

Towards the Use of Eulerian Field PDF Methods for Combustion Modeling in IC Engines

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ABSTRACT

Detailed chemistry and turbulence-chemistry interaction need to be properly taken into account for a realistic combustion simulation of IC engines where advanced combustion modes, multiple injections and stratified combustion involve a wide range of combustion regimes and require a proper description of several phenomena such as auto-ignition, flame stabilization, diffusive combustion and lean premixed flame propagation. To this end, different approaches are applied and the most used ones rely on the well-stirred reactor or flamelet assumption. However, well-mixed models do not describe correctly flame structure, while unsteady flamelet models cannot easily predict premixed flame propagation and triple flames. A possible alternative for them is represented by transported probability density functions (PDF) methods, which have been applied widely and effectively for modeling turbulent reacting flows under a wide range of combustion regimes. For IC engine simulations, the most promising ones are the Eulerian field PDF methods (SEF) whose formulation was originally proposed by Valiño and Sabel'nikov. Such models can be easily incorporated into CFD codes and are less computationally intensive with respect to Lagrangian approaches. In particular, Lagrangian particles are replaced by stochastic fields and transport equations are solved for them including a random process as a source term. Purpose of this work is the assessment of a SEF combustion model, that has been implemented into the Lib-ICE code, which is based on the OpenFOAM technology. To make the use of detailed chemistry possible in a reasonable amount of time, a multi-zone approach was incorporated in the combustion model and coupled with the TDAC technique, combining in-situ adaptive tabulation and dynamic adaptive chemistry. Experimental validation was carried out by simulating Diesel combustion experiments at constant volume conditions.

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INTRODUCTION

The continuous innovation towards the achievement of more efficient and less polluting engines has significantly extended the range of occurring combustion regimes and transitions from one mode to another in the same engine technology. Kinetically controlled combustion with or without spark-ignition such as HCCI, PCCI or SACI [1, 2, 3], Diesel engines with multiple injections and/or high EGR [4], GDI engines operating with a lean stratified charge [5, 6, 7] are examples of such a trend. On the modeling point of view, this evolution is motivating the definition of a unique and high fidelity combustion models that should be applicable in all relevant combustion regimes [8]. With such a premise, it is clear the need to incorporate in the proposed model a detailed chemistry

approach, but also to account at some stage of the non-linear interaction between fluid mixing and finite-rate chemistry. On the other hand, in literature there are many studies [9, 10, 11, 12] in which successful simulations of Diesel, HCCI and premixed combustion were achieved by neglecting any sub-grid interaction between turbulence and chemistry, especially emphasis was given on the capability of well predicting auto-ignition rather than the flame structure. In this sense, very common alternative approaches, mainly for Diesel combustion simulations are the multiple Representative Interactive Flamelet Model (mRIF) and the Conditional Moment Closure (CMC). The first approximates the flame structure as a set of multiple unsteady laminar diffusion flames (*flamelets*). Their evolution is computed in the mixture fraction space, where species and energy equations are solved. Effects of

mixing are incorporated in the scalar dissipation rate, which is computed as a conditional average of its distribution in the CFD domain. Use of multiple flamelets ensures a better prediction of both flame structure and auto-ignition, since spatial variations of the scalar dissipation rate are properly taken into account [14]. The CMC model introduces a further level of detail, since flamelet equations are solved including also a term accounting for flow-field effects. This requires a simplified 1D, 2D or coarse 3D mesh of the studied geometrical domain, and suitable mapping techniques to interpolate computed solution on the real mesh. CMC model is very powerful, but computationally very demanding due to the need to solve flamelet equations directly in the CFD domain [15, 16]. For this reason its application is limited to small chemical mechanisms operating only with simplified surrogate fuels, like n-heptane [17]. Incorporating detailed chemistry in premixed or partially-premixed combustion is more complicated since flame propagation takes generally place in a thin wrinkled laminar flame front. Application of the flamelet concept to SI combustion (premixed or stratified) is not immediate, due to the need to properly account for both ignition process and pressure effects in post-flame kinetics governing both soot and NO_x formation. Finally, the third possible approach to model turbulent combustion, accounting for multi-regime conditions, is based on the application of probability function methods (PDF), which offer compelling advantages for modeling chemically reacting turbulent flows, providing an effective resolution to the closure problems that arise from averaging the highly nonlinear chemical source terms. Most developments of PDF models derive from Pope's original work [18] and are extensively discussed in [19, 20]. A comprehensive review and a perspectives on recent advances and trends can be found in [21, 22]. In a composition PDF method, a modelled transport equation is solved for the one-point, one-time joint PDF of the composition variables describing the local thermochemical state of the reacting system. The main advantage of PDF methods is that the chemical source term appears in closed form. Multiple strategies were proposed to solve PDF transport equations: most of the work was carried out by Lagrangian particle Monte Carlo methods where the PDF is represented by a large number of notional particles that evolve according to stochastic equations, and local mean quantities are estimated as appropriately weighted averages over the particles in a small neighborhood. However, implementation of Lagrangian particle methods into conventional CFD codes is complex and consistency issues might arise [21]. Moreover, a large number of particles is required to simulate statistically non-homogeneous systems, and particle-based PDF methods are computationally demanding. Examples of applications of Lagrangian PDF methods for IC engine simulations can be found in [23, 24]. A possible alternative is represented by Stochastic Eulerian Field PDF (SEF) methods, which might be more compatible and efficient when implemented into conventional CFD codes. Valiño presented such approach in [25], demonstrating its equivalence with Lagrangian methods. Examples of application of the SEF to spray combustion [26, 27], turbulent non-premixed [28] and premixed combustion [29] can be found in literature. In this work, a novel methodology to

simulate modern IC engine combustion with Stochastic Eulerian Field PDF method and detailed chemistry is presented. The SEF method was implemented into the LibICE code, based on the OpenFOAM® technology and extensively applied in the past for simulations of both premixed and non-premixed combustion in IC engines [30, 31, 32]. In particular, a novel, fully parallelized technique for on-line chemistry tabulation was employed, integrating the chemistry in a very limited set of points. Computational overheads were limited to the solution of a large number of transport equations which are multiple of the number of adopted stochastic fields. The proposed methodology was assessed and validated simulating Diesel combustion experiments. First, non reacting conditions were simulated to understand how the model predicts the mixture fraction distribution and its variance. Then combustion simulations were carried out and the flame structure computed by the SEF model was compared with the ones from well-mixed and the multiple RIF approaches.

NUMERICAL MODELS

Stochastic Eulerian Field (SEF) PDF Method

In an open, ideal-gas, single-phase, multi-component reacting mixture containing N_s chemical species, the local thermochemical state and the species chemical production rates Ω can be determined from the N_s species mass fractions Y and the mixture specific enthalpy h . This set of variables will be referred to as *composition variables* denoted by ϕ a vector whose dimension is $N_\phi = N_s + 1$. The corresponding composition joint PDF is denoted by $f_\phi = f_\phi(\psi; \mathbf{x}, t)$. Conventional (denoted using angled brackets, $\langle \rangle$) and mass-weighted or Favre-averaged (denoted using a tilde, $\sim$) mean values of any function of the composition variables, $Q = Q(\phi)$, can be expressed as integrals of the PDF over its sample space.

The starting point is a modeled transport equation for the joint PDF of the N_s species mass fractions Y the mixture specific enthalpy h :

$$\frac{\partial \rho f_\phi}{\partial t} + \frac{\partial \rho \tilde{u}_i f_\phi}{\partial x_i} + \frac{\partial \rho \Omega_\alpha f_\phi}{\partial \psi_\alpha} = \frac{\partial}{\partial x_i} \left[\Gamma_{T\phi} \frac{\partial (\rho f_\phi / \langle \rho \rangle)}{\partial x_i} \right] + \frac{1}{2} \frac{\partial \left[C_\phi \omega (\psi_\alpha - \tilde{\phi}_\alpha \rho f_\phi) \right]}{\partial \psi_\alpha} \quad (1)$$

Here summation is implied over repeated Roman (Cartesian coordinate index) or Greek (composition variable index) subscripts within a term. Transport in physical space by the mean velocity $\tilde{u}_i$ and transport in composition space by chemical reaction Ω_α appear in closed form on the left-hand of Eq. 1. The first term on the right-hand side corresponds to a gradient transport model for turbulent velocity fluctuations, and the second term corresponds to an interaction-by-exchange-with-the-mean (IEM) model [33] for molecular transport and mixing.

In the stochastic Eulerian field (SEF) PDF method, N_F notional Eulerian fields evolve according to stochastic PDFs. The system of stochastic PDEs is designed such that its one-point, one-time Eulerian joint PDF evolves according to [Eq. 1](#). The number of PDEs to be solved is equal $N_\phi \times N_F$, and standard Eulerian CFD algorithms are employed to solve stochastic PDEs of the method [28]. In this work, the SEF method was implemented following the approach introduced by Valiño where the SEF equation corresponding to [Eq. 1](#) is written as:

$$\begin{aligned} d(\langle \rho \rangle \phi_\alpha^\#) = & -\frac{\partial \langle \rho \rangle \tilde{u}_i \phi_\alpha^\#}{\partial x_i} dt + \Omega_\alpha(\phi^\#) dt + S^\# dt \\ & -\frac{1}{2} C_\phi \omega (\phi_\alpha^\# - \tilde{\phi}_\alpha) dt \\ & + \frac{\partial}{\partial x_i} \left[\Gamma_{T\phi} \frac{\partial \phi_\alpha^\#}{\partial x_i} \right] dt + \left(\frac{2\Gamma_{T\phi}}{\langle \rho \rangle} \right)^{1/2} \frac{\partial \phi_\alpha^\#}{\partial x_i} dW_i^\# \end{aligned} \quad (2)$$

the superscript # refers to any one of the fields in the vector ϕ ; $S^\#$ is the source term due to spray evaporation, different for each species but identical for each stochastic field; ω is the turbulence mixing frequency defined as the ratio between turbulent kinetic energy k and dissipation rate ε . $\mathbf{W}^\#$ denotes a vector-valued Wiener process that varies in time, but is independent of spatial location. Purpose of the Wiener vector is to introduce a stochastic noise in transport equations and generate a consequent PDF for enthalpy and each chemical species. The last two terms on the right hand side of [Eq. 2](#) involve the apparent turbulent diffusivity $\Gamma_{T\phi}$ and correspond to a gradient transport model for turbulent velocity fluctuations.

In the absence of the Wiener term $\mathbf{W}^\#$, [Eq. 2](#) is equivalent to a PDE. However, the stochastic field equations are written in increment form to emphasize that the stochastic term is not differentiable with respect to time. A key point in the Valiño formulation is that each field must be smooth (twice continuously differentiable) at the scale of the computational mesh. To be consistent with this statement, the same random increment is applied uniformly in each coordinate direction for each field by approximating $\mathbf{W}^\#$ at the beginning of each computational time-step and to treat explicitly the last term on the rhs in [Eq. 2](#). Following earlier SEF modeling studies, the $dW_i^\#$ is approximated as $dt^{1/2} \eta_i$, where η_i is a $\{-1, +1\}$ dichotomic vector. An operator-splitting strategy is used for the chemical and spray source terms, the mixing term and the random term in [Eq. 2](#). Density-weighted mean quantities are then obtained by ensemble averaging over the fields:

$$\tilde{Q} = \tilde{Q}(\mathbf{x}, t) \approx \frac{1}{N_F} \sum_{n=1}^{N_F} Q(\phi^n(\mathbf{x}, t)) \quad (3)$$

An important difference between Lagrangian particle and SEF methods is that, in the former, turbulent transport is represented by a stochastic term in physical space, while in the

latter, turbulent transport is represented in part by a stochastic term in composition space ([Eq. 2](#)). This can result in unphysical field compositions, and measures must be taken to minimize these excursions. Here the maximum magnitude of the stochastic term in the species equations is limited to the difference between the current value of the species mass fraction and the nearest physical bound on the species (either zero or unity) [34]. Despite very promising, Eulerian field PDF methods require specific developments mainly for what concerns the possible mixing models that can be adopted. In particular, the spatial smoothness has to be preserved and this aspect imposes some restrictions in case of models having stochastic processes with jumps, like the Curl's model. Another very promising model is the EMST, where the change of particle composition is determined by particle interactions along the edges of a Euclidean Minimum Spanning Tree constructed in composition space. However, implementation of the EMST model into the Eulerian stochastic method requires proper development efforts and detailed verifications about its assumptions. For all such reasons, the IEM (Interaction by Exchange with the Mean) mixing model was used in this work, since it ensures spatial smoothness. So far, SEF methods were only applied to model simplified configurations and, due to the need to use a large number of stochastic fields to properly represent the PDF distribution of the chemical species involved, small mechanisms were generally adopted to achieve results in a reasonable amount of computational time.

CPU Time Reduction

To compute chemical reaction rates in [Eq. 2](#), an operator splitting technique is used. In particular, an ODE stiff solver takes the thermodynamic conditions (composition and temperature) of each stochastic field in any cell and integrates the chemical problem within the time-step, solving the species and energy equations. Then species mass fractions are updated as:

$$\phi_\alpha^\#(t + \Delta t) = \phi_\alpha^\#(t) + \int_t^{t+\Delta t} \dot{\omega}^\# \frac{W^\#}{\rho_\alpha} dt' \quad (4)$$

where ρ_α is the density related to a stochastic field, $\dot{\omega}^\#$ is the reaction rate and $W^\#$ is the molecular weight of the chemical species. Solution of [Eq. 4](#) is carried out by means of a multi-step, Semi-Implicit Bulirsch-Stoer method, *S/BS* [35].

Finally, the reaction rate Ω_α is estimated as:

$$\Omega_\alpha = \frac{\phi_\alpha^\#(t + \Delta t) - \phi_\alpha^\#(t)}{\Delta t} \quad (5)$$

and it is included in the chemical species and enthalpy transport equations as a source term. Direct-integration of chemistry introduces significant computational overheads in the simulation when SEF methods are used. As a practical

example, the use of 20 stochastic fields in a Diesel combustion simulation (~ 20000 cells during main combustion) and a 100 species mechanism will require to integrate 40 millions of stiff equations for each CFD time step taking time-scales of the 0.1 - 10 μ s order into account. This is not feasible and for this reason solutions to reduce the CPU time need to be found. To this end, two different approaches are generally followed: in the first one, chemical composition or reaction rates are retrieved from large tables including pre-computed reaction rates or flamelet solutions [36, 37, 38, 39] while the second approach computes on-line the chemical species reaction rates by means of stiff integrators [40, 30, 41]. Tabulated kinetics make simulations very fast mainly when applied to constant-pressure conditions. However, the need to include pressure, equivalence ratio, progress variable and EGR variations in them grows their size significantly and makes their application complicated due to the need to load, store and retrieve a very large amount of data even shared by different processors. Possible recent improvements were proposed in [42]. When using direct-integration, CPU time can be drastically reduced by the use of on-line techniques for mechanism reduction and tabulation [43, 44, 30, 45] preserving the accuracy of the results and the flexibility of the method with respect to the adopted kinetic mechanism. In this work, a novel parallel methodology was developed which combines three different chemistry acceleration techniques: a multi-zone method, known as Chemistry Coordinate Mapping (CCM), Dynamic Adaptive Chemistry (DAC) and In-Situ Adaptive Tabulation (ISAT).

To integrate the stiff ODEs of elementary reactions and estimate the source term in the species transport and energy equations for each stochastic field, the CCM method works as follows [31, 45]: first, a phase space consisting of three principal variables $\tilde{T}$, J_H and $\beta = \log_{10}(\nabla J_H \cdot \nabla J_H + 1)$ is constructed. J_H is elemental mass fraction of hydrogen atom defined as:

$$J_H = \sum_{k=1}^N \frac{W_H}{W_k} \beta_{H,k} \tilde{Y}_k, \quad (6)$$

where W_H and W_k are the atomic and molecular weights of the hydrogen and the k -th species, respectively. $\beta_{H,k}$ is the number of H-atoms in the k -th species. Note that variables β and $\nabla J_H \cdot \nabla J_H$ are uniquely related each other. In this way, for each stochastic field, computational cells are mapped into a three dimensional $(T, \nabla J_H, \beta)$ space.

Let the phase space be discretized by N_T number of temperature zones, N_J number of J_H zones, and N_β number of β zones. The (i, j, k) cell in the physical domain is mapped to the (l, m, q) zone in the $(\tilde{T}, J_H, \beta)$ space. In discretized form the mapping is between the index $(i, j, k)_a$ of the cells for each stochastic field in the physical domain to the index (l, m, q) of the zones in the phase space. For each cell in the physical domain, cell indices, i.e., the value of $i_T(i, j, k)$, $i_J(i, j, k)$, and $i_\beta(i, j, k)$ in the phase space are stored on line at each time-step

during the simulation, and they will be used later for the procedure of mapping back results from the phase space to physical space. The mean values of the variables in the phase space zones are determined and used as the initial condition for integrating the reaction rates. The mean reaction rate is then computed for each zone and mapped back to the cells in the physical space using the stored mapping index. Differently from many of the available multi-zone approaches [46, 47], using only a two-dimensional tabulation that accounts for mixture fraction and temperature, in the CCM approach local flow and mixing conditions are also taken into account through the $\nabla J_H \cdot \nabla J_H$ term. This makes the proposed tabulation method more oriented to the combustion mode that is going to be simulated. CCM reduces the computational time since the size of the $(\tilde{T}, J_H, \beta)$ space where chemistry equations are integrated is generally 1-2 orders of magnitude lower than the number of employed CFD cells. Furthermore, compositions from all stochastic fields are mapped onto a single $(\tilde{T}, J_H, \beta)$ space and then integration is performed on multiple processors, with each one of them receiving approximately the same number of points to be integrated with almost the same range of thermodynamic conditions. In this way, different decomposition methods are used between flow solution and chemistry integration, with this last one performed with a very good load balancing on a relatively small number of points. Application of parallel CCM to chemistry integration with SEF model is displayed in Fig. 1.

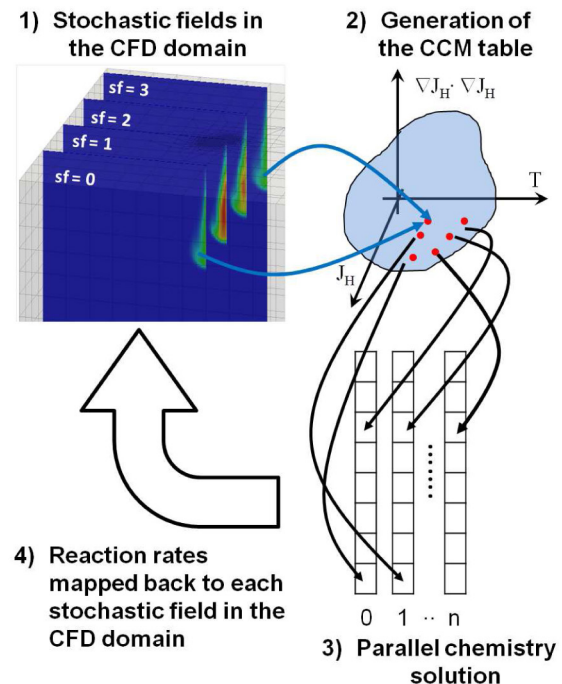


Figure 1. Application of parallel Chemistry Coordinate Mapping technique (CCM) to chemistry integration with the SEF combustion model.

Accuracy of the CCM method was extensively verified by the authors in [31, 45] where it was applied to RANS and DNS non-premixed combustion simulations. To reduce the CPU time for chemistry integration, the CCM method operates