Comparison of linear, non-linear and generalized RNG-based k-epsilon models for turbulent diesel engine flows

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Abstract

In this work, linear, non-linear and a generalized renormalization group (RNG) two-equation RANS turbulence models of the k-epsilon form were compared for the prediction of turbulent compressible flows in diesel engines. The object-oriented, multidimensional parallel code FRESCO, developed at the University of Wisconsin, was used to test the alternative models versus the standard k-epsilon model.

Test cases featured the academic backward facing step and the impinging gas jet in a quiescent chamber. Diesel engine flows featured high-pressure spray injection in a constant volume vessel from the Engine Combustion Network (ECN), as well as intake flows in a high-swirl diesel engine. For the engine intake flows, a model of the Sandia National Laboratories 1.9L light-duty single cylinder optical engine was used. An extensive experimental campaign provided validation data in terms of ensemble averages of planar PIV measurements at different vertical locations in the combustion chamber, for different swirl ratio configurations during both the intake and the compression strokes.

The generalized RNG k-epsilon model provided the best accuracy trade-off for both swirl and shear flows, thanks to the polynomial expansion of coefficients \( C_1 \) and \( C_2 \) in the RNG k-epsilon model with an effective ‘dimensionality’ of the strain rate field. Similar performance was seen across linear and non-linear RNG models, which achieves good prediction of in-cylinder swirl flows; however, they noticeably underpredict jet penetration in the case of high-pressure sprays, suggesting the additional computational cost and lower stability of the non-linear model do not justify greater suitability for engine calculations.

Introduction

Improvements in computing hardware and scientific software design are constantly driving more and more parts of the engine development workflow towards using computer simulation before expensive experimental campaigns need to be established. In recent years, greater computational capabilities have allowed internal combustion engine simulations to benefit from more accurate and predictive models for turbulence (i.e., Large Eddy Simulation), combustion chemistry (detailed kinetics solvers and large reaction mechanisms), sprays (Eulerian simulations), mostly thanks to the capability of modern computing platforms to solve millions to billions of equations simultaneously [1].

However, even if these advancements are allowing light to be shed on the interactions between the many physical phenomena acting at the smallest spatial and temporal scales, this type of simulation – which require ultra-large computing facilities and correspondingly long CPU times – does not fit typical industrial design workflows which requires turnaround times no more than ten or twenty hours for a simulation. Focus of the current study is modeling of light-duty diesel engines; for these simulations, it was previously shown that sector mesh models do not represent in-cylinder flow features appropriately, which leads to poor ignition development and pollutant formation predictions when moving from conventional diesel combustion towards low-temperature combustion strategies [2].

In this framework Reynolds-Averaged Navier Stokes (RANS) turbulence models can play a significant role towards achieving the best possible accuracy for ensemble-average cycle simulations, while keeping simulation times under control by balancing the computational grid resolution with enough physics having been embedded in the models. Employing two-equation models hence appeared to be an appropriate first bet, because they combine limited computational demands, extensive usage and validation for practical engineering simulations, as well as robust solution convergence properties. Hence, the accuracy of some two-equation k-epsilon turbulence models was assessed in the present work for flow configurations relevant to diesel engines: standard k-epsilon model, compressible renormalization group (RNG), renormalization group with second-order Reynolds stress tensor expansion, as well as a recently developed generalized renormalization group model (GRNG).

As reported in Figure 1, typical injection strategies in state-of-the-art light-duty diesels feature high-pressure fuel injection into the chamber, directed towards the piston bowl rim, such that the fuel spray jet can be partly directed downward within the piston bowl, and partly upward towards the squish region [3]. In this configuration, shear flows due to fuel injection and deflection along the walls, as well as in-cylinder swirl, coexist with compression flows due to piston movement, as well as jet impingement against the wall. Two academic and three engine-related test cases were selected to reproduce these configurations: channel flow sudden expansion or backward-facing step, gas jet impingement against a wall, high-pressure fuel injection in a quiescent environment in non-reactive and reactive conditions, as well as in-cylinder flows in a light-duty optical diesel engine. The results show that the standard k-
All simulations were performed using FRESCO [4], a new, object-oriented parallel platform for multidimensional engine simulations written in Fortran, being developed at the University of Wisconsin-Madison. The code implements an unstructured, parallel volume-of-fluid solver for the Navier Stokes equations with automatic domain decomposition for variable-topology meshes. Spray models for fuel injection feature advanced parallel algorithms for breakup, collision, vaporization and near-nozzle flow dynamics [5]. Combustion chemistry is handled by a sparse analytical Jacobian chemistry solver and high-dimensional-clustering based chemistry dimensionality reduction [6,7]. A list of the sub-models employed for the current simulations is reported in Table 1.

The solver implements an explicit first-order time integration scheme using the Arbitrary Lagrangian-Eulerian splitting of Hirt et al. [13], useful for advection-dominated flows such as those in internal combustion engines. First, the Lagrangian derivatives for the momentum (including spray particle coupling), mass conservation, energy and turbulence equations are solved in an implicit fashion, using a second-order central differencing scheme for the face quantities. Pressure coupling is iterated with the momentum equation using the SIMPLE procedure. Then, the advection terms are computed during a rezing step by fluxing quantities from the fictitious Lagrangian mesh to the actual, Eulerian node positions using an upwind scheme with van Leer’s minmod flux limiter [14].

The paper is structured as follows. First, the equations defining all turbulence models tested are presented. Then, each validation test case is discussed, and the performance of each turbulence model compared with available experimental measurements. Finally, recommendations for turbulence model usage in diesel engine simulations are given.

**Turbulence model implementation**

**Computational setup**

All simulations were performed using FRESCO [4], a new, object-oriented parallel platform for multidimensional engine simulations written in Fortran, being developed at the Sandia light-duty optical diesel engine, equipped with either a conventional omega-shaped piston bowl (left) or a stepped-lip bowl (right). Dashed lines represent piston movement during injection; black solid outline an approximate fuel vapor region.

**k-epsilon turbulence closures**

Turbulence model equations are solved in a finite-volume-integral sense in the same way as all other fields, i.e., by subdividing the substantial derivative into a Lagrangian and a Eulerian step, all production terms on the right-hand-side being solved implicitly during the Lagrangian stage, once the Lagrangian flow field has been updated. All turbulence models implemented in the current work belong to the class of two-equation k-epsilon models, where turbulence closure is achieved using two transport PDEs for the turbulence kinetic energy $k$ and turbulence dissipation $\epsilon$ scalars:

$$\frac{\partial (\rho k)}{\partial t} + \mathbf{u} \cdot \nabla (\rho k) = \nabla \cdot (\mu \nabla k) + P_{\text{spray}}$$

$$\frac{\partial (\rho \epsilon)}{\partial t} + \mathbf{u} \cdot \nabla (\rho \epsilon) = \frac{C_p}{k} (C_{\epsilon} P - C_{\epsilon} \epsilon) - 2 \rho R + C_{\epsilon} \rho \epsilon \nabla \cdot \mathbf{u} + \nabla \cdot (\alpha_s \mu \nabla \epsilon) + c_s P_{\text{spray}}$$

where $P$ represents production of turbulence kinetic energy due to strain,

$$P = -\rho u_i \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} = -\mathbf{\tau} : \nabla \mathbf{u} ;$$

and $P_{\text{spray}}$ due to the relative motion between liquid spray particles and the fluid phase. Following the Boussinesq eddy viscosity assumption, the Reynolds stress tensor $\mathbf{\tau}$ in the standard k-epsilon model is a linear function of the traceless mean strain rate tensor:

**Table 1. Computational model setup employed for the current study.**

<table>
<thead>
<tr>
<th>Phenomenon</th>
<th>Sub-model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spray breakup</td>
<td>Hybrid KH-RT instability, Beale and Reitz [8]</td>
</tr>
<tr>
<td>SGS near-nozzle flow</td>
<td>Unsteady gas-jet model with implicit momentum coupling [5]</td>
</tr>
<tr>
<td>Spray angle</td>
<td>Reitz and Bracco [9]</td>
</tr>
<tr>
<td>Drop drag</td>
<td>Analytical with Mach number effects [5]</td>
</tr>
<tr>
<td>Droplet collision</td>
<td>Deterministic impact with extended outcomes, [10], dynamic ROI (radius-of-influence), [5]</td>
</tr>
<tr>
<td>Chemistry solver</td>
<td>Sparse Analytical Jacobian (SpeedCHEM), Perini et al. [6]</td>
</tr>
<tr>
<td>Chemistry grouping</td>
<td>High-Dimensional Clustering, Perini et al. [7]</td>
</tr>
<tr>
<td>Piston compressibility</td>
<td>Static, Perini et al. [12]</td>
</tr>
</tbody>
</table>
\[ \tau = 2\mu S - \frac{2}{3} \rho k \delta_3, \quad (3) \]

\[ \mathbf{S}' = \mathbf{S} - \frac{1}{3} (\nabla \cdot \mathbf{u}) \delta_3 = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \frac{1}{3} (\nabla \cdot \mathbf{u}) \delta_3 \]

It is worth remembering that the mean strain rate tensor \( \mathbf{S} \) represents the deviatoric components of the Cauchy strain tensor, i.e., the hydrostatic contributions due to compression/expansion – which only appear in compressible flow, where \( (\nabla \cdot \mathbf{u}) \neq 0 \) – have been subtracted.

ReNormalization group. The source term \( R \) for the dissipation equation is present in the renormalization group model of Yakhot [15] only, and is meant to compensate for the energy not closed by the iterative wavelength filtering procedure, which was done to characterize all other constants of the RNG model:

\[ R = \frac{C_r \eta^4 (1 - \eta / \eta_0)}{1 + \beta \eta} \frac{\varepsilon^2}{k}. \quad (4) \]

\[ \eta = \sqrt{\frac{\beta}{E}} \frac{k}{E}. \]

\( \eta \) representing the ratio between turbulent and mean strain timescales, and subscript \( F \) a Frobenius norm operator. In practice, the \( R \) term of Equation (4) is not added explicitly to the dissipation equation, but is actually absorbed into the first term of the right-hand-side by replacing \( C_1 \) with an "augmented" coefficient \( C_{1R} \):

\[ C_{1R} = C_1 - C_\eta = C_1 - \frac{\eta (1 - \eta / \eta_0)}{1 + \beta \eta}. \quad (5) \]

In this way, the RNG term to the dissipation equation can act as a sink of dissipation when \( C_{1R} \) is positive. In general, for large mean strain rates, \( R \) will be a source of dissipation, hence reducing the turbulent viscosity.

The RNG k-epsilon model was extended to account for compressibility effects by Han and Reitz [16], which added a \( C_3 \) term pre-multiplying the flow divergence term, i.e., the flow expansion rate. An equation for \( C_3 \) was developed in their work following the rapid distortion limit procedure [17]:

\[ C_3 = \frac{-4 + 2C_1}{3} + \frac{\partial \nu_0}{\partial t} \frac{1}{\nu_0 (\nabla \cdot \mathbf{u})} \frac{\sqrt{6C_\nu}}{3 \beta \eta_0} \sgn(\nabla \cdot \mathbf{u}) \quad (6) \]

where the kinematic viscosity rate of change term was evaluated assuming an isotropic compression/expansion process for an ideal gas, for which \( \gamma = 1.4 \) and \( \mu \propto T^m \), with \( m = 0.5 \):

\[ \frac{\partial \nu_0}{\partial t} \frac{1}{\nu_0 (\nabla \cdot \mathbf{u})} \approx 1 - m(\gamma - 1) \approx 0.8. \quad (7) \]

Hence, the compressible RNG k-epsilon model of Han and Reitz produces a \( C_3 \) coefficient which only depends on the sign of the flow divergence:

\[ C_3 = \begin{cases} 1.726, & \nabla \cdot \mathbf{u} < 0, \\ -0.90, & \nabla \cdot \mathbf{u} > 0. \end{cases} \quad (8) \]

However, as observed in [18], in some codes such as the KIVA family of codes, the \( C_3 \) formulation was misinterpreted. In the rapid distortion limit \( (\nabla \cdot \mathbf{u}) k / \varepsilon \gg 1 \), and \( C_3 \eta \rightarrow -1/(\beta \eta_0) \), but it was implemented as

\[ C_3 = \frac{-4 + 2C_1}{3} + \frac{\partial \nu_0}{\partial t} \frac{1}{\nu_0 (\nabla \cdot \mathbf{u})} \frac{\sqrt{6C_\nu} \eta}{3 \beta \eta_0} \sgn(\nabla \cdot \mathbf{u}), \quad (9) \]

hence replacing the last term to \( C_3 \) with a linear term of the strain factor \( \eta \), whose actual values will reduce significantly the effects of that additional term, making the actual predictions closer to those of the standard \( k \)-epsilon model. In the current study, both formulations were considered: the formulation from Equation (9), as found in the KIVA codes, will be referred to as "RNG", while the correct one as from Equation (6) will be named "RNG-fix".

Nonlinear RNG model. In an attempt to overcome the limitations (but also the effectiveness) of the Boussinesq hypothesis associated to \( k \)-epsilon models, Speziale [19] proposed an extension of the Reynolds stress tensor to second-order terms, which could better model turbulent stresses by increasing the order of the stress tensor expansion versus the mean strain rate:

\[ \tau_y = 2\mu S' - \frac{2}{3} \rho k \delta_3 + 4 \rho C_\epsilon L^2 \left( S' \cdot S' \frac{1}{3} \| S \|_F^2 \delta_3 \right) \]

\[ + 4 \rho C_\epsilon L^2 \frac{\varepsilon}{k \beta \eta_0} \left( S - \frac{1}{3} \| S \|_F^2 \delta_3 \right), \quad (10) \]

where the \( \alpha \) superscript represents an Oldroyd derivative, which is frame indifferent, i.e., it has the same value either in a Eulerian or Lagrangian perspective; standard conventions for vector-tensor and tensor-tensor dot products apply; \( L = C_\omega k^{0.5} / \varepsilon \) indicates the integral length scale of turbulence, and two more constants were added, \( C_D = C_E = 1.68 \).

In the present study, Speziale’s extension to the Reynolds stress model was added to the implicit solution of the momentum equation, exploiting the vector and tensor field algebra embedded in FRESCO. However, this second-order term brings a two-fold increase in computational complexity: first, more storage and many more calculations are needed at each iteration of the momentum equation solver, as well as to store the time derivatives of the velocity field needed for computing the time derivative of the strain tensor; furthermore, this non-linear term renders the system of equations for the finite-volume momentum equation non-linear. In practice, the Conjugate Gradient iterative solver for linear equations, such as implemented in FRESCO, converged in most simpler cases; however, it was found to diverge for some of the complex flow configurations, as will be discussed next.
Generalized RNG model (GRNG). In an attempt to introduce flow anisotropy effects to turbulence, while still retaining the Boussinesq assumption for the Reynolds stresses and its implicit ease of computation, Wang et al. [18] proposed a generalized closure for the RNG k-epsilon equations, which incorporates the effects of a non-isotropic mean strain rate tensor through augmenting the RNG model coefficients by effective dimensionality coefficients, $n$ and $a$, of the strain rate field:

$$a = 3(S_{11}^2 + S_{22}^2 + S_{33}^2 - |S_{11}| + |S_{22}| + |S_{33}|)^{1/3} - 1$$

$$n = 3 - \sqrt{2a}$$

which were defined to match some template flow structures: $n=1$ for unidirectional axial compression, $n=2$ for cylindrical-radial compression (squish), $n=3$ for spherical compression. Based on validations from experimental and DNS data from various basic flow configurations, including homogeneous turbulence under adiabatic unidirectional and spherical compression, jet flows and engine flows, polynomial fits for the RNG model constants were derived:

$$C_{2,G} = b_0 + b_1 n + b_2 n^2$$

$$C_{3,G} = -\frac{n+1}{n} + \frac{2}{3} C_1 + \sqrt{\frac{2+2a}{3}} C_2 C_3 \eta \text{sgn}(\nabla \cdot \mathbf{u})$$

with $b_0=2.496$, $b_1=-0.686$, $b_2=0.11$. In this way, the GRNG k-epsilon equations can be solved in the same way as the RNG k-epsilon model, where the constants $C_2$ and $C_3$ have been replaced by their augmented counterparts from Equations (12) and (13).

In summary, the model constants for all four turbulence models employed in the current study are reported in Table 1. In the following, they will be referred to as: ‘standard’ for the original k-epsilon model; ‘RNG’ for the renormalization group with uncorrected distortion limit assumption; ‘RNG-fx’ for the renormalization group with fixed distortion limit assumption; ‘GRNG’ for the generalized RNG model; ‘non-linear’ for the RNG model with Speziale’s nonlinear Reynolds stress tensor extension.

### Table 2. Summary of model coefficients employed for different k-epsilon turbulence closure formulations.

<table>
<thead>
<tr>
<th></th>
<th>Std.</th>
<th>RNG</th>
<th>RNGf x</th>
<th>GRNG</th>
<th>Non-lin</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>1.00</td>
<td>1.39</td>
<td>1.39</td>
<td>1.39</td>
<td>1.39</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.769</td>
<td>1.39</td>
<td>1.39</td>
<td>1.39</td>
<td>1.39</td>
</tr>
<tr>
<td>$C_1$</td>
<td>1.44</td>
<td>1.42</td>
<td>1.42</td>
<td>1.42</td>
<td>1.42</td>
</tr>
<tr>
<td>$C_2$</td>
<td>1.92</td>
<td>1.68</td>
<td>1.68</td>
<td>Eq. (12)</td>
<td>1.68</td>
</tr>
<tr>
<td>$C_3$</td>
<td>-1.00</td>
<td>Eq. (9)</td>
<td>Eq. (8)</td>
<td>Eq. (13)</td>
<td>Eq. (8)</td>
</tr>
<tr>
<td>$C_4$</td>
<td>1.50</td>
<td>1.50</td>
<td>1.50</td>
<td>1.50</td>
<td>1.50</td>
</tr>
<tr>
<td>$C_5$</td>
<td>0.09</td>
<td>0.0845</td>
<td>0.0845</td>
<td>0.0845</td>
<td>0.0845</td>
</tr>
<tr>
<td>$\beta$</td>
<td>-</td>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
</tr>
<tr>
<td>$\eta_0$</td>
<td>-</td>
<td>4.38</td>
<td>4.38</td>
<td>4.38</td>
<td>4.38</td>
</tr>
</tbody>
</table>

### Academic Test Cases

#### Backward-Facing Step

Since k-epsilon models are well known for underpredicting recirculatory flows, the common academic sudden channel flow expansion case, or backward-facing step, was chosen as a first test case for the different turbulence model formulations. The experimental setup of Adams and Eaton [20] was used: the channel height to step height ratio was 3:1, and the step Reynolds numbers was $Re_h=45,000$. The pipe outlet was located 30 step heights downstream. The study provided measured velocity and turbulence intensity profiles 6 step heights upstream of the step; however, it was chosen to let turbulence naturally develop from the turbulence model.
and hence include a total upstream channel length of 60 steps, and initialize a flat velocity profile at the channel inlet. A schematic representing the model configuration is reported in Figure 2. A uniform, two-dimensional Cartesian grid with cell size H/15 was used for all computations, as reported in Figure 3.

Figure 3 also reports predicted flow structures with all turbulence models but the non-linear one, which did not successfully converge for this simulation. Predictions of the reattachment region were in line with the literature: x/H being 5.93 for the standard k-epsilon model, 7.06 for RNG k-epsilon, 6.73 for the fixed RNG k-epsilon, and 6.67 for the GRNG k-epsilon model, versus the measured experimental value of 6.6. Corresponding axial velocity profiles are reported in Figure 4. The axial velocity profile predictions reflect measured profiles reasonably well for all cases, the differences among them highlighting the causes for the slight discrepancies in predicting reattachment: the standard k-epsilon exhibits the smallest axial velocity gradient along the vertical line, while the GRNG model exhibits the strongest one. These results confirmed the unsuitability of the standard k-epsilon model in capturing recirculation flows, and the closest result was achieved by the GRNG k-epsilon model implementation. Both RNG model implementations, with or without rapid distortion limit fix, provided accurate results; the fix helped improve prediction accuracy for the recirculation bubble noticeably. In general, all RNG turbulence models appeared equally able to model this type of recirculation flows, the GRNG yielding the optimal simulation results.

**Impinging Gas Jet**

The second academic test case featured an impinging gas jet stream, descending from a long circular channel and impacting against a wall normal to the stream direction, following the experiments of [21,22]. A schematic of the domain employed for the current test case is reported in Figure 4: the flow field was initialized as quiescent, and a uniform bulk inlet velocity boundary condition corresponding to a Reynolds number $Re_d =$
23,000 was used. The simulation was run for 5 channel flow-thru times, where a total channel length of 80 diameters was employed to let the turbulence model develop a fully turbulent channel velocity and turbulence kinetic energy profiles, as well as to achieve proper steady-state solution convergence. The wall configuration featured distance to the pipe outlet h/d = 2, the channel diameter being d = 2.6 cm as from the experiments. Far from the jet impingement regions, zero gradient boundary conditions were imposed for all field quantities. A uniform computational mesh with cell size dx=d/25 was used.

A representation of the resulting steady-state flow field in the proximity of the pipe outlet and wall impingement region is represented in Figure 5, for the GRNG turbulence case. The jet at the channel outlet owns an unperturbed, parabolic velocity profile with peak velocity magnitude at the centerline of about 30% greater than the average bulk inlet velocity. Velocity reaches zero at the stagnation point, while the jet is being deflected outward and backward.

The accuracy of all turbulence models was assessed versus experimentally measured average velocities and turbulent fluctuation velocities, available at fixed radial distances from the pipe centerline along vertical lines of sight located at x/d = 0.5, 1.0, 2.5, as reported in Figure 6. The non-linear model again did not converge.

Figure 4. Two-dimensional domain representation and boundary conditions for the impinging gaseous jet test case.

Figure 5. Axisymmetric vertical cross-section of velocity magnitude contours at pipe outlet and jet impact region, normalized by average inlet bulk velocity. GRNG k-epsilon turbulence model. Lower-left corner highlights stagnation point.
The first radial coordinate, x/d = 0.5, is located exactly at the pipe radius, and the bulk velocity profile is almost flat, only slightly increasing towards the wall, z=0. All turbulence models predict nearly-identical bulk velocities close to the pipe (z↑), while slightly overpredicting it as moving towards the wall (z↓). The standard k-epsilon model, typically over-dispersive, consistently shows lower velocities, more in line with what seen in the experiments.

However, these lower velocities come at the price of much higher predicted turbulence fluctuations. All turbulence models exhibit a tendency towards over-predicting turbulence fluctuations, as also observed in [22], but with different patterns. Along the stagnation line (or symmetry axis in the 2D simulation), as from Figure 7, the predicted fluctuations yield better results closer to the pipe outlet, while overpredicting turbulence fluctuations closer to the stagnation point. At stagnation, the RNG models over-predict uprime by up to 100%, while the standard k-epsilon model reaches a >300% overestimation immediately before the wall.

In Figure 6, farther from the stagnation line, typical gaseous jet profiles become evident. At x/d = 1.0 and x/d = 2.5, the generalized RNG k-epsilon model represents very accurately the bulk velocity profiles, which suggests superior performance in capturing shear jet flows. The standard k-epsilon model shows again the greatest over-dispersion, and the highest turbulence levels correspondingly. Again, all turbulence models match turbulent fluctuation velocity trends fairly accurately, especially at the x/d=1.0 location, where the GRNG model provides very good predictions. However, all RNG models tend to overpredict turbulent fluctuations when moving outward from the centerline, until at x/d=2.0 near-wall uprime is underpredicted by more than 35% for all models. This could indicate inadequacies of the turbulent law of the wall boundary condition formulation for these wall-dominated flows. Also, it should be noted that employing a non-uniform, more refined resolution in the near-wall region than the current d/25 (or z/D = 0.04) could help better represent the steep gradients experienced at the stagnation point and in general close to the wall surface.

**Diesel Engine Test Cases**

**In-cylinder Flow in a Light-Duty Diesel Engine**

Experiments and modeling of the Sandia National Laboratories optical light-duty diesel engine were performed in order to...
characterize in-cylinder flow structures for a swirl-supported engine configuration. The experimental assembly features a single cylinder, optically accessible engine, adapted from a production General Motors 1.9L light-duty engine, which has undergone extensive research during recent years [23,24]. Optical access to the cylinder is granted through fused silica windows (50.7 mm x 25 mm), located at the top of the liner, as well as a fused silica piston. The optical piston shape resembles the production engine’s geometry, including piston bowl shape and valve cut-outs on the piston surface, the only difference being a wider crevice as well as larger top land height, which cannot be avoided to allow imaging within the piston bowl. A summary of the engine specifications is reported in Table 3.

The experimental setup for in-cylinder flow measurements features charge conditions relevant to a moderately boosted, low-load operating condition (“LTC3”), also reported in Table 3, which has been subject to a number of studies devoted at achieving an understanding of low-temperature combustion strategies in light-duty engine configurations [25]. The experimental campaign targeted in-cylinder flow structure via Planar Image Velocimetry (PIV) during the intake and compression stroke: each image being generated as the ensemble average from a statistically significant number of compression strokes, owning an average cell resolution of 0.7 mm in the combustion chamber near TDC, similar to what was found in a previous study to guarantee appropriate convergence of the spray combustion simulations in the same engine, when a sector mesh model was employed [28]. The mesh resolution in the valve regions was also previously tested, and it was found that it could provide converged predictions of the intake mass flows when 27 cell layers were employed for the full valve lift [2].

Comparisons of in-cylinder flow field predictions with the different turbulence models are reported in Figures 8 and 9. Both figures do not report results from the nonlinear RNG k-epsilon model, since the solver diverged at any accuracy tolerances tested. The RNG-fix turbulence model predictions have also been omitted for clarity reasons, since they provided nearly identical results as those from the classic RNG model implementation. Flow patterns were visualized by decomposing the Cartesian coordinates \((u, v)\) of the horizontal flow field at the measurement planes into tangential and radial velocity scalars, \((v_\theta, v_r)\):

\[
\begin{bmatrix}
-r \sin \theta \\
 0 \\
 r \cos \theta \\
 -\sin \theta \\
 \cos \theta
\end{bmatrix}
= \begin{bmatrix}
u \\
v_r
\end{bmatrix},
\]

then

\[
v_\theta = \theta r \\
v_r = \dot{r}
\]

in order to decompose the flow field into features which relate to strain, which in the cylinder is a result of swirl flow, or compression, as represented by the radial, or squish flow induced by piston motion. For clarity, three lines-of-sight were selected: one running below the exhaust valves, one at the cylinder centerline, and one below the intake valves.

Figure 8 reports the decomposed flow patterns for a fixed horizontal location 10 mm from the fire-deck at three crank angles during the intake stroke. All turbulence models overestimate peak tangential velocity values, with the GRNG model predicting larger tangential velocity components especially early during the intake stroke. At 240 degrees bTDC, the standard k-epsilon model yields the best predictions, especially at the centerline. All models seem to predict faster bulk swirl motion: PIV shows that bulk tangential motion entering from the tangential port (in the left-hand-side of the plot) is still below the intake port, while all simulations show this bulk flow motion has already reached the centerline.

Smaller differences are seen in the radial components, but some effects of the different formulations for the compression flow term are still visible: the RNG model features larger low flow compression at the centerline (negative radial velocity components), as a result of the imbalance towards compression in Equation (8); in the GRNG model, even larger compression is seen by the addition of the dimensionality term. In any case, the predicted flow structures get closer to each
other towards the late induction stroke, where the valve lift is reducing significantly, and by bottom dead center only slight deviations are seen in the tangential velocities between the standard k-epsilon model and the similar two predictions from the renormalized ones.

Results during the compression stroke are reported in Figure 9 at 60 degrees before TDC and three different horizontal locations in the cylinder. This crank angle was selected towards the end of the compression stroke, but still before significant squish flow can take place. Here, in-cylinder motion is represented by a well-established, nearly-vertical swirl vortex. All turbulence models capture flow properties acceptably well compared with PIV. Nonetheless, the
Figure 8. In-cylinder flow in the Sandia light-duty engine during the intake stroke, at (left to right) 240, 210 and 180 degrees bTDC: (top) tangential velocity, \( v_\theta \) (bottom) radial velocity, \( v_r \) at a horizontal plane located 10 mm from the fire-deck [27].

Figure 9. In-cylinder flow in the Sandia light-duty engine during late compression stroke, at 60 degrees bTDC: (top) tangential velocity, \( v_\theta \) (bottom) radial velocity, \( v_r \) at three horizontal planes located 3, 10, 18 mm from the fire-deck [27].
RNG and GRNG turbulence models have converged to very similar predictions, while the standard k-epsilon model exhibits some differences. In particular, very close to the fire-deck, only the standard k-epsilon model appears to capture correctly both the tangential and radial velocity profile, both at the centerline and below the valves. However, the two renormalized turbulence models show acceptably accurate predictions below the valves, but miss capturing the inversion in radial components near the centerline.

Overall, all three models provided acceptable accuracy versus the PIV measurements, with the standard k-epsilon model yielding the smoothest flow behavior in any configuration. Its over-dispersive behavior might not necessarily aid accuracy during the intake stroke, when severe distortion and compression effects coexist because of the near-sonic intake flow, swirl generation and piston motion. However, this seems to lead to more accurate predictions later during the compression stroke, where most of the initial non-uniformities are dissipated into a well-defined shear-and-compression flow configuration.

**Non-reacting ECN Spray A**

The first validation featuring a fuel spray was performed by modeling the Engine Combustion Network non-reacting Spray A experiments, which use n-dodecane as a fuel, T=900K ambient temperature, and 0% oxygen [29]. The constant-volume chamber geometry was discretized with a fully three-dimensional mesh instead of the commonly-adopted two-dimensional or azimuthal mesh, to achieve a more similar simulation setup to a typical engine simulation configuration. The mesh has a locally refined central jet-shaped core, and the minimum cell height exists near the nozzle, geometrically increasing along the jet axis and radially outward, as represented in Figure 10. The inner core extends conically with a semi-cone angle of 5.5 degrees. The grid resolution, intentionally similar to that of the full engine model, has an average near-nozzle cell size of 1.0 mm, and a total of about 19 thousand cells.

Turbulence model comparisons for vapor and liquid penetration results are reported in Figure 11. Because a direct comparison between the imagery-based measurements and simulation data is not possible, we compiled to the Engine Combustion Network guidelines. The liquid penetration predictions were evaluated computing the downstream location where the cumulative liquid mass reached 90% of the total instantaneous liquid fuel in the chamber; vapor penetration was computed as the farthest cell centroid location where a fuel volume fraction of at least 10 ppm was present. In the simulations, no change in spray model constants was applied for the breakup, collision and sub-grid scale momentum coupling models, using the optimal configuration of [5].

Liquid phase predictions were not significantly affected by the turbulence model choice, even if slight deviations in near-steady-state liquid length could still be seen – in particular, the standard k-epsilon model yielded the lowest liquid length prediction. Significant deviations were instead seen for the vapor phase. Among all models, the generalized RNG model showed greatest vapor jet penetration downstream in the chamber, the only one matching measured vapor penetration correctly. All non-generalized RNG models, including the standard one and the nonlinear one, showed similar behavior, and underestimated vapor penetration by about 13% versus the measured value, with almost negligible differences between their formulations. Interestingly, the nonlinear RNG model led to a somewhat slower penetration of the fuel vapor jet into the quiescent chamber shortly after the start of injection: this is a sign that the second-order expansion of the Reynolds stress tensor enhances turbulence generation when
steep velocity gradients are present, in spite of the bulk flow motion. Later on during the steady-state part of the injection, all RNG models show similar liquid- and vapor-phase penetration, suggesting that adding second-order stress tensor terms might not be worth the additional computational burden and complexity.

Predicted mixture fraction distributions are reported in Figure 12 for the steady-state jet conditions taken at t=5.5 ms, i.e., not much before
the end of the injection. The axial penetration plot shows that all simulations have reached farther downstream locations than actually measured, confirming the acceptability of this snapshot for the steady-state region. Measured distribution profiles were extracted from an ensemble-averaged image of the mixture fraction distribution, integrated azimuthally, and provide averages and standard deviations versus distance from the injection axis at select downstream locations \(dz=20, 30, 40, 50\) mm, plus axially, along the jet centerline.

The generalized RNG k-epsilon model performs best at all observation planes, as correct vapor phase penetration seems to correspond to a correct jet structure prediction. All other models, which noticeably underestimate vapor penetration, also predict a much greater radial jet dispersion, with lower axial peak mixture fractions, and wider jet spreading angles. It should also be noted that linear and nonlinear RNG models predict a very similar gaseous jet structure as the GRNG model in the near nozzle region \(dz\leq15\) mm, i.e., both in ramp-up and peak mixture fraction distribution, suggesting that the differences exhibited downstream are specific of the turbulence model, and should not be related to upstream spray modeling: it could be possible to partially compensate for the overdispersion phenomenon in the RNG models by changing spray model constants so as to reduce the liquid spray cone angle, and consequently increase centerline mixture fraction, but the jet would likely still spread out sufficiently downstream.

Also, the nonlinear RNG model does not seem to be able to compensate for this phenomenon, as the predicted mixture fraction distributions essentially overlap with the linear RNG models. The standard k-epsilon model exhibits instead even more severe dispersion and lack of vapor penetration.

**Reactive ECN Spray A**

The same simulation was used to validate reactive and sooting Spray A experiments, employing the same n-dodecane fuel and similar high-pressure, high-temperature chamber conditions from [30]. In the reacting simulations, a reduced n-dodecane reaction mechanism previously validated against soot formation predictions was used. The soot formation rate was modeled according to the two-step approach of Hessel et al. [31], using the single-equation Hiroyasu model for the soot formation term, acetylene as the soot-forming species and the Nagle and Strickland-Constable model for the O2-based soot oxidation mechanism.

Flame lift-off length and ignition delay times for environments having 15% oxygen concentration and 22.8 kg/m\(^3\) density were analyzed according to the ECN guidelines by Skeen et al. [32], using the same mesh resolution as for the non-reactive conditions. Average OH radical concentrations versus axial distance from the nozzle is computed, and the instantaneous lift-off length is identified as the location at which OH concentration reaches 50% of the maximum concentration during the initial ramp-up region, i.e., before reaching the near-steady downstream plateau. Ignition delay was instead defined as the time at which the maximum temperature rise rate for the cell with maximum temperature in the chamber occurs. Chamber temperatures sweeping from 750K to 1200K were considered and compared with the experimental measurements in Figures 13 and 14 – as well as computational results from other Institutions – reported by Skeen et al. [32]. Finally, it should be noted that, as the focus of this paper is on turbulence model behavior, no modifications were introduced to the n-dodecane reaction mechanism, whose behavior was assumed to be ‘good and consistent enough’ for this test.
Chemical kinetics was coupled to the flow model using direct chemistry integration, i.e., assuming each cell is a well-mixed reactor.

Figure 13. Reacting Spray A validation: predicted ignition delay times from different turbulence models for a 15% O₂ and varying temperature environment, versus ECN as well as other institutions’ calculations.

Figure 13 reports predicted ignition delay times: all turbulence models behaved smoothly, reporting exponentially increasing ignition delay times with lower temperatures, as seen in the experiments. However, some significant deviations are seen especially at temperatures lower than 1000K, where the standard, RNG and GRNG turbulence models exhibit comparatively similar behavior as the experiments, while the nonlinear and RNG-fix model predict noticeably higher ignition delay times. The RNG and GRNG models predicted identical behavior across the whole temperature range, highlighting that their differences in mixture fraction distribution might affect the location of the first ignition point, but not its timing.

Looking at flame lift-off lengths gives a more comprehensive idea of the models’ behavior, as reported in Figures 14 to 16. The temperature sensitivity of the steady-state lift-off length is reported in Figure 14, and highlights relevant differences in behavior: the standard k-epsilon model predicts noticeably lower lift-off length than any other k-epsilon model at all temperatures in the range. Again, the RNG and GRNG models exhibited closest behavior to the

Figure 14. Reacting Spray A validation: predicted lift-off length values from different turbulence models for a 15% O₂ and varying temperature environment, versus ECN as well as other institutions’ calculations.

Figure 15. Predicted temperature profiles from different turbulence models for a 15% O₂, 800K environment. White dots represent spray.
In order to compare model behavior in predicting steady state flame structures, two temperature values of interest, 800K and 1200K, were chosen where the largest discrepancies among turbulence models were seen, as reported in Figures 15 and 17. Corresponding measured flame structure from OH chemiluminescence is reported for reference in Figure 16 [33].

At both temperatures, different flame structures are seen. The RNG and GRNG turbulence models predict a less radially disperse flame, consistently with the more compact mixture fraction distribution in the non-reactive case, as well as deeper penetration, which is in line with what seen in the experiment. At the highest temperature, these models also show better agreement in lift-off length development, happening immediately downstream of the liquid spray jet. Similar considerations apply also for the RNG-fix and nonlinear models, which however, predict a slightly smaller penetration, and in particular do not capture the ‘bubbly’ flame tip structure, i.e., the amount of high-temperature mixture at z>8cm, also seen in the experiments. This ‘bubbly’ tip is best predicted by the GRNG model, resulting from the expansion of the high-temperature gases immediately upstream.

The standard model shows instead the worst predictions both in penetration, dispersion, and lift-off length, the latter having advanced towards the injector and into the liquid core region, likely as a result of the predicted excessive air entrainment into the jet. This behavior is seen at both temperatures, and explains the severe underestimation of lift-off length seen at all cases.

Overall, both un-corrected RNG and GRNG models agreed best with the experimental measurements at all temperature ranges, confirming the better suitability of these models for jet shear flows. While meeting the flame lift-off well, the GRNG model was also able to predict correct jet dispersion and jet tip structure, which were instead slightly overdispersed by the RNG model.

**Concluding Remarks**

In this work, several two-equation turbulence models of the k-epsilon class were implemented in an object-oriented parallel engine CFD simulation platform, and compared to assess their suitability for simulations of turbulent combustion in diesel engines. Focus was on understanding whether introducing anisotropies in the modeled Reynolds stress tensor could enhance simulation accuracy for complex turbulent flow configurations equally dominated by shear and normal stresses due to swirling motion, jet flow (either from a spray or from intake ports), and wall impingement.

The set of test cases featured: channel flow with a sudden expansion, gaseous jet impingement, high-pressure fuel spray injection in non-reactive and reactive environments, as well as in-cylinder flows in a light-duty optical diesel engine. Based on the results, the following observations could be drawn for each model:

- The standard k-epsilon model provided essentially the worst agreement at all tested cases except for the case of in-cylinder flow motion, where it exhibited...
somewhat better predictions when in presence of large flow nonuniformities. It failed in capturing reattachment in the backward facing step and predicted too over-disperse jet flows, which also led to augmented entrainment and incorrect prediction of lift-off length in diesel spray flames;

- The standard RNG k-epsilon model predicted consistent flow structures across all cases, confirming its robustness to model a wide variety of flows without changing any calibration constants, also suggesting that the coarse-graining procedure at the basis of its renormalization method applies well to engine-type turbulence;

- Fixing the RNG model’s rapid distortion correction only affected the simulations of high-pressure jets, reactive or non-reactive. In these cases, the fix led to predicting slightly more disperse jets; still, the slight deviations from the non-corrected case did not add up to meaningful quantitative differences;

- The additional computational complexity due to the second-order expansion of the Reynolds stress tensor in the non-linear RNG model introduced instability in the linear system solver, which often led to failure to reach convergence. Even in the cases where the simulation could be completed successfully, no significant improvements over other linear RNG formulations could be achieved, even at the price of substantially higher computational time;

- Finally, the GRNG turbulence model provided beneficial improvements in all test cases, without compromising on computational demands or robustness from the original RNG model. It often yielded extremely close results to experimental values, for example in capturing the reattachment location downstream of the backward-facing step, and the fuel vapor jet structure and penetration behavior, as well as flame structure in the reactive spray cases, where none of the isotropic k-epsilon models provided such a high accuracy.

In conclusion, the present results suggest the adoption of the GRNG model for achieving reliable ensemble-averaged diesel engine flow and combustion simulations, while not requiring computational overhead in comparison with other common two-equation turbulence models.

References


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Nomenclature

δij  Kronecker operator [-]
ε  Turbulence kinetic energy dissipation rate [cm²/s²]
φ  generic finite-volume field quantity
k  Turbulence kinetic energy [cm²/s²]
L  Integral turbulence length scale [cm]
ν  Spatial derivative [1/cm]
µt  Eddy viscosity [g/cm/s]
ν  Kinematic viscosity [cm²/s]
P  Turbulence kinetic energy production [g/(cm s²)]
ρ  Density [g/cm³]
Re  Nondimensional Reynolds number [-]
u, u  velocity vector [cm/s]
u'  Turbulence fluctuation velocity [cm/s]
S, Sij  Mean strain rate tensor
τ  Reynolds stress tensor [g/cm²]

Definitions/Abbreviations

CFD  Computational Fluid Dynamics
ECN  Engine Combustion Network
https://ecn.sandia.gov/
FRESCO  Fast, Robust Engine Simulation COde
GRNG  Generalized Renormalization group.
LES  Large Eddy Simulation
PTV  Particle Image Velocimetry
RANS  Reynolds-Averaged Navier Stokes
RNG  Renormalization group
TDC Top dead center