Numerical study using detailed chemistry combustion comparing effects of wall heat transfer models for compression ignition diesel engine

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Abstract

The present work highlights the effect of wall heat transfer models on numerical predictions of combustion phenomenon in compression ignition diesel engine. A comparison of engine's performance is made using *O'Rourke and Amsden*, *Han and Reitz* and *Angelberger* heat transfer models. A detailed chemistry model employed comprises of 61 species and 235 reactions for n-heptane/diesel combustion. RANS RNG k- ϵ turbulence model (*Reynolds-averaged Navier–Stokes*: RANS; *re-normalisation group*: RNG; *turbulent kinetic energy—rate of dissipation of turbulence energy*: k- ϵ turbulence model) is used here to model mass, momentum and energy transport equations for engine computational fluid dynamics simulations. The study performed is on turbocharged 130PS 5.675L diesel engine and presented against experimental findings. Effect of different wall treatment models on accuracy and inherent computational time requirement for predicting engine $P-\theta$ (cylinder pressure vs. crank angle) curve, indicated mean effective pressure and AHRR (apparent heat release rate) is discussed in this paper. This comparative study facilitates in choosing optimum heat transfer model for in-cylinder combustion study vis-à-vis the trade-offs between solution accuracy (which drives product quality) versus computational time (which drives time to market).

Keywords IC engine combustion · Wall heat transfer model · Chemical kinematics · CFD · Solution accuracy

1 Introduction

S. Šarić, B. Basara et al. proposed in their work “*Advanced near-wall heat transfer modelling for in-cylinder flows*” in International Multidimensional Engine Modelling User's Group about the effect of the wall heat transfer model on the heat flux and validated in the spark ignition engine [1], whereas Chris Angelberger et al. proposed their advanced model in their article on “*Improving Near-Wall Combustion and Wall Heat Transfer Modeling in SI Engine Computations*” which proposes an approach towards improving near-wall heat transfer model in SI engine combustion [2]. Although there are much studies which suggest the advancement in the model as “*A Spray/Wall Interaction*

Submodel for the KIVA-3 Wall Film Model” by P. J. O'Rourke et al. [3, 4], we have very limited literature which gives us a comparative analysis of each wall heat transfer model. Sanjin Šarić et al. further in their work “*A Hybrid Wall Heat Transfer Model for IC Engine Simulations*” explained the limitations of Han and Reitz heat transfer model and suggested modifications [5]. A Sircar et al. in their work “*An assessment of CFD-based wall heat transfer models in piston engines*” illustrated the effect on prediction behaviour with Angelberger wall heat transfer model and stated further comparison is required for turbulence quantities [6]. Wall heat transfer model's references are widely illustrated for spark ignition engines [7], but at the same time for compression ignition engines, for reference the literature

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resources are limited. The work highlights the importance of choosing wall heat transfer model and the effect in predicting performance characteristics of the model. Each wall heat transfer model is applied on the geometry with the same mesh upon performing a grid independency test [8]. The work can act as a reference for simulation performed across the globe for compression ignition diesel engine. The simulation results are compared with the experimental data. The experimental data are taken from reference of a standard turbocharged 130PS 5.675L diesel engine (Table 1).

1.1 Engine specifications

The analysis is done at operating point, i.e. 2200 rpm, 547Nm torque, and at full load condition. The parameters are kept constant throughout the study both physical and chemical, and a comparative study is presented between three wall heat transfer models. As observed in the study with different wall heat transfers model used for compression ignition engine simulation, all fall in permissible error range, but at the same time we need to check the level of accuracy of each of them for a precise and accurate study; having an idea of the model to be used also saves the computational time. Each wall heat transfer model as is having a specific mathematical model implies different computation time. For example, Han and Reitz heat transfer model takes into account the dynamic density variation, and hence, the computation time increases as the validation for boundary condition increases in parallel. Our purpose is to validate wall heat transfer model for a compression ignition engine having performance characteristics as the benchmark.

2 Modelling approach

The modelling is done on a standard CFD in-cylinder combustion software having all the three wall heat transfer schemes with a rich library for turbulence model in which RNG k- ϵ is chosen for study. The solution is obtained from the set of governing equations, law of conservation of mass, momentum, energy and species in

a three-dimensional in-cylinder in a CRDI diesel engine [9–11]

The turbulence modelling approach picked here is RNG k- ϵ . The RNG model was developed using re-normalisation group (RNG) methods by Yakhot et al. to renormalise the Navier–Stokes equations, to account for the effects of smaller scales of motion. In the standard k-epsilon model, the eddy viscosity is determined from a single turbulence length scale, so the calculated turbulent diffusion is that which occurs only at the specified scale, whereas in reality all scales of motion will contribute to the turbulent diffusion. The RNG approach, which is a mathematical technique that can be used to derive a turbulence model similar to the k-epsilon, results in a modified form of the epsilon equation which attempts to account for the different scales of motion through changes to the production term [12–15].

The combustion modelling is done on a standard reduced Engineering Research Center-Mechanism. The Engine Research Center had developed reaction mechanism of n-heptane to simulate diesel fuel chemistry. The method used for mechanism development is a combination of SENKIN, XSENKPLLOT and genetic algorithm. The mechanism can be used efficiently for multi-dimensional engine CFD modelling of diesel engines.

The meshing used is adaptive mesh refinement. The meshing technique basically works on the immerse boundary condition and eliminates the general problem of predefined-mesh quantification which cannot be dynamic as per real-time solution generated. The maximum cell counts are restricted here to 15 millions cells after a grid enhancement testing validation (Fig. 1).

Fuel species used for study is diesel (in liquid phase) and n-heptane—C₇H₁₆ (in gas phase after evaporation) as full kinetic dual fuel model is too complex and data information availability is also limited, so n-heptane is used as fuel surrogate for primary fuel in gas phase. Flow, thermal and turbulence model is Reynolds-averaged Navier–Stokes model (RNG k- ϵ) for continuity, momentum and energy equations. Spray break model is based on Lagrangian transport equations, with KHRT droplet breakup and NTC-collision approach. Boiling–evaporation model adapted is Forssling evaporation model having spray wall interaction model as rebound and slide [16, 17]. Equation of state is Redlich Kwong which is an empirical, algebraic equation that relates temperature, pressure and volume of gases. Solver parameter used for pressure velocity coupling is Rhie–Chow scheme, which is mostly applied with the aim of improving computational efficiency and speeding the coupling process especially where non-Cartesian meshing is done.

Table 1 Engine specification

Engine displacement	5675 cc
Rated power	134.1bhp@2400 rpm
Number of cylinders	6
Type	Turbocharged
Operating fuel	Diesel
Rated torque	490 Nm 1400–1800 rpm

3 Experimental setup

4 Mathematical model

- 1) Angle Encoder mounted on Crank pulley
- 2) Aperture Pressure Sensor

shear speed (taken from the momentum law of the wall) (Fig. 3).

$$u_{\tau} = c_{\mu}^{1/4} k^{1/2}, \quad (1)$$

4.1 Han and Reitz wall heat transfer model

$$k \frac{dT}{dx_i} = \begin{cases} \frac{\mu c_p (T_f - T_w) n_i}{y \text{Pr}_m} & y^+ < 11.05 \\ \frac{\rho c_p u \tau \ln \left(\frac{T_f}{T_w} \right) n_i}{2.1 \ln(y^+) + 2.513} & y^+ > 11.05 \end{cases} \quad (2)$$

4.2 O'Rourke and Amsden wall heat transfer model

$$k \frac{\partial T}{\partial x_i} = \frac{\mu_m C_p F (T_f - T_w)}{\text{Pr}_m y} n_i \quad (3)$$

Fig. 3 Comparison of each wall heat transfer model curves pressure versus crank angle

where

$$F = \begin{cases} 1.0 & y^+ < 11.05 \\ \frac{\left(\frac{y^+ Pr_m}{Pr_t}\right)}{\frac{1}{\kappa} \ln(y^+) + B + 11.05 \left(\frac{Pr_m}{Pr_t} - 1\right)} & y^+ > 11.05 \end{cases} \quad (4)$$

$$y^+ = \frac{\rho \mu_\tau y}{u_m} \quad (5)$$

The O'Rourke and Amsden wall film model predicts film transport on complex surfaces, heating and vaporisation of the film, and separation and re-entrainment of the liquid film at sharp corners it also incorporates the effects associated with spray/wall interactions—including droplet splash, film spreading due to impingement forces, and motion due to film inertia. The model is specially design in a way to perform study for IC engine, and the computational time is also relatively lesser than the other two models and hence is optimised for operation [4].

4.3 Angelberger wall heat transfer model

$$k \frac{dT}{dx_i} = \frac{\rho_w c_p u_\tau \ln\left(\frac{T_t}{T_w}\right) n_i}{\theta^+} \quad (6)$$

where

$$\theta^+ = \begin{cases} Pr y^+ & y^+ \leq 13.2 \\ 2.075 \ln(y^+) + 3.9 & y^+ > 13.2 \end{cases} \quad (7)$$

The Angelberger model accounts for quasi-isothermal flow (e.g. in intake pipes or compression during engine simulations) and for non-isothermal wall flow (e.g. in the combustion chamber during combustion or in exhaust pipes). The Angelberger model consistently predicts lower wall heat fluxes than the Han and Reitz model [2].

5 Results

The result is plotted and pressure versus crank angle curve is compared, and further, the values of IMEP are compared and the wall heat transfer model with least error is taken for further study and analysis.

The Han and Reitz model underpredicts the indicated mean effective pressure value which is above the permissible limits as of more than 10% error. The O'Rourke Wall heat transfer model underpredicts the result by 2% which is nearly close to the actual value while the Angelberger wall heat transfer model overpredicts the value by 4% which is not acceptable for further study. Also as we

observe the apparent integrated heat release rate plotted from start of injection to exhaust valve opening, the mean curve follows the path of simulation curve obtained from O'Rourke model. So O'Rourke heat transfer model gives a close prediction for performance parameter (Fig. 4 and Table 2).

6 Discussion

The boundary conditions and the precise modelling enable the O'Rourke model for predicting the performance characteristics curve very close to that of the experimental result. On the other hand, Han and Reitz account for the compressible effects; in this particular model, there is a gap in predicting the result as compared to the O'Rourke model, whereas Angelberger is suitable for modelling the quasi-isothermal case where the gap between the film temperature and wall temperature is relatively lower as suggested by its physics and boundary conditions.

O'Rourke and Amsden wall heat transfer model predicts film transport on complex surfaces, heating and vaporisation of the film, and separation and re-entrainment of the liquid film at sharp corners. Vaporisation of the films is due to differences between the fuel vapour mass fraction

Table 2 Comparison between performance parameter with each wall heat transfer model

Wall heat transfer model	Han and Reitz	O'Rourke	Angelberger
Rotation per minute	2200	2200	2200
Indicated mean effective pressure (bar)	13.05	14.28	15.20
%Error	10.54	2.10	−4.20

in the bulk gas above the films and the vapour mass fraction at the surface of the film determined by its surface temperature. The film surface temperature is determined implicitly by a wall film temperature equation. The parameters such as mass, momentum and energy are also well predicted by the wall functions for turbulent boundary layers near the films which are in vaporising state.

7 Conclusion

Since the O'Rourke wall heat transfer is giving the most optimised result both from the point of 'accuracy' as illustrated and computational feasibility as the computation time for O'Rourke being X is $1.25X$ and $1.75X$ for

Fig. 4 Comparison of each wall heat transfer model for apparent integrated heat release rate

Angelberger and Han and Reitz, respectively. O'Rourke and Amsden wall heat transfer model is observed to be suitable for study for in-cylinder CFD combustion study for mapping performance parameter of a standard diesel engine.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

References

- Šarić S, Basara B et al. (2015) Advanced near-wall heat transfer modelling for in-cylinder flows. In: International multidimensional engine modeling user's group meeting at the SAE congress, Detroit, MI, 20 April 2015
- Angelberger C, Poinot T, Delhay B (1997) Diagnostics and modeling in SI engines improving near-wall combustion and wall heat transfer modeling in si engine computations. SAE technical papers. <https://doi.org/10.4271/972881>
- O'Rourke P, Amsden A (1996) A particle numerical model for wall film dynamics in port-injected engines. SAE technical paper 961961. <https://doi.org/10.4271/961961>
- O'Rourke P, Amsden A (2000) A spray/wall interaction sub-model for the KIVA-3 wall film model. SAE technical paper 2000-01-0271
- Sanjin Saruc et al. (2015) A hybrid wall heat transfer model for IC engine simulations. SAE technical papers
- Sircar A et al. (2017) An assessment of CFD-based wall heat transfer models in piston engines. In: 10th U. S. national combustion meeting
- Piazzullo D, Costa M, Allocca L, Montanaro A et al (2017) A 3D CFD simulation of GDI sprays accounting for heat transfer effects on wallfilm formation. SAE Int J Engines 10(4):2166–2175
- Sideri M, Berton A, D'Orrico F (2017) Assessment of the wall heat transfer in 3D-CFD in-cylinder simulations of high performance diesel engines. Energy Procedia 126:963–970
- Lakshminarayanan PA, Aghav YV (2010) Modelling diesel combustion. Springer Science and Public Media, Berlin
- Ahmadi-Befrui B, Uchil N, Gosman AD, Issa RI (1996) Modeling and simulation of thin liquid films formed by spray-wall interaction. SAE paper 960627
- Plengsa-ard C, Kaewbumrung M (2018) CFD modelling wall heat transfer inside a combustion chamber using ANSYS forte. In: IOP conference series: materials science and engineering. vol 297, p 012036. <https://doi.org/10.1088/1757-899x/297/1/012036>
- Ihme M et al. (2016) Non-equilibrium wall-modeling for large-eddy simulation of internal combustion engines. In: THIESEL 2016 conference on thermo—and fluid dynamic processes in direct injection engines
- Seo J, Lee JS, Choi KH, Kim HY, Yoon SS (2013) Numerical investigation of the combustion characteristics and wall impingement with dependence on split-injection strategies from a gasoline direct-injection spark ignition engine. Proc Inst Mech Eng Part D J Automob Eng 227(11):1518–1535
- Costa TJ, Nickerson M, Littera D, Martins J, Shkolnik A, Shkolnik N, Brito F (2016) Measurement and prediction of heat transfer losses on the XMv3 rotary engine. SAE Int J Engines 9(4):2368–2380
- Zhang Y, Liu Z, Zuo Q, Xiao B, Sun S, Fu J (2018) Heat transfer model for high power density internal combustion engine based on fluid-solid coupling model. Zhongnan Daxue Xuebao (Ziran Kexue Ban)/J Central South Univ (Sci Technol) 49:2330–2336. <https://doi.org/10.11817/j.issn.1672-7207.2018.09.028>
- Zhang Y (2014) Development of a new spray/wall interaction model for diesel spray under PCCI-engine relevant conditions. At Spray 24(1):41–80. <https://doi.org/10.1615/atomizspr.2013008287>
- Jia M, Gingrich E, Wang H, Li Y, Ghandhi JB, Reitz RD (2016) Effect of combustion regime on in-cylinder heat transfer in internal combustion engines. Int J Engine Res 17(3):331–346. <https://doi.org/10.1177/1468087415575647>
- Gokul Raj CR et al (2018) Combustion and emission characteristics of a direct injection diesel engine at various EGR conditions—a numerical and experimental study. Eur J Adv Eng Technol 5(1):35–42
- Deng P, Han Z, Reitz RD (2016) Modeling heat transfer in spray impingement under direct-injection engine conditions. Proc Inst Mech Eng Part D J Automob Eng 230(7):885–898

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