Introducing Combustion-Turbulence Interaction in Parallel Simulation of Diesel Engines

Paola Belardini[1], Claudio Bertoli[1], Stefania Corsaro[2], and Pasqua D'Ambra[3]

[1] Istituto Motori (IM)-CNR
Via Marconi, 8 I-80125 Naples, Italy
{p.belardini, c.bertoli}@im.cnr.it
[2] Department of Statistics and Mathematics for Economic Research
University of Naples "Parthenope"
Via Medina 40, I-80133 Naples, Italy
stefania.corsaro@uniparthenope.it
[3] Institute for High-Performance Computing and Networking (ICAR)-CNR
Via Pietro Castellino 111, I-80131 Naples, Italy
pasqua.dambra@na.icar.cnr.it

Abstract. In this work we focus on parallel combustion simulation in modern Common Rail Diesel engines when the interaction between complex chemical kinetics and turbulence is taken into account. We introduce a turbulence term in a detailed chemical reaction model and analyze the impact on the reliability of pollutant emission predictions and on the efficiency and scalability of our combustion software. The parallel combustion software we developed adaptively combines numerical schemes based either on Backward Differentiation Formulas or semi-implicit Runge-Kutta methods for the solution of ODE systems arising from the chemical reaction model. It is based on CHEMKIN-II package for managing detailed chemistry and on two general-purpose solvers for adaptive solution of the resulting ODE systems. Furthermore, it is interfaced with KIVA3V-II code in order to simulate the entire engine cycle.

1 Introduction

In recent years stringent limits on engines pollutant emissions have been imposed by Government laws, strongly conditioning motor industry. For this reason, the design of modern engines relies on even more sophisticated, complex technologies. In particular, in latest-generation Diesel engines the Common Rail technology is usually employed and an high level of Exhaust Gas Recirculation (EGR) rate is also established; moreover, multiple fuel injection mechanism is typically adopted in order to reduce soot emissions and combustion noise. The impact on engine modeling is the need of accurately simulating highly complex, different physical-chemical phenomena occurring in each engine cycle. Mathematical models for the description of the overall problem typically involve unsteady Navier-Stokes equations for turbulent multi-component mixtures of ideal gases, coupled with suitable equations for fuel spray and combustion modeling. The solution

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of the complex overall model usually relies on a time-splitting approximation technique, where different physical phenomena are conceptually decoupled and, consequently, different sub-models are solved separately one from each other on a suitable 3d computational grid representing engine cylinder and piston bowl.

In recent years much attention has been addressed to combustion: great effort has been devoted to the design of detailed chemical reaction models suitable to predict emissions in sophisticated, last-generation Common Rail Diesel engines. Therefore, the numerical solution of chemistry has become one of the most computational demanding parts in simulations, thus leading to the need of efficient parallel combustion solvers [1,15]. The typical main computational kernel in this framework is the solution of systems of non-linear Ordinary Differential Equations, characterized by a very high stiffness degree. The reaction model does not introduce any coupling among grid cells, in other words cells are supposed to be isolated when chemical reactions occur. This assumption actually neglects turbulence effects in combustion process, a quite severe approximation in the high temperature combustion phase.

In this work we discuss the impact of introducing, in multidimensional modeling of Diesel engines, based on a decoupled solution of transport and reaction phenomena, a model describing the combustion-turbulence interaction. We model the interaction between complex chemistry and turbulence following the approach discussed in [13,14], that is, splitting the characteristic times of the species involved in combustion into the sum of a laminar term and a properly smoothed turbulent term. This model does not introduce any coupling among computational grid cells, preserving locality in the solution of the turbulent combustion process. The simulations are obtained by a parallel combustion software [4,5,6], based on CHEMKIN-II package for managing detailed chemistry and on a multi-method ODE solver [7] for the solution of the ODE systems arising from the turbulent chemical reaction model. The software is interfaced with the KIVA3V-II code for the simulation of the entire engine cycle. In section 2 we briefly outline the turbulent combustion model, in section 3 we describe the solution procedure and the main features of the parallel software, in section 4 we discuss some results of numerical simulations on realistic test cases.

2 Turbulent Combustion Model

Diesel engine combustion is characterized by liquid fuel injection in a turbulent environment. Two main phases can be distinguished in the overall phenomenon. Fuel injection gives raise to chemical reactions that, under suitable temperature and pressure conditions, lead to fuel ignition. The period from the starting of fuel injection and fuel ignition is named ignition delay: in this phase chemical reactions occur without giving strong energy contributions, but high stiffness is the main feature, due to very different reaction rates among the reactant species. Kinetics occurring before ignition is usually referred to as low temperature combustion or cold phase, while combustion phase, or high temperature combustion, is the chain of reactions subsequent to ignition.

In a time-splitting solution procedure for simulation of Diesel engines, computational grid cells are supposed to be isolated during the solution of the chemical reaction equations driving combustion, thus, neglecting their interaction, turbulence is not properly considered. On the other hand, combustion is strongly influenced by turbulence, since it has significant effects on the transport properties and on the mixing of reactants. Neglecting turbulence can seriously affect results concerning the numerical simulation of combustion phase, when turbulence effects are more relevant: indeed, chemical species conversion rates estimation does not take into account mixture inhomogeneities, thus leading to overestimated combustion rates. As a consequence, the stiffness degree of the arising ODE systems increases in this case, that is, neglecting turbulence has considerable effects from the mathematical point of view as well.

We consider a turbulent combustion model in order to accurately predict the effects of both chemical kinetics and turbulent mixing. The model is based on a recent detailed kinetic scheme, which considers N-dodecane as primary fuel. It involves 62 chemical species and 285 reactions. The kinetic scheme considers the H abstraction and the oxidation of the primary fuel, with production of alchil-peroxy-radicals, followed by the ketoydroperoxide branching. In the model the fuel pirolysis determines the chetons and olefins formation. Moreover, a scheme of soot formation and oxidation is provided, together with a classical scheme of NOx formation. The reaction system is expressed by the following system of non-linear Ordinary Differential Equations:

$$\dot{\rho}_m = W_m \sum_{r=1}^{R} (b_{mr} - a_{mr}) \dot{\omega}_r(\rho_1, \ldots, \rho_m, T), \qquad m = 1, \ldots, M, \tag{1}$$

where R is the number of chemical reactions involved in the system, M is the number of species, $\dot{\rho}_m$ is the production rate of species m, W_m is its molecular weight, a_{mr} and b_{mr} are integral stoichiometric coefficients for reaction r and $\dot{\omega}_r$ is the kinetic reaction rate.

Production rate terms can be separated into creation rates and destruction rates[12]:

$$\dot{\rho}_m = \dot{C}_m - \dot{D}_m, \qquad m = 1, ...M, \tag{2}$$

where $\dot{C}_m$, $\dot{D}_m$ are the creation and the destruction rate of species m respectively. The latter can be expressed as

$$\dot{D}_m = \frac{X_m}{\tau_m}, \qquad m = 1, ...M, \tag{3}$$

where X_m, τ_m are respectively the molar concentration and the characteristic time for destruction rate of species m. Expression (3) shows that the eigenvalues of the Jacobian matrix of the right-hand side of system (1) are related to the characteristic times for destruction rates of species involved in the combustion model. Detailed reaction models involve a great number of intermediate species and no equilibrium assumption is made. Thus, the overall reaction systems include species varying on very different timescales one from each other;

this motivates the high stiffness degree that typically characterizes ODE systems arising in this framework. Moreover, relation (3) shows that if combustion rates are overestimated, that is, characteristic times are underestimated, then it results in a higher stiffness degree: this explains the impact of neglecting turbulence from the computational point of view.

We model interaction between complex kinetics and turbulence following the approach discussed in [13,14]. The model relies on the assumption that the characteristic time τ_m^c of each species involved in the combustion model depends both on a *kinetic timescale* and a *turbulent timescale*. The former is defined as the time needed by a species to reach equilibrium state under perfectly homogeneous conditions, the latter is the eddy breakup time. More precisely, we suppose that it holds

$$\tau_m^c = \tau_m^k + f\tau_m^t, \qquad m = 1, ...M \tag{4}$$

where τ_m^k, τ_m^t are the kinetic and the turbulent timescales of species m, respectively. The turbulent timescale is considered proportional to the eddy turnover time as estimated by the standard $k - \epsilon$ turbulence model employed in the KIVA3V-II code. The factor f serves as a delay coefficient that slows down reactions according to turbulence effects. It is assumed to be

$$\frac{1 - e^r}{0.632}, \tag{5}$$

where r is the ratio between combustion products and total reactant concentrations. It indicates the stage of combustion within specific regions: the value $r = 1$ corresponds to complete consumption of fuel and oxygen. Note that a reliable estimate of r is a key issue when detailed chemical kinetic models are used, since in that case combustion products have to be well established. The delay coefficient f changes accordingly to r, depending on the local conditions.

From relation (4) it follows that the densities ρ_m satisfy the equation

$$\frac{\partial \rho_m}{\partial t} = \frac{\rho_m^* - \rho_m}{\tau_m^k + f\tau_m^t}, \qquad m = 1, ...M \tag{6}$$

where ρ_m^* is the equilibrium concentration. Therefore, the main computational kernel in the turbulent combustion model is the solution, in each grid cell and at each splitting time step, of system (1) where the right-hand side is properly scaled, according to (6). Note that, for sake of efficiency, the kinetic timescale for all the species is assumed to be equal to that of the slowest species involved in the oxidation scheme.

In Figure 1 two graphics reporting stiffness degree estimations during the ignition delay period of a typical engine simulation are shown. One refers to a simulation where the detailed combustion model, without turbulence term, was employed. The other one shows the results of a simulation involving interaction between complex kinetics and turbulence. Figure reveals that, as expected, since the introduction of turbulence term in the model slows down reaction rates, it has, from the computational point of view, a smoothing effect on ODE systems.

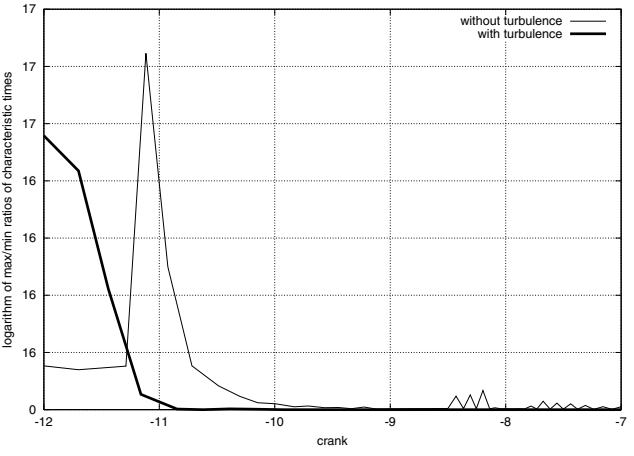

Fig. 1. Stiffness estimate

3 Parallel Solution of Turbulent Combustion

In this section we describe the main features of the parallel package we developed for the numerical simulation of turbulent combustion in Diesel engines. As also proposed in [1,15], parallelism is based on a domain decomposition technique where the computational grid is partitioned among the parallel processors; the main computational kernel arising from the turbulent combustion model is the solution of a system of non-linear Ordinary Differential Equations per each grid cell, at each time step of the splitting solution procedure, which can be solved concurrently, since there is no coupling among the cells. On the other hand, the approach followed for accounting interaction between complex kinetics and turbulence does not affect inherent parallelism in the solution process: indeed, the scaling procedure described in section 2 preserves the locality with respect to grid cells.

In our software, main contribution is related to the local stiff ODE solver. Indeed, we proposed a multi-method solver, based on an adaptive combination of a 5-stages Singly Diagonally Implicit Runge-Kutta (SDIRK) method [11] and variable coefficient Backward Differentiation Formulas (BDF) [8].

We tested SDIRK4 and VODE packages when no interaction between turbulence and chemical reactions was considered; main features of both solvers and some results are described in [6]. Those results showed that the VODE package is more accurate than SDIRK4 in the cold phase. From the mathematical point of view, low temperature combustion corresponds to the transient phase; Runge-Kutta based methods are well-known to loose accuracy in the very stiff phase [3], indeed we observed that SDIRK4 could overestimate ignition delay [6] and, consequently, underestimate pressure rise. On the other hand, SDIRK4 was, in all of our numerical simulations, more efficient than VODE in the high temperature combustion phase, therefore, we proposed and developed a multi-method solver

that automatically switches from VODE to SDIRK4 when ignition is approaching. First results on the use of the multi-method solver in the solution of detailed chemical kinetics in multidimensional Diesel engine simulations have been presented at [7]. Here we analyze the behaviour of the multi-method solver when the turbulence combustion interaction model described in section 2 is considered.

Note that physical stiffness is strongly related to local conditions, therefore, when adaptive solvers are considered in a parallel setting, grid partitioning becomes a critical issue for computational load balancing. To this aim, our parallel solver supports three partitioning strategies, namely, pure block, pure cyclic and random distribution. In the former, a block of contiguous cells, according to cell numbering into the grid, is distributed to each process, in the latter, cells are distributed among processes following a typical round-robin algorithm. In the case of random partitioning grid cells are reordered according to a permutation of indexes, deduced by a pseudo-random sequence, before grid distribution. Experiments on our test cases, when VODE or SDIRK4 were used as solver, revealed that random partitioning produces the best parallel performance results. Details on the performance analysis of different grid partinioning strategies on our test cases can be found in [5].

The parallel combustion software is written in Fortran and uses standard MPI API for message passing. Furthermore, it is based on CHEMKIN-II [12], a software package for managing large models of chemical reactions in the context of simulation software. It provides a database and a software library for computing model parameters involved in system (1).

Our parallel software has been interfaced with the KIVA3V-II code [2], in order to properly test it within real simulations. Details on the integration between the parallel combustion software and KIVA3V-II can be found in [4,6].

4 Numerical Results

In this section we show some results concerning simulations performed on a prototype, single cylinder Diesel engine, with IV valves, having characteristics similar to the 16 valves EURO IV Fiat Multijet. Simulations have been carried out at 1500 rpm. In order to fit a wide range of operating conditions both in the experimental measurements and in the numerical simulations, the production engine has been modified for having a swirl variable head. The engine is equipped with an external supercharging system to simulate intake conditions deriving from turbo-charging application. In addition, the exhaust pipe is provided with a motored valve to simulate the backpressure due to the turbocharger operation. In the experiments three test cases, corresponding to different operating conditions, reported in Table 1, have been considered. The position of the piston into the cylinder is measured by means of crank angle values, therefore, injection timing and injection period are expressed with respect to them. The limit positions of the piston, that is, the lowest point from which it can leave and the highest point it can reach, correspond to -180^o and 0^o crank angle values respectively. Numerical experiments have been carried out on a Beowulf-class Linux cluster,

Table 1. Engine operating conditions

	Rail Pressure (bar)	EGR	Injection timing (crank angle)	Injection period (crank angle)	Injected fuel (mg)
Test case 1	500	40%	-12.7	7.3	8.0
Test case 2	900	0%	-2.3	5.7	8.7
Test case 3	500	0%	-2.1	7.3	8.5

made of 16 PCs connected via a Fast Ethernet switch, available at IM-CNR. Eight PCs are equipped with a 2.8GHz Pentium IV processor, while the others have a 3.8GHz Pentium IV processor. All the processors have a RAM of 1 GB and an L2 cache of 256 KB. We used the GNU Fortran compiler (version 3.2.2) and the LAM implementation (version 7.0) of MPI.

ODE systems have been solved by means of the multi-method solver we developed. In the stopping criteria, both relative and absolute error control tolerances were considered; at this purpose, we defined two vectors, *rtol* and *atol*, respectively. In all the experiments here analyzed *atol* values were fixed in dependence of the particular chemical species. The reason motivating this choice relies on the very different concentrations characterizing chemical species involved in detailed reaction models. All the components of *rtol* were set to 10^{-3}, in order to satisfy the application accuracy request.

In Fig. 2 the in-cylinder combustion pressure graph is shown. Experimental pressure values are compared to predicted ones for testing results reliability. In order to analyze the impact of accounting for kinetics-turbulence interaction, two graphics are shown: on the left, results concerning simulations performed without turbulence term in kinetics model are reported. On the right, the represented pressure curves refer to numerical simulations involving the turbulent combustion model described in section 2. We observe that, for all the considered test cases, the introduction of chemistry-turbulence interaction term in the combustion model provides a better agreement between experimental and simulated pressure curves, confirming that the complex physical phenomena occurring during combustion are more accurately described in this case.

In Figure 3 we show some performance results on the Test case 1. In the experiments we are discussing, computational grid has been distributed according to random grid partitioning strategy. We show results of numerical simulations involving the detailed combustion model without the kinetics-turbulence interaction term and compare them with the ones obtained via the numerical solution of the turbulent combustion model in order to investigate the impact of accounting for kinetics-turbulence interaction on performance as well. In Fig. 3, on the top-left, we reported the total number of performed function evaluations for each process configuration, that is a measure of the total computational complexity of the combustion solver. More precisely, for a fixed number of processes varying from one to sixteen, we added the number of function evaluations performed by each process. On the top-right, simulation time, expressed in hours, versus number of processes is represented. We note that considering the turbulence term in

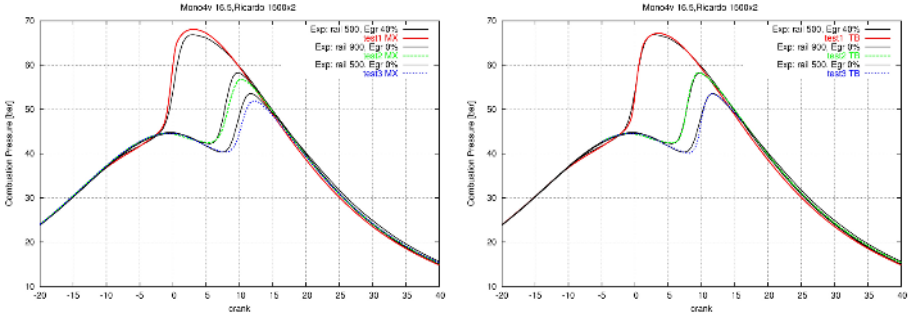

Fig. 2. Comparison between experimental and simulated in-cylinder pressure. Left: combustion simulation without turbulence term. Right: turbulent combustion model simulation results.

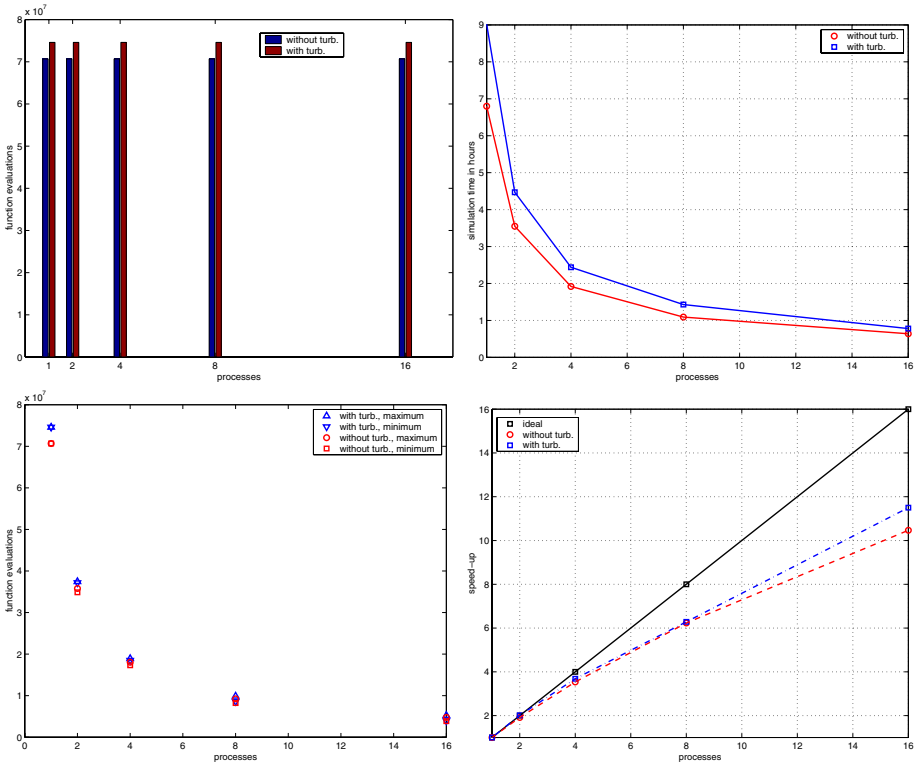

Fig. 3. Top-left: total number of performed function evaluations versus number of processes. Top-right: simulation time expressed in hours. Bottom-left: maximum and minimum number of performed function evaluations versus number of processes. Bottom-right: speed-up.

the combustion model results in an higher overall simulation time. Accounting for turbulence-chemistry interaction turns in a local scaling of the right-hand side of systems (1), which affects the properties of the involved ODE systems, leading to an increase of the computational load per processor. On the other hand, communication costs and serial computation overheads are not affected. Furthermore, accounting for turbulence-chemistry interaction seems to produce better load balancing: on the bottom-left of the figure we analyze the load balancing among the processes for each configuration. We reported the minimum and the maximum number of performed function evaluations, for each process configuration. More precisely, for a fixed number of processes, we computed the total number of function evaluations performed by each process and considered the maximum and the minimum among such values. We note that, when the turbulent term is introduced in the combustion model, the gap between those values is reduced. The whole previous analysis is in agreement with the speed-up lines, represented on the bottom-right of the figure, where we can observe that higher speed-up values are obtained when turbulence is considered.

5 Some Conclusions

In this work we have shown first results related to the effort of improving reliability of parallel simulations of combustion in Diesel engines. A chemistry-turbulence interaction model has been introduced in a decoupled solution of the chemical reaction and of the Navier-Stokes equations for the reactive fluid flow. Even though the chemistry-turbulence interaction term does not affect the inherent parallelism in the combustion solver, it seems to produce larger local computational complexity and better load balancing. Numerical results on realistic test cases show that the use of the model provides a better agreement between experimental and simulated results. Therefore, the impact of the chemistry-turbulence interaction term on the ODE systems arising in detailed combustion models has to be deeply investigated.

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