Development and Use of LES for Diesel Engine CFD

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Large eddy simulation is a promising advancement for IC engine modeling. This requires appropriate models for a many physical processes. This paper classifies and briefly describes the major types of models for turbulence, combustion, and sprays. Representative references are listed with an emphasis on engine applications. Recommendations for modeling approaches to use in engine LES are also provided.

Introduction

It is generally agreed that the next generation of turbulence modeling in computational fluid dynamics (CFD) for many applications will be some form of large eddy simulation (LES) [1,2]. For the appropriate applications, LES can offer significant advantages over traditional Reynolds Averaged Navier Stokes (RANS) modeling approaches. In internal combustion (IC) reciprocating engines LES can be used to study cycle-to-cycle variability, provide more design sensitivity for investigating both geometrical and operational changes, and produce more detailed and accurate results. There are also characteristics of IC engines such as inherent unsteadiness and a moderately sized domain that are well suited to LES. However, there can be many difficulties in using LES for the multi-phase, reacting, turbulent flows in complex internal combustion engine geometries. In addition, LES in IC engines is new and there are potential uncertainties and ambiguities since a generally accepted 'best practice' is still developing. This report lists current LES models that could have application to IC engines and briefly evaluates their suitability and potential predictive capability for engine CFD.

LES Turbulence Models

The turbulence model in LES simulations is for sub-grid stresses in the momentum equation. It is the primary model in LES since it should allow for flow structures in the solution. Table 1 classifies the major approaches to LES turbulence models and briefly states advantages and disadvantages. This table does not list more esoteric but includes only modeling approaches that are likely to find use in practical applications.

LES Combustion Models

There is a rich tradition of combustion modeling [10] much of which has been adapted for engine simulations. In many cases, users have simply taken RANS combustion models and used them with LES turbulence models. This is a type of hybrid approach and has proven useful. However, as LES use in engines matures, more attention is being given to either adjusting or even reformulating basic combustion models for use in LES. Table 2 classifies and briefly describes the major approaches to combustion modeling that have either been used or could be used for engine CFD.

	Model type	Turbulent Viscosity	Transport equations	Advantages	Disadvantages	Refs.
T1	None	Numerical viscosity only	0	No model required.	Depends on grid and numerical dissipation; hard to control.	[3]
T2	Smagorinsky	Yes	0	Simple to implement.	Requires adjusting a viscosity coefficient.	[4]
T3	Dynamic Smagorinsky	Yes	0	Dynamically determines the viscosity coefficient.	Requires additional averaging to remain numerically stable.	[5]
T4	Detached Eddy	Yes	1	Combines RANS near wall model with LES in the freestream.	Ad-hoc transport equation for turbulent viscosity term.	[6]
T5	k-equation LES	Yes	1	Uses additional transport equation for more physics.	Requires adjusting a viscosity coefficient for each case.	[7]
T6	Dynamic k-equation LES	Yes	1	Dynamically adjusts the viscosity coefficient.	Still based on turbulent viscosity.	[8]
T7	Dynamic Structure	Non-viscosity	1	More physical; directly models stress tensor; no turbulent viscosity.	Requires additional effort for implicit time integration.	[9]

Table 1: Major LES turbulence modeling approaches. In this, and all tables, only a limited number of references are sited due to space constraints. Preference is given for engine applications.

General Approaches and Specific Models	Mode	Advantages	Disadvantages	Refs.
C1: Direct Integration				
"CHEMKIN" or other stiff ODE integrator	H	Uses detailed kinetic mechanisms; no special modeling required.	Ignores subgrid turbulence effects. Better suited for homogeneous combustion. Computationally expensive.	[11]
C2: Blended				
RIF	D	Better computational efficiency for detailed chemistry. Uses flamelet concepts to model subgrid mixing (C4d).	Not really a CFD method since model is not applied to each grid cell.	[12]
C3: Time Scale				
(a) Magnusson	P, D	Simple; uses both kinetic and turbulent time scales.	Requires using same time scales for all reactions within individual grid cells.	[13]
(b) CTC	P, D	Improves on Magnusson by integrating towards current equilibrium state.	Still requires same time scales.	[14]
C4: Transport Equation		Flamelet approaches. Sound mathematical descriptions.	Transport equations require modeling of scalar flux, source terms, and sink terms.	
(a) Progress variable, C	P	Sound modeling of turbulence effects on flame front.	No detailed chemistry. Better for high Reynolds number flows. Requires high grid resolution to resolve flame front	[15]
(b) Level set, "G Equation"	P, D	Similar to C4a for premixed flames but reduces grid resolution requirements.	Not suited for detailed chemistry. Requires model for turbulent flame speed.	[16]
(c) Flame surface area, Σ	P, D	Similar to G-equation approach (C4b) but uses the flame area for a more physical description.	(similar to C4b)	[17]
(d) Mixture fraction, Z	D	Can incorporate detailed chemistry through flamelet library. Uses prescribed PDF to model subgrid mixing effects.	Requires flows with fast chemical times scales (high Da number) unless unsteady effects are incorporated.	[18]
(e) Conditional Moment Closure – Z/n	D	Tries to improve on mixture fraction models (C5d) by using values from the reaction zone.	Increased complexity due to more terms that require modeling.	[19]
C5: PDF Transport	all	Provides direct closure without models for reaction terms.	Complex; Monte-Carlo method; requires phase space mixing model.	[20]

Table 2: List of major combustion modeling approaches that have potential for use in LES. Original or primary type of combustion application for each model is indicated by Mode in column 2: H for homogeneous, P for premixed, D for diffusion.

LES Fuel Spray Models

Until recently there has been little published work on spray models for LES simulations. Most simulations of applications have used existing RANS type spray models with simple modifications for use with LES turbulence and combustion models. Most practical applications for IC engines use the Lagrangian spray parcel methodology originally developed for RANS approaches (see Reitz [21]) in which the CFD grid is not resolved around individual spray particles. In this context the spray modeling issue is how to represent the sub-grid interaction of the Lagrangian spray particles with the continuous gas phase. This interaction includes momentum transfer (e.g. drag), kinetic energy transfer, heat and mass transfer during evaporation, and models for atomization, breakup, and collisions. This is a very extensive list of complex physical processes that require modeling. This is probably why most spray models are extensions of RANS approaches and, only recently, has work has been done on developing new spray model formulations specifically for LES applications.

	Model type	Advantages	Disadvantages	Refs.
S1	RANS correlations	Uses established turbulence models	Does not consider specific advantages of LES formulations	[22]
S2	LES modifications	Integrates spray models into LES methodology	Still early in development phase; more validation needed.	[23]
S3	Volume of Fluid (VOF)	Effectively represents dense spray region.	Numerical and resolution difficulties for drops in less dense regions.	[24]
S4	Continuous phase, non-particle models (Full Eulerian)	More authentic representation than Lagrangian parcel approaches	Computational very expensive and not applicable to full combustion chamber simulations.	[25]

Table 3: List of spray modeling approaches that could be used in LES.

Recommendations

The more advanced differential LES turbulence models (T5-T7) should be used. These do not require extremely fine grids and work well on the courser grids commonly found in engine applications. The most common LES models use simple viscosity formulations (T2, T3), do not take advantage of LES concepts, and perform poorly in engine applications unless unrealistic grid resolutions are used.

Use transport based combustion models (C4) since these models benefit from the large scale flow structures that occur in LES simulations. Use LES specific modification for major terms within the models such as mixing time scales, scalar dissipation rate, turbulent flame speeds, scalar flux, etc.

The development of LES spray models is significantly behind work on other LES models. Thus, it is hard to make a strong recommendation for use in IC engine applications. In practice, it appears that using RANS based spray models with some minor modifications to work with LES turbulence models may be adequate for the time being.

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