

The Impact of a Non-Linear Turbulent Stress Relationship on Simulations of Flow and Combustion in an HSDI Diesel Engine

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ABSTRACT

In-cylinder flow and combustion processes simulated with the standard k - ε turbulence model and with an alternative model—employing a non-linear, quadratic equation for the turbulent stresses—are contrasted for both motored and fired engine operation at two loads. For motored operation, the differences observed in the predictions of mean flow development are small and do not emerge until expansion. Larger differences are found in the spatial distribution and magnitude of turbulent kinetic energy. The non-linear model generally predicts lower energy levels and larger turbulent time scales.

With fuel injection and combustion, significant differences in flow structure and in the spatial distribution of soot are predicted by the two models. The models also predict considerably different combustion efficiencies and NO_x emissions. The turbulence model impacts entrainment and jet velocity; this is believed to be the major factor influencing the flow structure development and the formation of NO_x emissions. Like the motored simulations, major differences in the distribution and magnitude of turbulent kinetic energy and time scale are seen—differences which are likely to impact the modeled combustion behavior.

INTRODUCTION

Reynolds-averaged, Navier-Stokes (RANS) based flow modeling is the foundation on which most current simulations of engine flow and combustion are based. Although large-eddy simulation (LES) methods are also used—and have important advantages—the additional computational cost presently precludes their use for repetitive design and optimization simulations. The most widely used RANS-based model incorporates a two-equation (k - ε) turbulence model which is closed by adopting a linear constitutive relationship for the turbulent

stresses. While this model has the virtues of simplicity and relatively low computation cost, the accuracy with which it can predict complex, three-dimensional flows and flows with swirl is limited [1,2]. There is potential, however, to improve the model accuracy by adopting a more advanced turbulent stress relationship.

Assuming that the turbulent stress tensor can be represented solely as a function of the turbulent time scale and the mean velocity gradients, the most general model that can be adopted (preserving the desired transformation and contraction properties) consists of 10 independent terms, corresponding to polynomials in the mean velocity gradients up to fifth order [3]. In the linear constitutive relationship for the turbulent stress tensor, only the first term is retained. This simplification robs the model of its ability to capture the physics responsible for the re-distribution of turbulence energy among the various normal stresses. However, for two-dimensional flows, much of the re-distribution physics captured by full Reynolds stress closures is retained by including a second term, quadratic in the mean velocity gradients [1].

In a recent evaluation of the accuracy of various constitutive relations for the turbulent stresses in complex, swirling diesel engine flows, quadratic stress relationships are shown to significantly improve the prediction of the normal stress anisotropy as well as the shear stresses. Figure 1 presents a comparison of measured and predicted normal stress anisotropy. The predicted anisotropy is obtained by applying the two different constitutive relationships to experimental estimates of k , ε , and the mean velocity gradients. The model shown, a quadratic model developed by Wallin and Johansson (hereafter WJ), clearly represents a significant improvement in the prediction of the anisotropy, yet adds only modestly to the computational cost [4].



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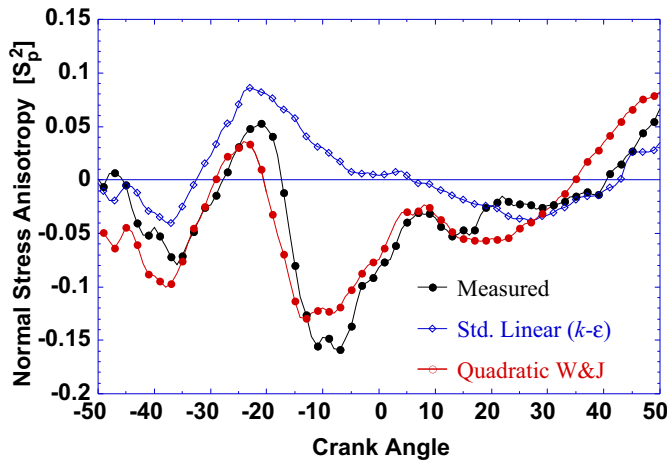


Figure 1 A comparison of the experimentally measured anisotropy in the radial and tangential normal stresses to that predicted with the standard linear stress relationship and the non-linear relationship of Wallin and Johansson [4]. The stress anisotropy is reported normalized by the mean piston speed S_p

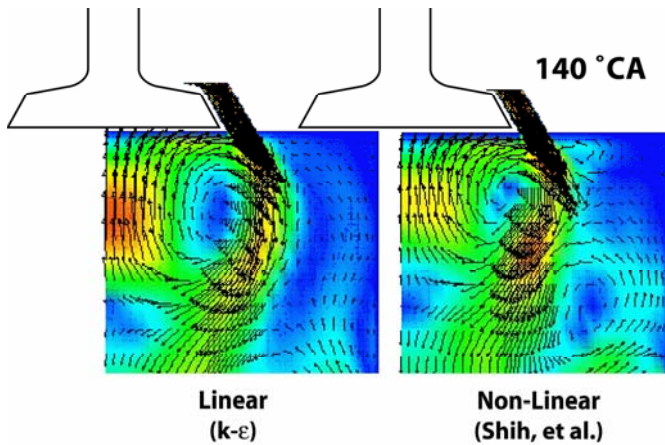


Figure 2 Flow computed through a stationary valve. Simulation results courtesy of C. Son and C. Rutland, University of Wisconsin. The non-linear stress relationship employed is that of Shih, et al. [7]

An important unanswered question is whether or not a more accurate model for the turbulent stresses will change the simulated mean flow structures and significantly impact the progress of the combustion event. Mean flows driven by the turbulent stresses are typically considered to be fairly weak, such as the transverse flows observed in turbulent flow through a square duct [5]. Application of non-linear stress relationships to the simulation of engine-like flows can result in significant structural changes to the mean flow, however [6]. An example is shown in Fig. 2, which illustrates the flow through a single, centrally-located valve. Even in this highly-directed flow, dominated by the valve jet, the non-linear model predicts a mean flow structure which differs significantly from that predicted with the standard linear model. A sizeable secondary vortex is observed in the non-linear model results, which

seems clearly capable of influencing the transport and mixing of both momentum and species on a large scale.

Motivated by the significant changes to the mean structure of engine intake flows predicted by non-linear stress models [6], and the improved agreement to in-cylinder measurements of the stress anisotropy, in this paper we investigate the potential impact of the turbulence model on the flow and combustion processes in the cylinder of an automotive class, high-speed, direct-injection (HSDI) engine. Based on its superior performance in predicting measured stress anisotropy, as shown in Fig. 1, the WJ model was selected for this exercise.

Predictions of the global combustion behavior, indicated by the heat release characteristics and the engine-out emissions, as well as the in-cylinder flow structures and spatial distributions of turbulence and pollutant emissions are analyzed and contrasted for both the WJ model and the standard k - ϵ model at various engine loads and swirl ratios. Our goal is to see if significant differences in the predictions—potentially justifying the increased complexity and cost of a more accurate model—arise when the non-linear constitutive relationship is employed. We further seek to examine the simulation results for specific features that can be employed to experimentally validate the model predictions.

TURBULENT STRESS MODEL OVERVIEW

The linear stress relationship employed in the standard k - ϵ model relates the (normalized) anisotropic part of the Reynolds stress tensor to the mean strain rate tensor through a simple, linear relationship

$$\frac{u_i u_j - \frac{2}{3} k \delta_{ij}}{2k} = -C_\mu \left(\frac{k}{\epsilon} \right) S_{ij}^* \quad (1)$$

where the constant $C_\mu = 0.09$ and the deviatoric part of the mean strain rate tensor S_{ij}^* is given by

$$S_{ij}^* = S_{ij} - \frac{1}{3} (\nabla \cdot \mathbf{U}) \delta_{ij} \quad (2)$$

In the WJ model [4], this relation is extended by the addition of a second term, quadratic in the mean velocity gradients

$$\frac{u_i u_j - \frac{2}{3} k \delta_{ij}}{2k} = -C_\mu \left(\frac{k}{\epsilon} \right) S_{ij}^* + \alpha_2 \left(\frac{k}{\epsilon} \right)^2 (S_{ik}^* \Omega_{kj} - \Omega_{ik}^* S_{kj}^*) \quad (3)$$

Ω_{ij} represents the various components of the mean rate-of-rotation tensor. It is important to reiterate that the WJ model is derived from a full Reynolds stress turbulence closure, and therefore retains much of the physical content of this more detailed closure.

Unlike the standard linear model, in the WJ model C_μ and α_2 are not constants, but vary with the characteristic mean flow strain and rotation rates non-dimensionalized with the turbulent time scale k/ε .

Defining the non-dimensional strain and rotation rates

$$S^* = \left(k/\varepsilon\right) \sqrt{S_{ij}^* S_{ij}^*} \quad \text{and} \quad \Omega = \left(k/\varepsilon\right) \sqrt{\Omega_{ij} \Omega_{ij}} \quad (4)$$

The Wallin and Johansson model constants are given by

$$C_\mu = -\frac{3}{5} \frac{g}{\beta_2} \left(\left(\frac{g}{\beta_2} \right)^2 - 2\Omega^2 \right)^{-1} \quad \text{and} \quad \alpha_2 = C_\mu / \left(\frac{g}{\beta_2} \right) \quad (5)$$

In turn,

$$\begin{aligned} \frac{g}{\beta_2} = & -\frac{3}{4} \left(\frac{C_1^0}{2} - 1 - \frac{2}{3} \frac{k}{\varepsilon} (\nabla \cdot \langle \mathbf{U} \rangle) \right) - (P_1 + \sqrt{P_2})^{1/3} \\ & - \text{sign}(P_1 - \sqrt{P_2}) |P_1 - \sqrt{P_2}|^{1/3} \end{aligned} \quad (6)$$

when $P_2 \geq 0$, and for $P_2 < 0$

$$\begin{aligned} \frac{g}{\beta_2} = & -\frac{3}{4} \left(\frac{C_1^0}{2} - 1 - \frac{2}{3} \frac{k}{\varepsilon} (\nabla \cdot \langle \mathbf{U} \rangle) \right) - \\ & 2(P_1^2 - P_2)^{1/6} \cos \left(\frac{1}{3} \arccos \left(\frac{P_1}{\sqrt{P_1^2 - P_2}} \right) \right) \end{aligned} \quad (7)$$

The quantities P_1 and P_2 are given by

$$\begin{aligned} P_1 = & \frac{9}{4} \left(\frac{C_1^0}{2} - 1 - \frac{2}{3} \frac{k}{\varepsilon} (\nabla \cdot \langle \mathbf{U} \rangle) \right) \\ & \left(\frac{3}{16} \left(\frac{C_1^0}{2} - 1 - \frac{2}{3} \frac{k}{\varepsilon} (\nabla \cdot \langle \mathbf{U} \rangle) \right)^2 + \frac{9}{20} S^{*2} - \frac{2}{3} \Omega^2 \right) \end{aligned} \quad (8)$$

and

$$\begin{aligned} P_2 = & P_1^2 - \\ & \left(\frac{9}{16} \left(\frac{C_1^0}{2} - 1 - \frac{2}{3} \frac{k}{\varepsilon} (\nabla \cdot \langle \mathbf{U} \rangle) \right)^2 + \frac{9}{10} S^{*2} + \frac{2}{3} \Omega^2 \right)^3 \end{aligned} \quad (9)$$

C_1^0 is a model constant with the value 3.6.

It is instructive to examine the behavior of the model constants as S^* , Ω , and $\nabla \cdot \langle \mathbf{U} \rangle$ vary. Isopleths of C_μ are presented in Fig. 3 for various values of S^* and Ω , computed with $\nabla \cdot \langle \mathbf{U} \rangle = 0$. Also plotted in the background of the figure are points (S^*, Ω) derived from measurements made in a motored, direct-injection engine [8]. Estimates of the dissipation, necessary to

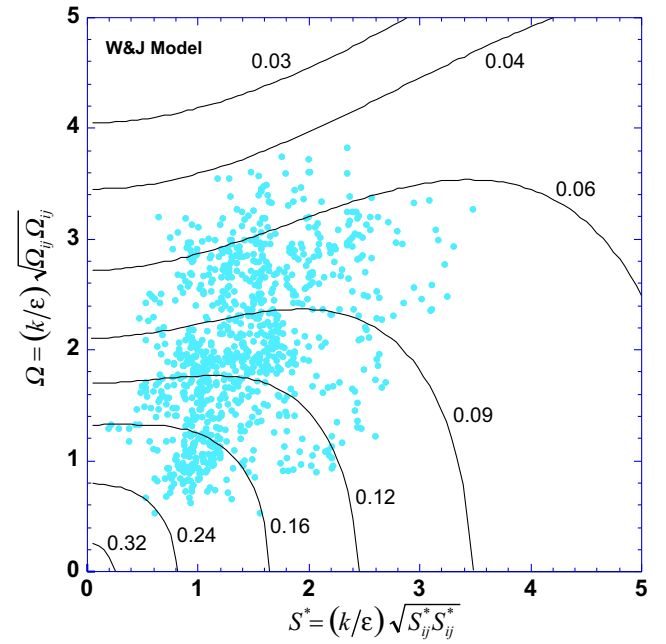


Figure 3 Variation of the constant C_μ as a function of the non-dimensional characteristic strain and rotation rate. $\nabla \cdot \langle \mathbf{U} \rangle = 0$

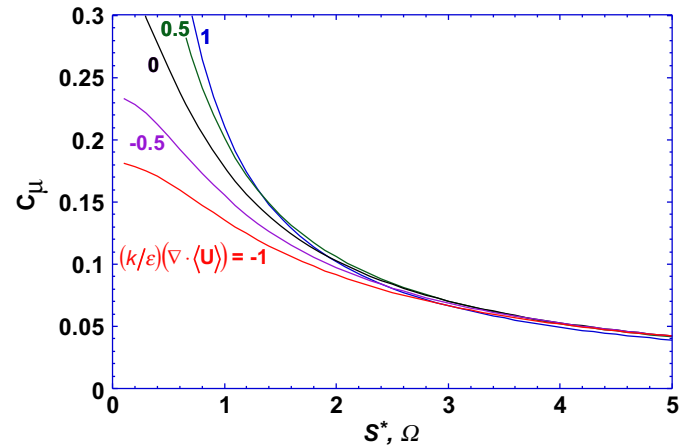


Figure 4 Variation of the constant C_μ as $\nabla \cdot \langle \mathbf{U} \rangle$ is varied with $S^* = \Omega$

form the turbulent timescale, were obtained from measured velocity-correlation length scales as described in [9].

From Fig. 3 we see that for “typical” values of S^* and Ω found in a motored engine flow, as determined from the centroid of the (S^*, Ω) pairs, the WJ model provides a value of C_μ very near the constant value of 0.09 employed in the standard linear model. Hence, under conditions when the higher order terms in Eq.(3) are insignificant, we anticipate that the Wallin and Johansson model will perform similarly to the standard linear model.

Eqs.(5)-(9) also indicate that C_μ will vary with $\nabla \cdot \langle \mathbf{U} \rangle$ as well as S^* and Ω . To investigate the influence of $\nabla \cdot \langle \mathbf{U} \rangle$ we have computed C_μ along the line $S^* = \Omega$ for various values of the normalized rotation $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$. The

results are shown in Fig. 4. For normalized strain and rotation rates greater than about 2 (that is, when mean flow processes occur over times that are short compared to turbulent time scales), $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$ has little influence on the coefficient C_μ . On the other hand, when turbulent time scales are comparable to or smaller than mean flow time scales, bulk flow compression will impact the value of C_μ considerably.

Like C_μ , the coefficient α_2 also varies with the normalized strain and rotation rate, as shown in Fig. 5. To understand how the importance of the linear terms in Eq.(3) changes relative to the quadratic terms as S^* , Ω , and $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$ vary, it is useful to examine the ratio of the magnitude of the two terms: $C_\mu/(\alpha_2 \Omega)$. This quantity is plotted in Fig. 6 for various values of $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$, with $S^* = \Omega$. Analysis of the data reported in [8] shows that during compression the normalized dilation is typically of magnitude -0.5, while during expansion it is somewhat larger, generally between 0.5 and 1.0.

Again like the coefficient C_μ , the influence of $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$ on this ratio is smaller for large normalized strain and rotation rates. However, it is significant at all values of S^* and Ω . For mean flow compression, the linear term dominates the stress relationship, particularly at small S^* , Ω . With bulk flow expansion and $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle) \approx 1$, however, the two terms are of nearly equal magnitude. Hence, we can anticipate that the influence of the non-linear terms will be more pronounced during the expansion stroke. Finally, we note that for a given value of $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$, the ratio of the two terms is relatively constant, provided that the turbulent time scale is roughly twice the mean flow time scale or larger.

NUMERICAL METHODOLOGY

Numerical simulations for this research are performed using KIVA-3V. This is an industry accepted code, capable of modeling transient two and three-dimensional flows with chemical reactions and spray fuel injection [10]. Checks were added to KIVA-3V to ensure weak realizability is met with each turbulence model.

For the KIVA-3V simulations with fuel injection and combustion, hybrid Rayleigh-Taylor and Kelvin-Helmholtz instabilities account for the fuel droplet breakup. The fuel injected is n-tetradecane. The Shell combustion model is used for autoignition and the mixing-controlled combustion is modeled with the characteristic time model. NO_x chemistry is described by the extended Zel'dovich mechanism and the soot model considers a one-step formation model coupled with a Nagel and Strickland-Constable oxidation model. These models are described in detail elsewhere [11]. The tangential mean velocities are initialized at $-55^\circ\text{CA}^\dagger$ to a solid-body-like radial velocity profile at the specified swirl ratio by setting the KIVA variable 'swipro' to 1. The turbulence field is initialized to a uniform distribution of k corresponding to a

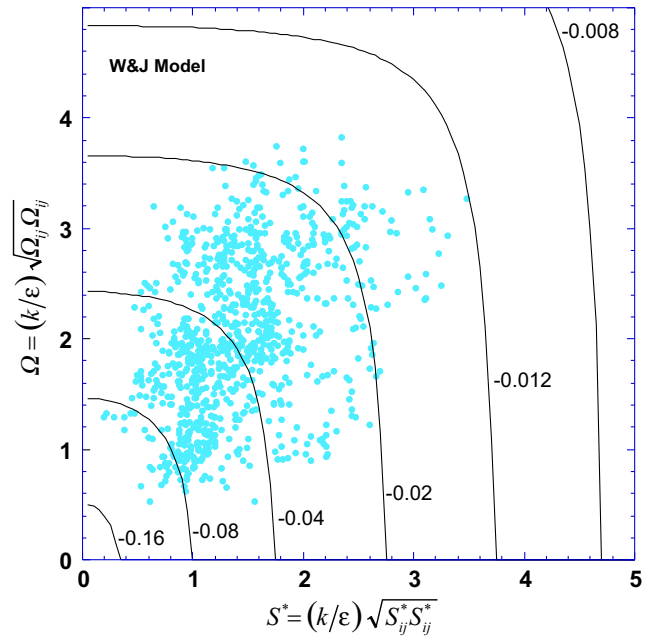


Figure 5 Variation of the constant α_2 as a function of the non-dimensionalized characteristic strain and rotation rate. $\nabla \cdot \langle \mathbf{U} \rangle = 0$

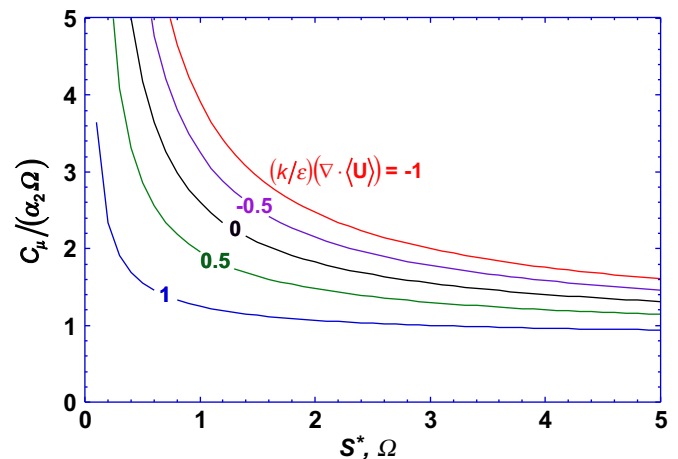


Figure 6 Variation of the ratio of the linear term to the quadratic term in the stress relationship of Eq.(3), for various values of the normalized bulk flow dilatation $(k/\varepsilon)(\nabla \cdot \langle \mathbf{U} \rangle)$

fluctuating velocity u' equal to 54% of the mean piston speed, and a uniform initial turbulence length scale equal to approximately 14% of the bore diameter.

Testing and validation of the Wallin and Johansson stress model, as implemented into KIVA-3V, was performed by considering two canonical flow configurations: the backward-facing step configuration explored experimentally by Driver and Seegmiller [12] and flow in a square duct as measured by Yokosawa and co-workers [5]. For the backward facing step, the accuracy of the mean and turbulent velocity profiles was not significantly improved over the accuracy of the standard k - ε model, though the predicted re-attachment

[†] Cited crank angles are referred to ATDC compression