The eulerian monte carlo approach for solving joint composition PDF equation for turbulent combustion applied to methane/air mixture ignition

M. Ourliac⋆ , V. A. Sabel'nikov⋆ and M. Habiballah⋆
⋆Office National des Etudes et Recherche Aérospatiale
Chemin de la Hunière, 91761 Palaiseau, France

Abstract

This paper describes an hybrid Reynolds Averaged Navier Stokes/ Eulerian Monte Carlo (RANS/EMC) numerical method, developed for the solution of the one-point joint composition probability density function (PDF). In this approach the conservation equations for mean density, momentum, total sensible energy and $k-\epsilon$ model are solved by RANS solver while EMC method is applied for solving composition and enthalpy PDF transport equation. Transport PDF method allow chemical sources terms, which are the driving ones in combustion and flame, to be treated exactly. This Monte Carlo method is eulerian in the sense that one solves Stochastic Partial Differential Equations (SPDE) to calculate the PDF. The mean velocity and turbulent scalars are supplied by the RANS code to the EMC one which in turns gives all the reaction and mixing terms needed in the RANS code. The main issues which are coupling, pressure calculation, boundary conditions and numerical methods are presented in this paper. Finally numerical results are obtained for an ignition model problem behind a backward facing step.

1. Introduction

In turbulent reactive flows, pollutant production, soot formation and ignition/extinction mainly arise from a conjunction of rare physical events and finite chemistry effects. Predicting these phenomena thus requires a precise knowledge of the statistics of the species concentration and temperature, as well as an accurate description of chemical reactions. Regarding both aspects, the one-point joint composition probability density function appears as a promising tool for computing ignition process: it contains the detailed one-point statistical information of the turbulent scalars and allows chemical sources terms to be treated exactly. These advantages are counterbalanced by a severe numerical constraint. The PDF transport equations has a completely different structure from traditional moment-closure model equations, being a high dimensional scalar equation. Thus traditional numerical techniques such as finite volume or finite element methods are not suitable to solve the PDF transport equations since their computational cost increases exponentially with the number of dimension. On the other hand, the Monte Carlo method has proven to be very useful for solving high dimensional equations.

So far in the field of turbulent combustion, Monte Carlo methods have mostly been considered under their Lagrangian form (LMC), following the seminal work of Pope[1] . In the LMC method, the PDF is represented by an ensemble of stochastic particles whose properties evolves according to Stochastic Ordinary Differential Equations (SODE's) such that, ideally, the particles exhibit the same PDF as occurs in turbulent flow they are modeling. However mean fields obtained from RANS or LES solver are required to close the PDF model equations and overcome statistical fluctuations. Numerous works[2–4] focused on the convergence, accuracy and consistency conditions of this so-called hybrid LMC method and its ability to compute complex flows was proven.

However, the development and evaluation of a new Eulerian Monte Carlo method is also useful and stimulating, since in this method problematic such as statistical convergence is expressed in a different way and then could push both approaches forward. EMC methods are based on stochastic fields which evolve from prescribed stochastic partial differential equations (SPDE's) stochastically equivalent to the PDF equation. These SPDE's are the Eulerian counterpart of the SODE's used in LMC methods. EMC has been firstly developed by Valino[5] . Sabel'nikov and Soulard[6] used Brownian advection velocity model to derive SPDE's and shed light upon EMC. Conservative form of SPDE's is derived later by Soulard and Sabel'nikov[7] . Conservative SPDE's are better suited for numerical integration of the

method in CFD codes. Last few years, hybrid RANS/EMC and LES/EMC models have been successfully applied to reactive flows and turbulent flames computation[8,9] and to ignition process[10] .

The focus of the current work is to develop an hybrid RANS/EMC solver under conservative form for simulating complex flow configuration. The remaining of the paper is organized as follows. First, modelled equations for the mean fields and the PDF equation are presented. Then a numerical scheme for each solver is proposed and peculiar interest is focused on the boundary conditions for stochastic fields and on the coupling strategy adopted. Finally, the hybrid method is applied to ignition model problem of a turbulent premixed methane flow behind a backward facing step.

2. Governing Equations

2.1 PDF formulation

The PDF transport equation is as follows[6] :

$$\frac{\partial}{\partial t}(\overline{\rho} f) + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{U}_j f) = \frac{\partial}{\partial x_j}(\overline{\rho}\Gamma_T \frac{\partial f}{\partial x_j}) - \frac{\partial}{\partial \psi_\alpha}(\overline{\rho} M f) - \frac{\partial}{\partial \psi_\alpha}(\overline{\rho} S_\alpha f), \tag{1}$$

where Ψ is the sample composition variables $\Psi = (Y_1, Y_2, ..., Y_{N_s}, h)$, Y_i and h being mass fraction and total enthalpy. $f(\Psi; x, t)$ is one-point pdf of the scalar Ψ. The symbol $\overline{Q}$ and $\widetilde{Q}$ denotes the Reynolds and Favre averaging of quantity Q, $\widetilde{Q} = \frac{\overline{\rho Q}}{\overline{\rho}}$. In this equation, the effects of molecular mixing and turbulent advection appears in unclosed form and require modelling, whereas chamical source term and mean advection do not require any modelling. Molecular mixing is here modeled by an operator denoted M. In the practical application described afterwards, the IEM model will be used. Turbulent advection is modeled with a gradient diffusion assumption.

2.2 Stochastic Partial Differential Equations

Conservative SPDE's stochastically equivalent to the PDF equation (Eq. 1) derived by Soulard and Sabel'nikov[7] are :

$$\frac{\partial r Y_k}{\partial t} + \frac{\partial (\widetilde{U}_j + u_j^*) \circ r Y_k}{\partial x_j} = r\omega(Y_k - \widetilde{Y}_k) + r S_k \tag{2}$$

$$\frac{\partial r h}{\partial t} + \frac{\partial (\widetilde{U}_j + u_j^*) \circ r h}{\partial x_j} = r\omega(h - \widetilde{h}) \tag{3}$$

$$u_j^* = \frac{\Gamma_T}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial x_j} + \frac{1}{2} \frac{\partial \Gamma_T}{\partial x_j} + \sqrt{2\Gamma_T}\dot{W}_j \tag{4}$$

In these equations $\widetilde{U}$, Γ_T and ω, the mean velocity, the turbulent diffusion coefficient and the turbulent frequency are supplied by the RANS solver. r is the stochastic density, $r = \sum r Y_k$, $\overline{r} = \overline{\rho}$. W_j are independant Brownian processes (also called Wiener process), $\overline{dW_j} = 0$, $\overline{dW_i(t) dW_j(t)} = \delta_{ij} dt$, $\dot{W}_j$ denotes time derivative.

2.3 Thermochemistry

Following Jenny et al.[3] , the mean over temperature interval $[0, T]$ mass heat capacity at constant volume is introduced:

$$e_s(T) = \int_0^T c_v(T) dT = \overline{c_v}(T) T, \tag{5}$$

where $e_s(T)$ is sensible energy. The above definition for $\overline{c_v}$ (with similar definition for $\overline{c_p}$) allows to write the equation of state in terms of e_s rather than T as:

$$p = \rho R \frac{e_s}{c_v} = (\gamma' - 1)\rho e_s \tag{6}$$

where $\gamma' = \frac{\overline{c_p}}{\overline{c_v}}$. A new averaged equation is added to the RANS solver with its source term computed from the stochastic fields.

2.4 Mean Conservation Equations

In the hybrid method, a RANS solver is used to solve the mean conservation equations for mass density, momentum and total sensible energy. The $k-\epsilon$ model is used to compute the turbulent stresses and turbulent diffusion coefficient, with k being the turbulent kinetic energy and ϵ the turbulent dissipation.

$$\frac{\partial}{\partial t}\overline{\rho} + \frac{\partial}{\partial x_j}\overline{\rho}\widetilde{U}_j = 0. \tag{7}$$

$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{U}_i + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{U}_i\widetilde{U}_j + \overline{P}) = \frac{\partial}{\partial x_j}\sigma_{ij}. \tag{8}$$

$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{E}_s + \frac{\partial}{\partial x_j}\widetilde{U}_i(\overline{\rho}\widetilde{E}_s + \overline{P}) = \frac{\partial \sigma_{ij}}{\partial x_j} - \overline{\rho}\widetilde{\sum_{k=1}^{N_s} S_k h_k^\circ} \tag{9}$$

$$\frac{\partial}{\partial t}\overline{\rho}k + \frac{\partial}{\partial x_j}\overline{\rho}k\widetilde{U}_j = \frac{\partial}{\partial x_j}(\overline{\rho}\frac{\nu_t}{Pr_k}\frac{\partial k}{\partial x_j}) + P_k - d_k. \tag{10}$$

$$\frac{\partial}{\partial t}\overline{\rho}\epsilon + \frac{\partial}{\partial x_j}\overline{\rho}\epsilon\widetilde{U}_j = \frac{\partial}{\partial x_j}(\overline{\rho}\frac{\nu_t}{Pr_\epsilon}\frac{\partial \epsilon}{\partial x_j}) + P_\epsilon - d_\epsilon. \tag{11}$$

In hybrid PDF/RANS solver, the main link between the hydrodynamic solver and the PDF solver is the pressure term in momentum equation. By using equation 2 and 3 one can calculate a mean stochastic temperature and then use equation of state with mean stochastic density or mean physical density to calculate pressure. However this kind of pressure calculation has been the cause of severe numerical difficulties, since temperature field computed from EMC is quite noisy. The method presented in this paper to solve this issue is to use transport equation for the total sensible energy (Eq. 9). With neglecting the turbulent kinetic energy, $\widetilde{E_s} = \widetilde{e_s} + \frac{1}{2}\widetilde{U_i}\widetilde{U_i}$.
Finally, the mean pressure is determined by:

$$\overline{P} = \overline{\rho}(\overline{\gamma'} - 1)\left(\widetilde{E}_s - \frac{1}{2}\widetilde{U}_i\widetilde{U}_i\right) \tag{12}$$

In summary the RANS solver is employed to solve the conservation equations for mean mass density (Eq. 7), the mean momentum (Eq. 8) , the mean total sensible energy (Eq. 9), the turbulent kinetic energy (Eq. 10), the turbulent dissipation (Eq. 11). EMC solver calculates the mean source term in Eq. 9.

3. Numerical solution procedures

This part concerns the numerics involved for solving the coupled EMC/RANS equations. We will first concentrate on the temporal integration and spatial discretisation of the SPDEs equations (the RANS part is already well documented), then on the coupling strategy employed in this work. The key point of the boundary conditions for the stochastic fields is then addressed and finally the numerical technique used for ignition simulation.

3.1 Finite volume method

To solve the Reynolds averaged quantities a cell centered finite volume solver named CHARME is used. The RANS equations are solved with a second order explicit Runge Kutta integration scheme with a preconditioning scheme based on that of Turkel. The preconditioning is needed to remove the well-known numerical difficulties due to eigenvalue stiffness caused by the large disparity between the characteristic wave speed at low Mach numbers.

3.2 SPDE's numerical scheme

The SPDE's are under the conservative form, the numerical method used to solve this equations is a finite volume one. The choice of the Stratonovitch form of the SPDE yields to use a predictor-corrector procedure generalizing the Heun scheme[7] . A *cfl* condifion is enforced:

$$\Delta t = cfl\frac{\Delta x^2}{\widetilde{U}\Delta x + 2\Gamma_T} \tag{13}$$

The source S_k in Eq. 2 are calculated using low Mach number approximation: thermodynamic pressure is replaced by constant value $p = 1bar$ over the domain.
For the spatial discretization, fluxes are calculated at the cell interface with Flux Difference Splitting (FDS) procedure. Equations 2 and 3 are solved for N stochastic fields with N independent noises. The Favre averaging of a function θ is simply computed by:

$$\widetilde{\theta} = \frac{\sum_{k=1}^{N} r\theta^{(k)}}{\sum r^{(k)}} \tag{14}$$

The number of stochastic field is a key parameter of the computation. For Monte Carlo methods the statistical error is of $\sqrt{N}$ order, so increasing N of a 2 factor decreases the stochastic error of $\sqrt{2}$, but increases the computation time for each iteration of 2. Consequently the value for N must be carefully chosen. For the application below, the calculation is performed with 25 stochastic fields.

3.3 Coupling

For LMC methods, many different strategies for coupling have already been tested[2] , in this work the hybrid EMC/RANS solver implemented can be either run in a loosely or tightly coupled manner. In a loosely coupled algorithm, a completed outer iteration is completed by running RANS code until convergence and the EMC code for a specified number of time steps. In tight coupling, RANS and EMC code are run for a single time step to complete an outer iteration. The goal of this work is to prove the ability of the method to simulate ignition, which is a unstationnary process. Therefore, only the tightly coupling will be presented and tested in this work. The overall solution sequence can be summarized as follows. Once EMC iteration is performed, this gives mean source term for the total sensible energy equation (Eq. 9) ; then an iteration for the RANS code is performed which gives, mean velocity, turbulent diffusion coefficient and turbulent frequency.

3.4 Boundary conditions for stochastic fields

In SPDE's the value of the noisy part of the stochastic velocity can be in every direction and its value is much larger than the mean velocity for subsonic flow. This changes completely the numerical treatment of boundary conditions.

3.4.1 Wall stochastic boundary condition

Usually for solving species mass conservation equation under conservative form with finite volume method, the boundary condition for a non-porous media, the mass flux are given to be zero at the wall; the mass is then conserved. However, in RANS and LES calculation, the mesh can be so coarse that the diffusion coefficient is non zero in the cell near the wall. There exists then a difference between the physical and the modelled behavior at the wall, but in most cases this error may be neglected. For Lagrangian PDF methods, stochastic particle behavior is supposed to be the same as physical particle one. If the stochastic particle impact a wall, then it will bounce on it. The question is now: what is the equivalent behavior for stochastic fields? The stochastic fields being non-local (in opposition to the stochastic particles) and the stochastic velocity being in the same direction in all the domain for a specific stochastic field at time t, there cannot be any bouncing. As in RANS calculation with coarse grid, the boundary layer is not resolved, in particular the turbulent diffusion coefficient is far from zero. Moreover the stochastic velocity is proportional to $\frac{1}{\sqrt{dt}}$ so that, in the calculation, this velocity is large in the cell near the wall. Contrary to the RANS case, the error is then large and may cumulate through the calculation and create very large stochastic density gradient. In order to prevent such behavior a "fictitious" stochastic flux was added at the wall (see Figure 2) . This "correction" by fictitious stochastic flux was validated on a "$1D$" diffusion process between two walls.

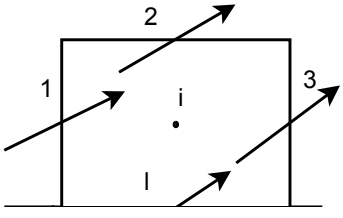

Figure 1: Fictitious Stochastic Flux at the wall

3.4.2 Inlet/Outlet stochastic boundary condition(I/O)

Due to the stochastic component of the velocity a "physical inlet" boundary condition can be alternatively an outflow condition and an inflow condition. It is the same for an "physical outlet" boundary condition. As shown by Sabel'nikov and Soulard[6] , the influence of boundary condition can lead to discontinuities inside the domain, but in real cases, due to mixing and numerical diffusion the amplitude of the discontinuities are weak. For a subsonic flow, SPDEs of the EMC solver are hyperbolic differential equation, boundary conditions have then to be specified on part of the domain where characteristic enter the domain. Therefore the treatment of the "I/O" boundaries is the following:

- if $\overrightarrow{\xi}.\widetilde{\overrightarrow{U}} > 0$ then nothing is changed from the usual case, density and mass fraction are imposed at the inlet and computed from the interior at the outlet.
- if $\overrightarrow{\xi}.\widetilde{\overrightarrow{U}} < 0$ then the flux at the "physical inlet" is decentred from the inside of the domain and the incoming flux at the "physical outlet" is also computed from the values inside the domain.

4. Model Ignition Problem

The ignition is simulated by the following model: an additional source term S_{add} is added in the SPDEs in several cells placed inside the recirculation zone.

$$\frac{\partial rY_k}{\partial t} + \frac{\partial(\widetilde{U}_j + u_j^*) \circ rY_k}{\partial x_j} = r\omega(Y_k - \widetilde{Y}_k) + rS_k + S_{k,add} \tag{15}$$

The fictitious source term is active only on the 100 first iterations. During this time the combustion products have been created in the recirculation zone. The fictitious source term is then turned off and the physical chemical source terms alone helps to the increasing the reacting zone.

4.1 Configuration and numerical mesh

The physical domain is $L = 1m$ horizontally and $H = 0.1$ vertically. The height of the step, placed at the lower wall is, is $h = 0.035m$. At inlet, a methane/air mixture is injected at $U_0 = 58m/s$ and $T_O = 525K$, with a stoichiometric equivalent ratio $\phi = 1$. The inlet values of the turbulent quantities are $k_0 = 15m^2/s^2$ and $\epsilon_0 = 500m^2/s^3$. At outlet, the pressure is fixed: $P_s = 1bar$. The geometry and inlet conditions correspond to the experimental ones[11] .
At the upper and lower wall, wall functions are applied for k and ϵ, while the wall boundary conditions for mass fractions are those presented in subsection **3.4.1**. The resolution of the mesh is chosen to be $\Delta x = 7.5 \cdot 10^{-3}m$ and $\Delta y = 5.0 \cdot 10^{-3}m$ (Δx and Δy are respectively the grid size in the horizontal and vertical direction). The time step for each solver is $\Delta t = 2 \cdot 10^{-06}s$ giving a cfl number equal to 0.01.

4.2 Chemical scheme

A 5 species - 1 reaction scheme is used to describe the complete combustion of the methane and air to CO_2 and H_2O:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2 \tag{16}$$

The source term for the progress variable is expressed as :

$$S = AY_{CH_4}^a Y_{O_2}^b exp(-\frac{T_a}{T}) \tag{17}$$

where A,a,b and T_a are the Arrhenius law constants: $a = 0.2$, $b = 1.3$, $A = 6.7 \cdot 10^9 mole^{-0.5}/s$, and $T_a = 22800K$.

4.3 Results

To see the temporal evolution of the ignition process instantaneous snapshots of the mean temperature and root mean square temperature for several elapsed time are presented in Figure 2. After 10 iterations a small hot kernel due to the additional source term is formed. This kernel grows with time, and after 10000 iterations which correspond to a physical of $0.02s$, the whole domain behind the step is ignited.

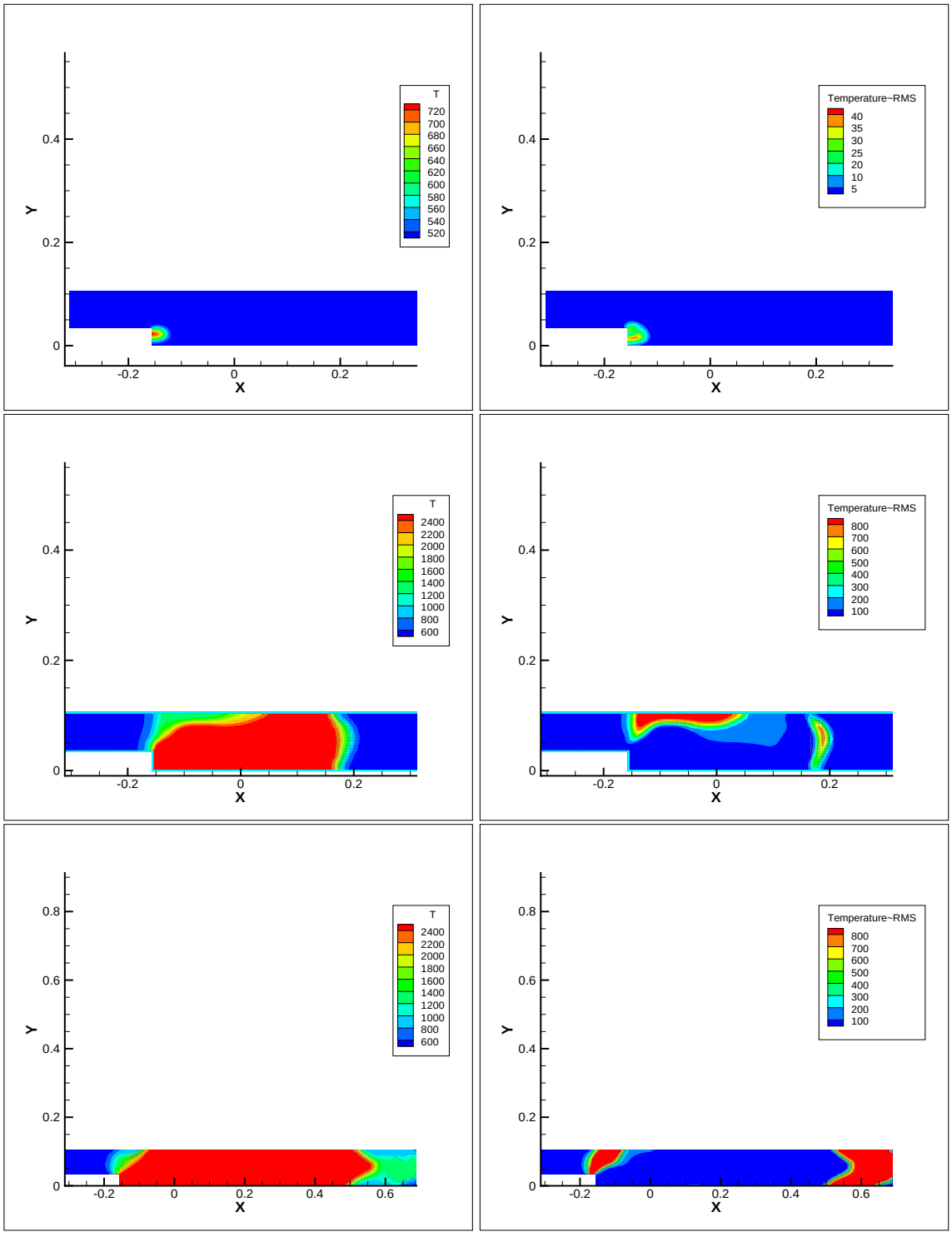

Figure 2: Instantaneous snapshots of the mean temperature (left column) and root mean square temperature (right column) for 10, 2000 and 6000 iterations (from top to bottom)

5. Conclusion

Hybrid numerical method for solving coupled RANS/EMC equations and its implantation in the code CEDRE from ONERA is presented. The ability, at a qualitative level, of the hybrid RANS/EMC solver to simulate ignition was proven. Our interest was mainly focused on the two principal aspects : the coupling strategy and the boundary conditions treatment. Event if no quantitative results are presented here, the method seems very promising for simulating unstationnary chemically driven phenomena. In the future, a calculation of a physical ignition on the DLR micro chamber configuration will be performed.

References

[1] Pope, S. B. PDF methods for turbulent reactive flows. In *Progress in Energy and Combustion Science*, Vol. 27, pages 119–192, 1985.

[2] Muradoglu, M., Jenny, P., Pope, S. B. and Caughey, D. A. A Consistent Hybrid Finite-Volume/Particle Method for the PDF Equations of Turbulent Reactive Flows. In *Journal of computational Physics*, Volume 154, pages 342–371, 1999.

[3] Jenny, P., Pope, S. B., Muradoglu, M. and Caughey, D. A. A Hybrid Algorithm for the Joint PDF Equation of Turbulent Reactive Flow. In *Journal of computational Physics*, Volume 166, pages 218–252, 2001.

[4] Muradoglu, M., Pope, S. B. and Caughey, D. A. The Hybrid Method for the PDF Equations of Turbulent Reactive Flows: Consistency Conditions and Correction Algorithms. In *Journal of computational Physics*, Volume 172, pages 841–878, 2001.

[5] Valiño L. A field Monte Carlo formulation for the calculating the pdf of a single scalar in a turbulent flow. In *Flow, Turbulence Combustion*, Volume 60, pages 157-172, 1998.

[6] Sabel'nikov, V. A. and Soulard, O. Rapidly decorrelating velocity field model as a tool for solving Fokker-Planck PDF equations of turbulent reactive scalars. In *Physical Review*, E, Volume 72, 016301, 2005.

[7] Soulard, O. and Sabel'nikov, V. A. Eulerian Monte Carlo methods for solving joint velocity-scalar PDF equations in turbulent reacting flows. In *ECCOMAS CFD*, TU Delft, Netherland, 2005.

[8] Mustata, R., Valino L., Jimenez, C., Jones, W.P. and Bondi, S. A probability density function Eulerian Monte Carlo field method for large eddy simulations: Application to a tubrulent piloted methane/air diffusion flame (Sandia D). In *Combustion and Flame*, Volume 145, pages 88–104, February 2006.

[9] James, S., Zhu, J., Anand, M.S. Large Eddy simulation of turbulent flames using the filtered density function modeld. In *Proceedings of the combustion institute 31*, 2007.

[10] Jones, W.P., Navarro-Martinez, S., Rohl, O. Large Eddy simulation of hydrogen auto-ignition with a probability density function method. In *Proceedings of the combustion institute 31*, 2007.

[11] Magre, P., Collin, G. Application de la drasc a l'operation A3C, Technical Report, ONERA 7.3608 EY, ONERA/DEFA, 1994.

This page has been purposedly left blank