On simulating scalar transport by mixing between Lagrangian particles

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Lagrangian particles with mixing can be used as direct numerical simulations (DNS), large eddy simulations (LES), or filtered density function (FDF) methods depending on conditions of the simulations. We estimate major parameters associated with the DNS, LES, and FDF regimes and demonstrate that, under certain conditions specified in the paper, simulations using different mixing models approach the DNS limit. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2711233]

The results presented in the most recent "Turbulent Nonpremixed Flames Workshop"[1] indicate a very interesting trend: the sensitivity to different mixing models is reduced when used in conjunction with large eddy simulations (LES). We believe that this is not a coincidence—in the LES framework,[2] mixing models operate in more local conditions and this localness improves the performance of conventional mixing models. A similar improvement[3] is observed in the multiple mapping conditioning (MMC) approach,[4] where localness is forced upon conventional mixing operators by using MMC reference variables. In this Letter, we consider a class of models involving mixing between Lagrangian particles and demonstrate that this behavior should be expected. We show first that, under certain conditions, Lagrangian mixing models approach solutions of the scalar transport equations and, thus, can be used as direct numerical simulations (DNS) of scalar transport. The error in approximating the scalar transport is estimated. We then consider Lagrangian simulations when turbulent scalar fields are not fully resolved and distinguish two regimes in these simulations—large eddy simulations (LES) (Ref. 2) and filtered density function (FDF) (Ref. 5)—depending on how parameters of the model are selected.

Our present analysis focuses on conceptual issues and, for the sake of simplicity, we consider constant density flows. We begin our consideration with the continuous scalar transport equation,

$$\frac{\partial Z}{\partial t}+u_i\frac{\partial Z}{\partial x_i}-D\frac{\partial^2 Z}{\partial x_i\partial x_i}=0, \tag{1}$$

where $i=1,2,3$ and the sum is taken over repeated indices. The velocity field is presumed to be fully described, i.e., the flow can be laminar or turbulent but, if it is turbulent, all the smallest scales are resolved in the representation of the velocity field $u_i=u_i(\mathbf{x},t)$. At this stage, the velocity field is treated as fully specified and no stochasticity associated with the velocity field is considered. Equation (1) can be seen as a Fokker-Planck (direct Kolmogorov) equation that specifies the number density of particles moved according to the following system of stochastic (Ito) equations:[6]

$$dx_i^*=u_i(\mathbf{x}^*,t)dt+(2D)^{1/2}dw_i, \tag{2}$$

where w_i represent independent stochastic Wiener processes. Assuming that a number of particles is distributed randomly with initial probability proportional to $Z_0(\mathbf{x})\equiv Z(\mathbf{x},t_0)$, the probability of finding a particle at a particular location is proportional to $Z(\mathbf{x},t)$. Equivalently, $Z(\mathbf{x},t)$ can be interpreted as the value that is proportional or equal to the average number density of particles $\rho_p=\rho_p(\mathbf{x},t_0)$. If the total number of particles n_p is very large, then the actual number of particles within a given volume is indicative of the average number of particles within this volume and this value is linked to the integral of $Z(\mathbf{x},t)$ over the volume. This equivalence of continuous deterministic diffusion (1) and stochastic differential equations (2) (representing particle random walk) is one of the principal properties of nature known in physics and mathematics.[6] In fluid mechanics, approaches (1) and (2) are generally referred to as Eulerian and Lagrangian.

The Lagrangian formulation presented above does not involve any mixing but can be modified so that mixing appears as an essential part of the simulations. Indeed, we do not need to distribute particles according to certain initial conditions but may well use uniformly distributed particles having an average number density of $\rho_p^\circ=\text{const}$. In this case, we simply mark the particles so that the average number density of the marked particles ρ_p is initially determined by the continuous initial distribution $Z_0(\mathbf{x})$. This marker, which can be denoted by Z^*, is 1 for the marked particles and 0 for the particles that are not marked. The function $\rho_p(\mathbf{x},t_0)$ represents the required solution of (1). The same value ρ_p can be equivalently interpreted as an average Z^*-weighted density of all particles defined by $\rho_p=\langle\Sigma_{(p)}^{n_V}Z_{(p)}^*|\mathbf{x},t\rangle/V$, where the sum is taken over $p=1,\ldots,n_V$ particles located in a small volume V. Here, we use conditional expectations to emphasize that averaging is performed at a given location and time. Since the scalar transport is linear, one can consider superposition of different markers with arbitrary weighting coefficients and this superposition remains compliant with Eq. (1). We conclude that Z^* does not have to be zero or one and can take any other value. At this point we obtain a new formulation of the stochastic problem that remains equivalent to the continuous formulation of the scalar transport. In the new formulation, the particles are uniformly distributed in the flow and each particle has a weight, Z^*, that remains constant once

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the simulation is started. Assuming that $Z_0(\mathbf{x})$ is a smooth function and that the number of particles is sufficiently large, we set the weight values to $Z^*=Z_0(\mathbf{x}^*)$ for each particle. The value ρ_p (defined as the average Z^*-weighted density of particles) remains to be a solution of (1). This relationship can be written as $\rho_p=\langle Z^*|\mathbf{x},t\rangle\rho_p^\circ$, where $\rho_p^\circ=\langle n_V|\mathbf{x},t\rangle/V=\text{const}$. We conclude that $Z(\mathbf{x},t)=\langle Z^*|\mathbf{x},t\rangle$, since $\langle Z^*|\mathbf{x},t\rangle$ complies with both the transport equation (1) and the initial conditions.

While the initial conditions are set so that the values Z^* do not have any scattering around $Z_0(\mathbf{x}^*)$, the random component of particle motion introduces such scattering. The scattering grows in time and this makes evaluation of the conditional averages more and more difficult. It is logical to use a mixing procedure to suppress the unrestricted growth of the scattering. Indeed, if at a certain moment $t=t_1$ the positions of two random trajectories coincide, then, due to the Markov properties, the process can be terminated at this moment and restarted with the initial conditions that correspond to the particle distribution at the moment of termination. The two particles located at the same point can be assigned any new values $Z^{*+}_{(1)}$ and $Z^{*+}_{(2)}$, instead of the old values $Z^*_{(1)}$ and $Z^*_{(2)}$, provided the total weight of these particles is preserved, $Z^{*+}_{(1)}+Z^{*+}_{(2)}=Z^*_{(1)}+Z^*_{(2)}$, although $Z^{*+}_{(1)}=Z^{*+}_{(2)}=(Z^*_{(1)}+Z^*_{(2)})/2$ corresponds to maximal reduction of scattering. If n_m particles with weights $Z^*_{(p)}$ $(p=1,\ldots,n_m)$ have the same location then multiparticle mixing can be used,

$$Z^{*+}_{(p)}=Z^*_m+\alpha\Delta Z^*_{(p)}, \tag{3}$$

where $Z^*_m\equiv n_m^{-1}\Sigma^{n_m}_{(p)}Z^*_{(p)}$, $\Delta Z^*_{(p)}=Z^*_{(p)}-Z^*_m$, and $0\leqslant\alpha\leqslant 1$ represent the extent of mixing ($\alpha=0$ for complete mixing and $\alpha=1$ when no mixing occurs). The extent of mixing α can be random or deterministic. If $n_m=2$ this mixing is similar to Curl's and modified Curl's mixing, while mixing with large n_m would approach the interactions by exchange with conditional mean [IE(C)M] model (specific information about these and other models can be found elsewhere[1,2,5,7,8]). Mixing in (3) is conservative (i.e., preserves the total weight of the particles) and results in the following decrease of the conditional variance $\Omega=\langle(Z^{*\prime})^2|\mathbf{x},t\rangle$, $Z^{*\prime}=Z^*-\langle Z^*|\mathbf{x},t\rangle$:

$$\frac{\Delta\Omega}{\Omega}=\left(1-\frac{1}{n_m}\right)\langle 1-\alpha^2\rangle. \tag{4}$$

This can be characterized by the mixing time τ_m,

$$\tau_m=\frac{\Omega}{N}=\frac{2\Delta t}{\Delta\Omega/\Omega}=\frac{2\Delta t}{\left(1-\frac{1}{n_m}\right)\langle 1-\alpha^2\rangle}, \tag{5}$$

where $\Delta\Omega/\Delta t=2N$ is the dissipation of the scalar over duration of the time interval Δt associated with the mixing event and $\Delta\Omega=\Omega-\Omega^+$ is the dissipated variance. The equilibrium value of the variance can be determined from the balance of the generation and dissipation terms[3,8]

$$2DG^2-2\frac{\Omega}{\tau_m}=0,\quad G^2\equiv\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}, \tag{6}$$

where G denotes the magnitude of the gradient of the scalar. Due to Markov properties, resetting the values of $Z^*_{(p)}$ to $Z^{*+}_{(p)}$ is a legitimate operation that reduces scattering but does not affect the link between the discrete and continuous formulations. While the original approach (2) required an additional set of particles to simulate another scalar, the system of stochastic particles with mixing can be used to simultaneously simulate n_s scalars with the same set of particles by assigning several values of Z^*_I $(I=1,2,\ldots,n_s)$ to every particle. Mixing operator (3) is independently applied to each value Z^*_I that corresponds to I^{th} scalar. The initial conditions $Z^*_I(t_0)=Z_I(\mathbf{x}^*,t_0)$ are, generally, different for different scalars but all simulated scalars satisfy the same equation (1).

Practically, particle trajectories can intersect only in low-dimensional spaces and we have to account for the fact that particles have to interact at nonzero distances. The numerical errors associated with incomplete localness of mixing need to be assessed. Mixing involves the exchange of the values Z^* (or fractions of these values) and this generates additional diffusion that is herein referred to as numerical diffusion. Indeed, assuming that only a single particle has a nonzero value of Z^* in a mixing group, complete mixing would result in redistribution of the following fraction $\varkappa=(1-n_m^{-1})(1-\alpha)$ of this value between all particles of the mixing group while the fraction of $1-\varkappa$ remains assigned to the particle. Due to incomplete localness of the model the fraction $\varkappa$ performs random jumps to the location of other particles in the group. The effective numerical diffusion coefficient that is associated with this process is given by $D_m=\langle\varkappa\rangle d_m^2/(2\Delta t)$, where d_m^2 is the average of the squared distance between the particles in the mixing groups along a selected direction. If d_m is small, mixing is localized in physical space. Taking into account Eqs. (4) and (5) results in

$$D_m=\frac{d_m^2}{\beta\tau_m},\quad \beta\equiv\frac{\langle 1-\alpha^2\rangle}{\langle 1-\alpha\rangle}. \tag{7}$$

The parameter β depends on the type of mixing model used in simulations but it is easy to show that $\beta\sim 1$. Indeed, we note that $1-\alpha^2=(1+\alpha)(1-\alpha)$ and $1\leqslant 1+\alpha\leqslant 2$, hence $\langle 1-\alpha^2\rangle\leqslant 2\langle 1-\alpha\rangle$ and $\langle 1-\alpha^2\rangle\geqslant\langle 1-\alpha\rangle$, resulting in $1\leqslant\beta\leqslant 2$. Thus, the specific form of the mixing model has only a limited effect on the intensity of the numerical diffusion.

We considered the system of stochastic differential equations (particles) with values $Z^*_{(p)}$ assigned to each of the particles. The values are subject to mixing which is required to be (1) conservative (preserving the sum of $Z^*_{(p)}$); (2) local (mixing is performed within the distance of d_m in physical space); (3) linear with respect to $Z^*_{(p)}$; (4) independent (if several scalars are introduced, mixing is independent for each of the scalars); (5) preserving boundedness of scalars (i.e., $0\leqslant\alpha\leqslant 1$); and (6) applied to all particles in a stochastic or deterministic manner but without discrimination so that the scalar variance is consistently reduced as characterized by a certain mixing time scale τ_m. Most of these conditions are well known.[7] The calculated values approach the solution

of continuous transport equation (1) provided $\tau_m \to 0$ and $d_m \to 0$ in a way so that $d_m^2/\tau_m \to 0$. The condition $\tau_m \to 0$ ensures that variation of Z^* around Z determined by $\Omega = DG^2\tau_m$ in (6) tends to zero while the condition $d_m^2/\tau_m \to 0$ minimizes the bias introduced by numerical diffusion D_m associated with mixing. Substituting $\tau_m = \beta^{-1}d_m^2/D_m$ into $\Omega = DG^2\tau_m$ introduces a new interpretation of Eqs. (6) and (7),

$$\Delta Z_m^2 = \beta\Omega\frac{D_m}{D}, \tag{8}$$

where $\Delta Z_m \equiv Gd_m$ determines localness of the mixing operation in the scalar space. The uncertainty of stochastic simulations Ω and the relative value of numerical diffusion D_m/D can be small at the same time only when mixing is local and ΔZ_m is small. We can introduce the characteristic cutoff scale $d_c = \Omega^{1/2}/G$ so that the scales $\Delta x \gg d_c$ are resolved in simulations while the scales $\Delta x \lesssim d_c$ are not resolved due to stochastic variations of Z^* around Z. Equations (6) and (7) indicate that $d_c^2 = D\tau_m = d_m^2\beta^{-1}D/D_m$. Since physical diffusion D should be dominant over numerical diffusion D_m, we obtain $d_c \gtrsim d_m$, i.e., the spatial resolution d_c is limited by the mixing scale d_m. Practically, even if only the closest particles are selected for mixing, d_m^2 cannot be smaller than d_1^2/n_d, where d_1 is the characteristic distance between particles and n_d is the dimension of the physical space. (When $d_m \approx d_1$, mixing between just mixed particles, which does not reduce the variance, can still be avoided assuming D_m/D is sufficiently small.) Hence, in order to make d_m^2 smaller and smaller we have to decrease spacing between particles by increasing the number of particles n_p used in the calculations.

The previous consideration proves that particle tracing with mixing can be used to solve the scalar transport equations and a large class of mixing models can be used for this purpose, provided mixing becomes localized $\Delta Z_m \to 0$ and τ_m is adequately selected. If the flow is turbulent, then calculations resolving the viscous (Kolmogorov) scales in the flow become DNS of the scalar transport (note that averaging is performed only over the Brownian-type fluctuations simulating molecular diffusion, but not over realizations of the velocity field). Performance of different mixing models varies significantly when the long-distance mixing is allowed, but as localness of the models is enforced by allowing interactions only at smaller and smaller distances, different mixing models should converge to DNS. Using Lagrangian particles with mixing as a DNS tool is, however, not always practical. Ideally, to enforce strict localness, the particles should be spaced from each other by a distance that is much smaller than the Kolmogorov scales. This would require very large computational resources. Even if characteristics of the dynamic field are fully resolved (this is by default presumed throughout the paper), resolving all small-scale details for tens or even hundreds of reacting species in a realistic stiff chemical kinetic mechanism is, and will remain, extremely difficult.

At this point, we consider a more practical situation when the characteristic distance between the particles d_1 belongs to the inertial interval of turbulence. Whether or not the velocity field is fully resolved in simulations, the scalar fields cannot be resolved at distances smaller than d_1. This means that, under these conditions, the scalar simulations become LES (Ref. 2), rather than DNS. Thus, Lagrangian simulations of scalar transport have a cutoff scale, d_c, which is presumed to belong to the inertial interval. The fluctuations with length scales smaller than d_c are not resolved and can be conventionally called subgrid or subfilter fluctuations (we refer to the "Lagrangian grid" that is represented by moving particles and is different from the Eulerian grid that is used for velocity simulations). The scalar fluctuations of scales greater than d_c are resolved in simulations. If the velocity field is fully resolved, and this is what we assume in our analysis, then particles move according to the algorithm (2); but if the fluctuations of the velocity field are filtered out below a certain scale of d_v, then D in (2) has to be replaced by the effective coefficient $D_v \sim (\varepsilon_t d_v^4)^{1/3}$ that simulates the influence of subgrid diffusion. Here ε_t is the dissipation of energy, averaged over realizations of the velocity field (turbulence averaged). The mixing model is characterized by the mixing scale d_m that, presumably, also belongs to the inertial interval of turbulence. If the characteristic mixing time τ_m is selected so that $d_m^2 \sim \varepsilon_t\tau_m^3$, then, as discussed below, $d_c \sim d_m$. If τ_m increases while d_m remains the same, d_c increases according to $d_c^2 \sim \varepsilon_t\tau_m^3 > d_m^2$. Indeed, both fields Z and Z^* have the same large-scale structure and, therefore, the same turbulence-averaged scalar dissipation N_t (although local values of the dissipation may be quite different for Z and Z^*). According to the definition of τ_m we obtain that $\Omega \sim N_t\tau_m$ increases with τ_m introducing a greater uncertainty into simulations (Ω is the variance of $Z^{*\prime} = Z^* - Z$). The scale d_c is linked to the scales τ_m and Ω by the equations $d_c^2 \sim \varepsilon_t\tau_m^3$ and $d_c^2 \sim \varepsilon_t N_t^{-3}\Omega^3$ of the inertial interval of turbulence. Decreasing τ_m below $d_m^{2/3}\varepsilon_t^{-1/3}$ reduces scattering Ω but does not improve resolution due to the bias introduced by numerical diffusion $D_m \sim d_m^2/\tau_m$. In this case $d_c \sim (D_m^3/\varepsilon_t)^{1/4} \sim \varepsilon_t^{-1/4}d_m^{1/2}\tau_m^{-3/4}$ increases when τ_m decreases. Assuming that d_m is fixed, the resolution of $d_c \sim d_m$ is achieved in Lagrangian LES when $\tau_m \sim \varepsilon_t^{-1/3}d_m^{2/3}$ and both the random scattering and numerical bias are of the same order of magnitude. Scattering $\Omega \gtrsim N_t\tau_m$ is inherently present in simulations, and any further reduction of Ω by decreasing τ_m below $\varepsilon_t^{-1/3}d_m^{2/3}$ worsens the resolution due to increasing D_m. The scattering Ω is more obvious when many particles are located within the mixing distance d_m from each other but, even if $d_m \sim d_1$, the value Z^* still has some scattering around Z due to $\Omega \sim N_t\tau_m > 0$. We will term the fluctuations $Z^{*\prime} = Z^* - Z$ as "minor fluctuations." Any further increase in the range of resolved scales requires reduction of d_m. A progressive reduction of d_m can be achieved only by decreasing d_1 and increasing the number of particles n_p.

The variables used in LES represent resolved values with subgrid fluctuations being filtered out. Hence, from a LES perspective, minor fluctuations represent a numerical noise that needs to be reduced as much as possible. The diffusing clouds model[4] is a mixing scheme that uses distance-dependent exchanges between particles and is more complicated than (3). This model was introduced in an attempt to reduce the level of minor fluctuations but had a rather limited success. It appears that the best approach is not

in trying to reduce these fluctuations but in utilizing minor fluctuations in a way simulating certain features of the subgrid fluctuations of the scalars (we should note that the second author of Ref. 4 always held this view). Since combustion models have to deal with a large number of reactive scalars, we may wish to see that the joint probability of minor fluctuations matches the joint probability of subgrid scalar fluctuations. In this interpretation, the Lagrangian particles with mixing becomes an FDF model[2,5] irrespective of the number of particles present within a subgrid cell. In LES, the parameter τ_m was selected to maximize, for given n_p, the range of resolved scales while, in the FDF approach, τ_m is to be selected to provide a most realistic joint distribution of scalars and these goals are not identical. We consider now two scalars, Z and Y, where Z can be interpreted as a mixture fraction and Y is one of reactive scalars. The conditional variance $\Theta=\langle(Y'')^2|Z\rangle$, where $Y''\equiv Y-Q$ and $Q\equiv\langle Y|Z\rangle$ is the conditional expectation, is positive when Q is not a simple linear function of Z. Generation of the conditional variance is, to a large extent, associated with small-scale fluctuations of the scalar dissipation, and correct simulation of the conditional variance Θ is particularly important when dealing with extinction and reignition.[3] It seems that, if a Lagrangian mixing model is subject to the FDF interpretation, matching the physical level of subgrid-generated conditional variance (rather than enforcing a certain specific value of Ω) is the most important criterion for selecting τ_m and other mixing parameters.[8]

The MMC version[4,8] of the FDF approach[5] gives a good illustration of differences between LES and FDF interpretations of mixing models. If the number of particles used in simulations is not sufficiently large, the value ΔZ_m increases and localness of the mixing model is compromised. The localness of the model can be improved without increasing the number of particles if we take into account that reactive scalars are, typically, more dependent on the mixture fraction than on physical coordinates. In MMC,[4] the localness of mixing is achieved by using reference variables and this approach can be used in conjunction with LES. The simplest MMC model, which is used in conjunction with DNS/LES and effectively incorporates the features of subfilter conditional moment closure (CMC)[9,10] into the FDF framework, involves simulation of the continuous mixture fraction field $Z(\mathbf{x},t)$. It must be stressed that the Lagrangian value $Z(\mathbf{x}^*,t)$ is interpreted in MMC as a reference variable, while the particle property Z^* [but not $Z(\mathbf{x}^*,t)$] is used as the physical mixture fraction during evaluation of chemical source terms.[8] We presume that all details of the mixture fraction and velocity fields are fully simulated (if subgrid fluctuations of Z are filtered out, these fluctuations can be emulated by a Markov process as discussed in Ref. 8). The variables $\boldsymbol{\xi}^*$ are introduced so that $\xi_0^*\equiv Z(\mathbf{x}^*,t)$ and $\xi_i^*=x_i^*$ for $i=1,2,3$, and the distance between two particles "p" and "q" is defined by $d_{(pq)}^2=g^{jk}\Delta\xi_j^*\Delta\xi_k^*$, where $j,k=0,\ldots,3$ and $\Delta\boldsymbol{\xi}^*=\boldsymbol{\xi}_{(p)}^*-\boldsymbol{\xi}_{(q)}^*$. The metric tensor g^{jk} is selected to increase resolution in the mixture fraction space and decrease ΔZ_m, although these improvements come at the price of reduced localness in the physical space. Mixing is localized in this new space and two particles can be mixed only if $d_{(pq)}^2\lesssim d_m^2$. The mixing parameters are selected to match the level of conditional variance. Discarding accurate Z and using approximate Z^* (which coincides with Z only at the resolved scales) in chemical calculations may seem odd from the LES/DNS point of view. This treatment is, however, very logical if the FDF-based criteria are applied: Z has inherently inaccurate joint distributions with reactive scalars Y^* simulated by the mixing model due to the differences between Z and Z^* determined by the presence of minor fluctuations.

Depending on parameters of the model, Lagrangian particles with mixing can be used for DNS, LES, or subgrid FDF simulations. It is shown that, if the number of particles used in simulations increases, the simulated scalars will approach DNS while the differences between mixing models gradually disappear (provided the mixing models are properly localized in the physical space). In the LES framework, the performance of a subgrid FDF model can be enhanced intensively [by improving the quality of the mixing model as, for example, done in MMC (Ref. 3)] or extensively (by increasing the number of particles used in simulations).

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