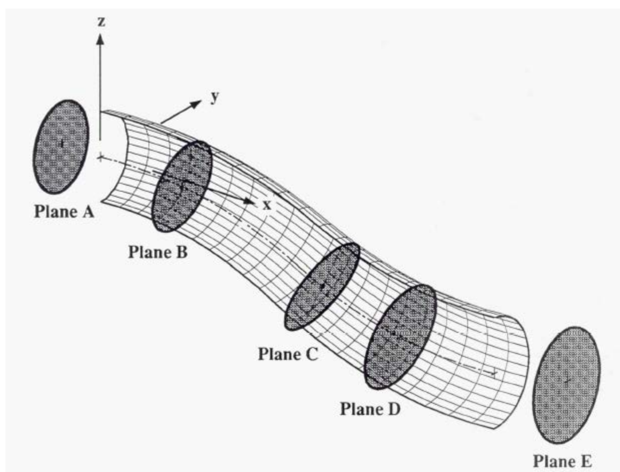

Fig. 6: S-Duct geometry with planes of interest [12].

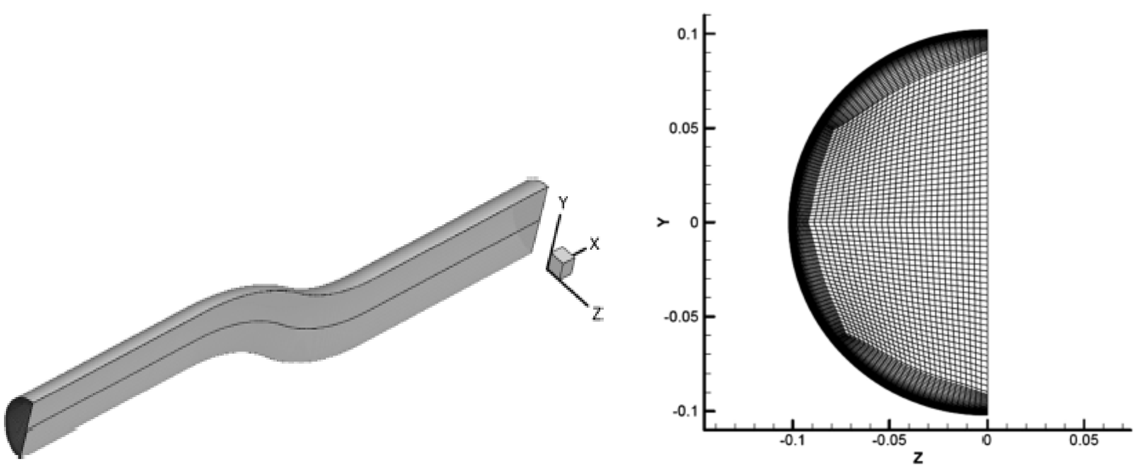

Fig. 7: S-duct full view (left) and cross-section (right) with grid structure [13].

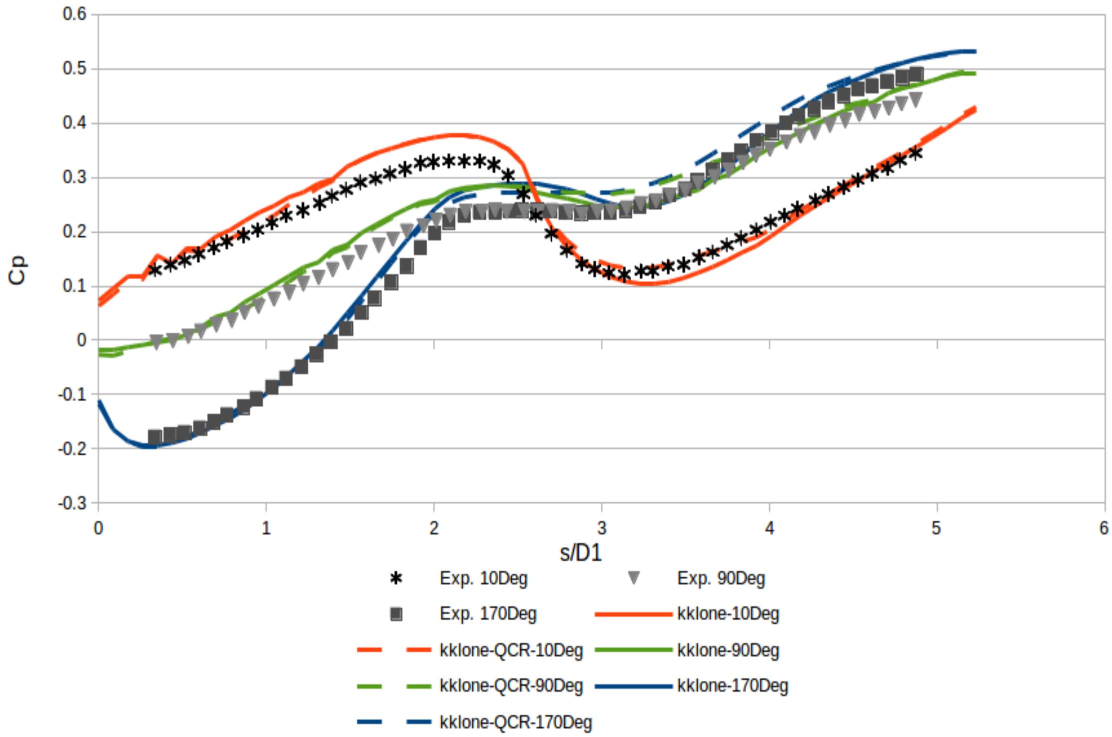

Fig. 8: Experimental and computed C_p using one-equation k-kL and one-equation k-kL-QCR model along the duct walls at $\phi = 10^o$, 90^o and 170^o.

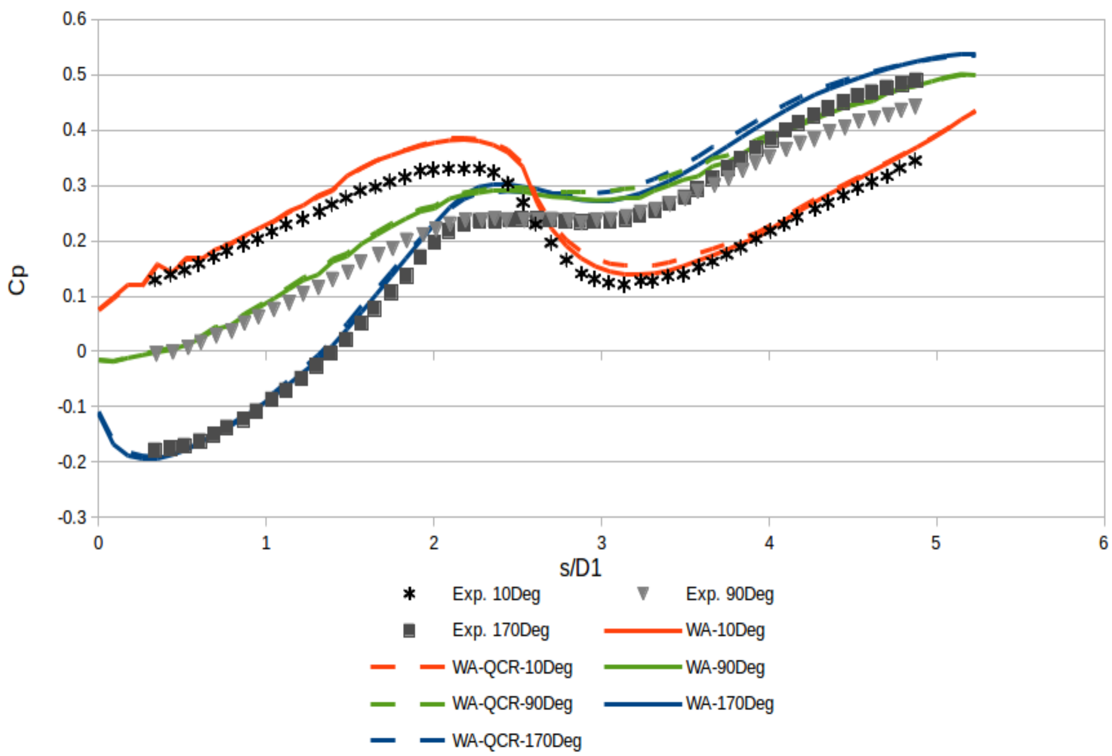

Fig. 9: Experimental and computed C_p using WA and WA-QCR model along the duct walls at $\phi = 10^o$, 90^o and 170^o.

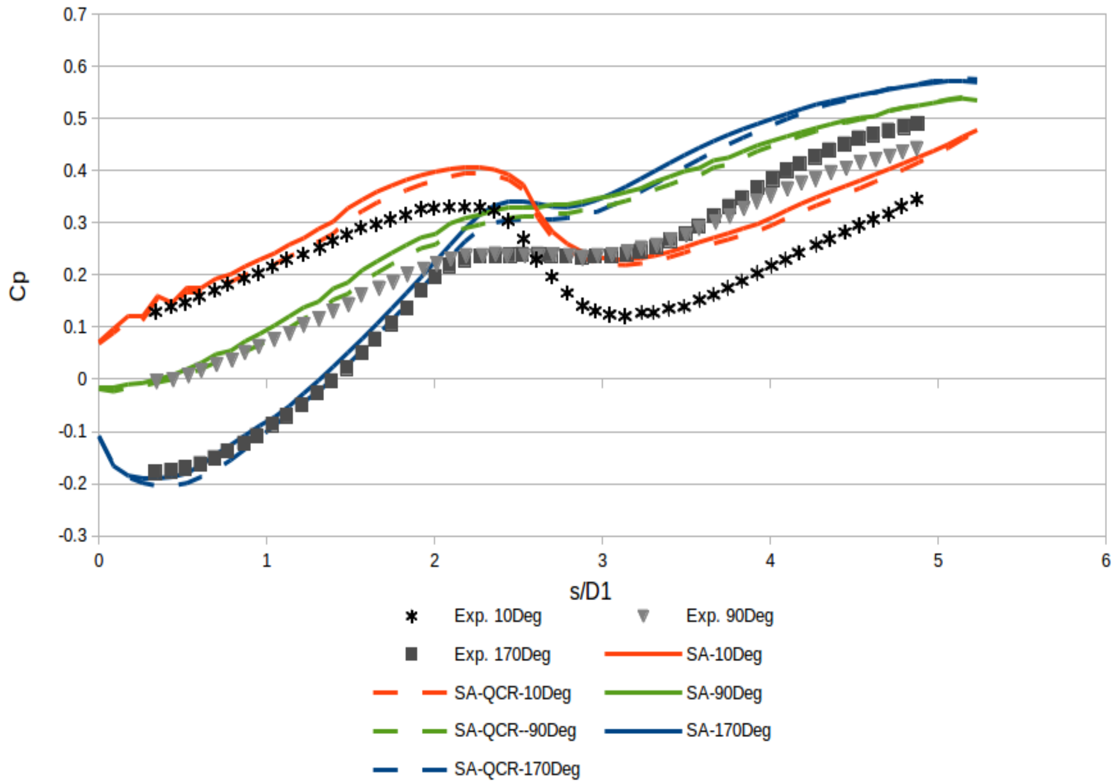

Fig. 10: Experimental and computed C_p using SA and SA-QCR model along the duct walls at ϕ = 10°, 90° and 170°.

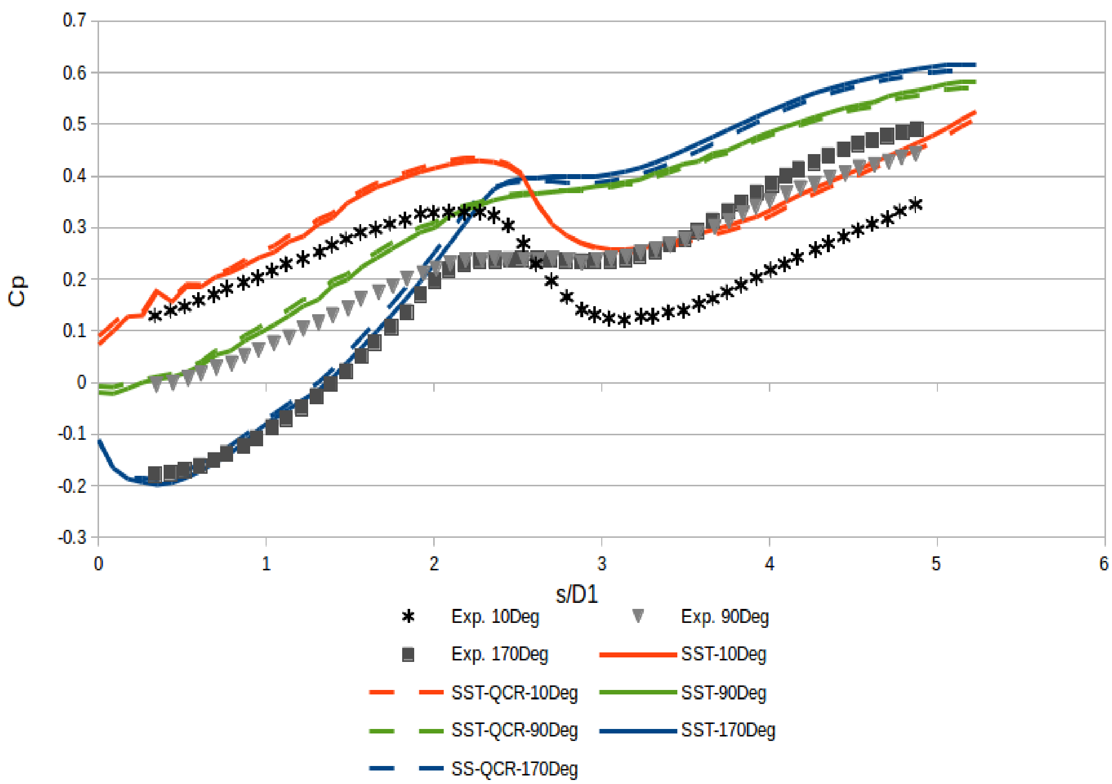

Fig. 11: Experimental and computed C_p using SST and SST-QCR model along the duct walls at ϕ = 10°, 90° and 170°.

V. Conclusions

It In this paper, the Quadratic Constitutive Relation (QCR) was successfully implemented in OpenFOAM with one-equation k-kL model. The accuracy of one-equation k-kL-QCR model was compared to the standard one-equation k-kL model and one-equation k-kL-ARSM model, as well as other turbulence models namely the WA, SA and SST k-ω models. The computation of 3D supersonic flow in a square duct showed substantial improvement in accuracy when QCR was used instead of ARSM in one-equation k-kL model. The computation of 3D subsonic flow in NASA Glenn S-Duct also showed good potential of both one-equation k-kL and k-kL-QCR models. Also, compared to SA-QCR model and WA-QCR model, the new one-equation k-kL-QCR was found to be slightly more accurate for some other test cases from NASA TMR not reported in this abstract. They will be reported in the complete paper at the time of the conference. Based on the results presented in this paper, one-equation k-kL turbulence model with QCR has enormous potential waiting for computing complex vertical flows and wall bounded flows with small regions of separation.

References

[1] Han, X., Rahman, M. M., and Agarwal, R. K., "Development and Application of a Wall Distance Free Wray-Agarwal Turbulence Model," AIAA Paper 2018-0593, AIAA SciTech Forum, Kissimmee, FL, 8-12 January 2018.

[2] Shuai, S. and Agarwal, R. K., “A One-Equation Turbulence Model Based on k-kL Closure,” AIAA 2019-1879, AIAA Scitech 2019 Forum, San Diego, CA, 7-11 January 2019.

[3] Menter, F. R. and Egorov, Y., "The Scale-Adaptive Simulation Method for Unsteady Turbulent Flow Predictions. Part 1: Theory and Model Description," Flow, Turbulence, and Combustion, Vol. 85, 2010, pp. 113-138.

[4] Menter, F.R., “Eddy viscosity Transport Equations and their Relation to the k–ε Model,” NASA-TM-108854 , 1994.

[5] Spalart, P. R., "Strategies for Turbulence Modelling and Simulation," International Journal of Heat and Fluid Flow, Vol. 21, 2000, pp. 252-263.

[6] Gatski, T. B., Rumsey, C. L. & Manceau, R., “Current Trends in Modelling Research for Turbulent Aerodynamic Flows,” Phil. Trans. R. Soc. A 365, 2007, pp. 2389–2418.

[7] Nagapetyan, H., Wray, T., & Agarwal, R. K., “Application of the Quadratic Constitutive Relation to Various Turbulence Models in OpenFOAM,” AIAA Paper 2016- 3476, AIAA 46th AIAA Fluid Dynamics Conference, Washington D.C, 13-17 June 2016.

[8] Abdol-Hamid, K. S., "Development and Documentation of kL-Based Linear, Nonlinear, and Full Reynolds Stress Turbulence Models," NASA TM-2018-219820, April 2018.

[9] Wen, T. and Agarwal, R. K., “Development of a One-Equation Algebraic Reynolds Stress Model based on k-kL Closure,” AIAA Paper 2019 – 3325, AIAA Aviation 2019 Forum, Dallas, TX, 17-21 June 2019.

[10] Davis, D. O. and Gessner, F. B., "Further Experiments on Supersonic Turbulent Flow Development in a Square Duct," AIAA J., Vol. 27, No. 8, August 1989, pp. 1023-1030.

[11] http://turbmodels.larc.nasa.gov [retrieved Oct. 2019]

[12] Wellborn, S.R., Reichert, B.A, and Okiishi, T.H., “An Experimental Investigation of the Flow in a Diffusing S-Duct,” AIAA Paper 92-3622, 28th Joint Propulsion Conference and Exhibit, Nashville, TN, 6-8 July 1992.

[13] Han, X., Wray, T. J., Fiola, C., and Agarwal, R. K., “Computation of Flow in S-Ducts with Wray-Agarwal One-Equation Turbulence Model,” Journal of Propulsion and Power, Vol.31, No. 5, 2015, pp. 1338-1349.

[14] Nagapetyan, H., “Development and Application of Quadratic Constitutive Relation and Transition Crossflow Effects in the Wray-Agarwal Turbulence Model,” Ph.D Thesis, Washington University in St. Louis, August 2018.