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Turbulent mixing simulation using the Hierarchical Parcel Swapping (HiPS) model

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ABSTRACT

A computationally efficient and novel turbulent mixing model termed Hierarchical Parcel-Swapping (HiPS) was introduced by A.R. Kerstein [J. Stat. Phys. 153, 142-161 (2013)]. HiPS simulates the effects of turbulence on time-evolving, diffusive scalar fields. The interpretation of the diffusive scalar fields or a state space as a binary tree structure is an alternative approach compared to existing mixing models. The characteristic feature of HiPS is that every level of the tree corresponds to a specific length and time scale, which is based on inertial range scaling. The state variables reside only at the base of the tree and are understood as fluid parcels. The effects of turbulent advection are represented by stochastic swaps of sub-trees at rates determined by turbulent time scales associated with the sub-trees. The mixing of adjacent fluid parcels is done at rates consistent with the prevailing diffusion time scales. We present an overview of the HiPS model for the simulation of passive scalar mixing and show the generated scalar power spectra with forced turbulence. Additionally, preliminary results for the mean square displacement and scalar dissipation rate will be presented as well as a model extension to account for variable Schmidt number effects.

Keywords: differential diffusion, hierarchical parcel swapping, HiPS, mixing model, passive scalar mixing

NOMENCLATURE

L_0	$[m]$	integral length scale
L_i	$[m]$	length scale of level i
L_η	$[m]$	Kolmogorov length scale
Re	[-]	Reynolds number
Sc	[-]	Schmidt number
Y	[m]	displacement
k_i	$[m^{-1}]$	wavenumber at level i
n	[-]	number of levels
u	[m/s]	velocity
χ	[1/s]	scalar dissipation rate
ϵ	$[m^2/s^3]$	dissipation rate
Γ	$[m^2/s]$	scalar diffusion constant
ϕ	[-]	variable value
ϕ^{**}	[-]	variable value before a swapping event
ϕ^{*}	[-]	variable value after a swapping event
τ	$[s]$	time
τ_0	$[s]$	integral time scale
τ_i	$[s]$	time scale of level i
τ_{mix}	$[s]$	time since last mixing process

1. INTRODUCTION

Turbulent mixing plays an important role in our daily life and ranges, as [1] suggests, "from supernovae to cream in coffee". As of today, there is a large number of mixing models which can be found in the literature [2]. Most of them are formulated in the context of transported Probability Density Function (PDF) methods. The most distinctive representatives are the Interaction by Exchange with the Mean (IEM) model [3], the Euclidean Minimum Spanning Trees (EMST) model [4], Curl's model [5], and the Fokker-Planck type models [2].

The central challenge of these stochastic models is the representation of the mixing processes in a way that is computationally efficient, and which is able to retain a significant level of physics. The constraints for a good mixing model can be derived directly from the statistical analysis of the conditional fluctuating diffusion flux in the composition PDF transport equation, see [2]. Among others, we mention that the molecular mixing model must not modify the scalar mean $\langle\phi\rangle$, and yield the correct joint scalar dissipation rate $\chi_{\alpha\beta}$ (for scalars α and β). Additionally, [2] also lists some desirable properties for good mix-

ing models, among which we mention the bounding of scalars to the so-called allowable region (e.g. positivity), the locality of the mixing in composition space, dependence of the mixing rate on scalar length scales and the incorporation of parametric dependencies such as Reynolds *Re* and Schmidt number *Sc* dependencies.

In Curl's model [5], pairs of particles are randomly selected from an ensemble of particles and their compositions are fully mixed. An alternative to Curl's model is the IEM model [3] and the Linear Mean Square Estimation model (LMSE) [6]. In the IEM mixing model, all of the individual particles gradually evolve to an average state. In terms of desirable properties, Curl's and the IEM model have some serious limitations. The biggest deficiency of these models becomes apparent when considering reactive flows. The constraint that scalar mixing should be local in composition space is violated by both models [2]. The violation of the localness principle of Curl's model produces a discontinuous jump of the fluid-particle composition during a mixing event [2]. This is a clear limitation of the model and causes unphysical conditions in flame sheet simulations. Cold fuel can enter into regions of cold oxidizer without reacting. In reality, the fuel must pass the high temperature region of the flame sheet and is reacting before it can reach the cold oxidizer. The IEM mixing model also violates the locality principle, since it predicts that composition variables vary continuously in composition space under the influence of the mean composition. The Euclidean minimum spanning tree (EMST) mixing model is local in composition space and seeks to address the problems encountered in flows with simultaneous mixing and reactions [4]. However, as in Curl's and IEM mixing models, EMST does not address the problem of the dependency on scalar length scales directly. Note that [7] attempted to introduce length scale dependency in the IEM model by means of a spectral model for the scalar dissipation rate. However, this introduces additional modeling assumptions and complications.

The understanding of the construction mechanism of the PDF of scalar concentrations, and of its time evolution is vital [8]. As [8] explains, "history matters", in the sense that, stirring and diffusion being two distinctive phenomena, it is an urgent need to account for the advection of fluid parcels in the mixing modeling. Statistically, this is a multi-time or multi-point correlation for the diffusion and dispersion of individual fluid parcels [9]. Consider a key issue affecting the IEM and Curl's models: the fact that two fluid parcels that are relatively close to each other are generally in a similar chemical composition state. How can it be that these two parcels are in relatively similar chemical composition if they never mixed before? Therefore, "history matters" [8, 9]. However, multi-point correlations are not considered in pure composition-space stochastic mixing models such as the Curl, IEM or EMST models.

At this point, the Hierarchical Parcel Swapping (HiPS) [10] model provides an efficient mixing model which is able to incorporates the correct physics, including the dynamics of the small scales in physical space. HiPS uses a hierarchical and stochastic mechanism of swapping fluid parcels to incorporate turbulence. Unlike other purely stochastic composition-space mixing models typically used in chemical reaction engineering, HiPS incorporates, by construction, multi-point or multi-parcel correlations. This will allow the understanding of issues such as scaling laws on different regimes of scalar turbulence, structure functions, high order statistics, as well as multi-point Lagrangian statistics.

HiPS as a flexible mixing model could be incorporated in the future as a closure for higher fidelity stochastic turbulence models, hybrid stochastic and Large Eddy Simulation (LES) approaches, or as a subgrid closure in hybrid LES or Reynolds-averaged Navier–Stokes (RANS) methods.

In this work, the functionality of a stand-alone HiPS formulation is first detailed. Preliminary results for passive scalar mixing with forced turbulence are shown. This includes the scalar power spectrum, the mean square displacement and the scalar dissipation rate. Additionally, a model extension of HiPS to take into account differential diffusion (variable Schmidt numbers) is given in the Outlook.

2. HIPS MODEL

HiPS was developed as a turbulent mixing model [10] by A.R. Kerstein. The core principle of HiPS is based on the representation of effects of turbulence on time-evolving scalar fields by a binary tree structure. Interestingly, this idea of the binary tree was postulated by Obukhov [11], according to his considerations on discrete models of turbulence. As in the discrete representation suggested by [11], dynamic parcels are tracked, allowing a consistent Lagrangian treatment. Variable values reside at the base level of the tree, the leaf level, which is a representation of the physical solution. An exemplary representation of the HiPS binary tree with 4 levels is detailed in Fig. 1a. Assuming that every node has exactly 2 children, there are 8 leaves at the leaf level. The number of levels n determines the number of leaves 2^{n-1}. In Fig. 1a, each leaf is understood as a fluid parcel and contains a variable value ϕ_α, where α is an index between 0 and 7. The variable values only reside at the base of the tree.

Every level i of the tree is associated with a specific length scale L_i and time scale τ_i. The length scale of a sub-node is simply half the length of the considered node, though other so-called scale reduction factors may be used. The associated time scales follow Kolmogorov's inertial range scaling law [12],

$$\epsilon \sim \frac{u^2}{\tau} \sim \frac{L^2}{\tau^3}. \tag{1}$$

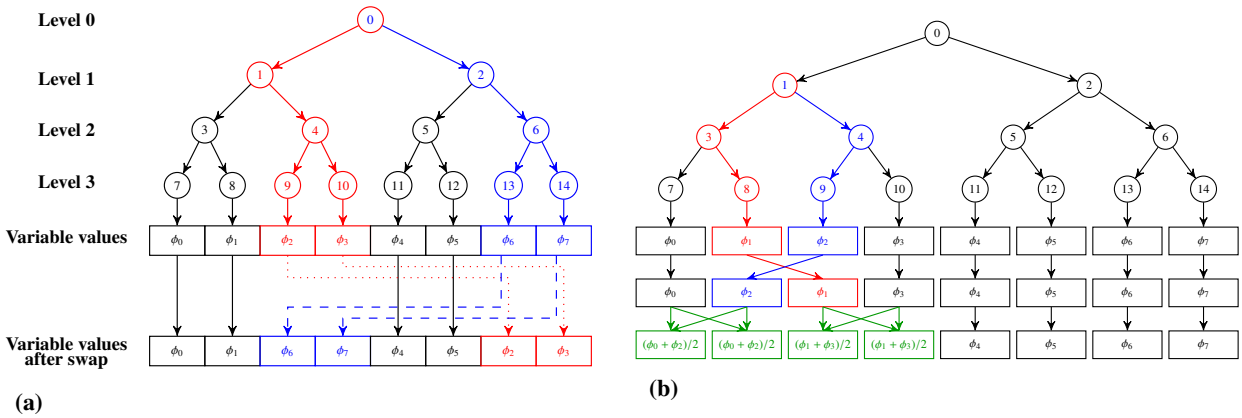


Figure 1. (a) Schematic illustration of a 4 level binary tree used in HiPS with a swapping event originated at node 0 with select grandchildren 4 and 6. (b) Schematic illustration of a swapping event originated at node 1 and a subsequent mixing process. The swapping event changes the proximity of adjacent fluid parcels and requires a subsequent mixing event, which is simply done by intermixing the contents of two adjacent fluid parcels.

In Eq. 1, u stands for the velocity and ϵ for the dissipation rate which is taken to be constant in the inertial range. Table 1 lists the length and time scales for an n level binary tree.

Table 1. Length and time scales of the binary tree used in HiPS.

level	length scale	time scale
0	L_0	τ_0
1	$L_0/2$	$\tau_0/2^{2/3}$
2	$L_0/4$	$\tau_0/4^{2/3}$
i	$L_0/2^i$	$\tau_0/(2^i)^{2/3}$
...	...	...
$n-1$	$L_0/2^{n-1}$	$\tau_0/(2^{n-1})^{2/3}$

The model rules for the representation of the effects of turbulence, which we will refer to as swapping events, are implemented by first selecting a grandparent node. A grandparent node is characterized by its children and grandchildren, such that only node 0 on level 0, as well as nodes 1 and 2 on level 1, can be considered grandparent nodes in Fig. 1a. The grandparent nodes are sampled in time as a Poisson process with a mean rate $\lambda_i = 2^i/\tau_i$, set by time scales assigned to each level i of the tree, based on Kolmogorov's inertial range scaling law [12],

$$\tau_i = \tau_0 \left(\frac{L_i}{L_0} \right)^{(2/3)} . \tag{2}$$

In this scaling law, L_0 and τ_0 are the integral length and time scales assigned to level 0 of the tree, and L_i and τ_i are the length and time scales of the i-th level of the tree. Based on Kolmogorov's hypothesis [13], the Reynolds number represented by the HiPS tree is defined by the tree size,

$$Re^{3/4} = \frac{L_0}{L_\eta}. \tag{3}$$

L_η stands for the Kolmogorov length scale, which is the length scale of the leaf level for the case of unity Schmidt number. The handling of variable Schmidt numbers is outlined in Section 4. After the grandparent node is selected, the swapping event is performed. For this purpose, a grandchild node is randomly selected from each of the left and right branches (children) of the grandparent node. The grandchildren of the grandparent node are then exchanged, or swapped along with their respective subtrees.

Fig. 1a shows this process at the selected parent node 0 with grandchildren 4 and 6. Note that nodes 3 and 5 could also have been selected as grandchildren. The exchange of fluid parcels taking place at the leaf level, the only physically relevant level of the tree, and the only level of the tree which is computationally stored, is an abstraction for the scale-reduction and advective rearrangement of fluid parcels in real turbulent mixing. Fluid properties stored at parcels located at the leaf level, undergo local modifications in their scalar gradients constructed from the discrete fluid properties stored at the leaf level. Considering one velocity component as a scalar, this would be the model analogy of increased strain due to turbulent advection. This complies with a local wavenumber increase, as in Kolmogorov turbulence [10].

The example in Fig. 1a shows a swap involving grandchildren at tree levels higher than the leaf level. Another situation occurs when the grandparent node 1 is selected, and, as an example, grandchildren nodes 8 and 9 are selected accordingly. The swapping event takes place at the leaf level, which corresponds to the smallest represented physical length scale. The parcel swapping changes the proximity within a fluid parcel pair and causes a mixing process. This is the case of Fig. 1b. A similar swapping event could occur if node 2 were selected as the grandparent node.

The mixing process, which is termed mixing

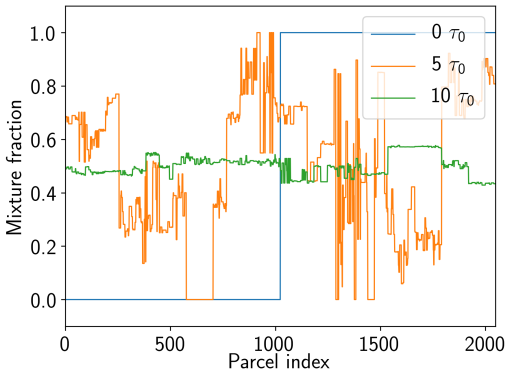


Figure 2. Illustration of passive scalar mixing in HiPS. The mixture fraction of the passive scalar is given at three different times along the fluid parcels.

event, is represented by intermixing the contents of two adjacent fluid parcels (constituting a node-joined pair). Mixing events can be implemented either instantaneously or at rates consistent with the prevailing diffusion time scales. Instantaneous mixing is a particularly efficient way to perform mixing. In the binary tree in Fig. 1a, an instantaneous mixing event would result in the scalar values of the adjacent parcels being replaced with the mean of the two parcels.

One salient feature of HiPS is that the mixing process itself is not restricted to a specific operation or rule. In [10, 14], and in the example presented in Fig. 1b, the mixing rule is equivalent to Curl's model. With this, HiPS effectively incorporates all features of Curl's model, plus the desired scale locality, representation of the correct joint scalar dissipation rate and the dependency of the mixing rate on scalar length scales. The mixing process could also be adapted to implement any existing mixing rule, e.g., IEM, without loss of generality. Additionally, the binary tree representation of the model allows the most efficient way to treat parcel advection from a computational point of view. That is, parcel movements can be simply represented by a bit shift in an index array pointing to locations in the various variable arrays. The efficient implementation of HiPS and its physical basis opens the door for the evaluation of higher order statistics in scalar turbulence in large parameter investigations, e.g., the skewness and hyperskewness of the scalar derivative required in order to discuss anomalous behavior of scalar structure functions [1].

In Fig. 2, the temporal evolution of a scalar mixing simulation is shown. The binary tree used for this simulation spans 12 levels. The plot illustrates the mixture fraction of the scalar against the fluid parcel indices. The scalar profile is initialized with a step function. All scalar values in the parcels at the left-hand sub-tree of the root node 0 are set to the value of 0 and all scalar values in the parcels at the right-hand sub-tree of the the root node 0 are set to the value of 1. This is indicated in Fig. 2 by the blue solid line ($0\tau_0$). At a later time ($5\tau_0$), the effects of the swapping and mixing events on the mixture fraction can be seen. The mixture fraction approaches the mean value of 0.5 with increasing time. After sufficiently long time ($>10\tau_0$), the flow is nearly mixed (approaching the mean value of 0.5) and only minute fluctuations can be seen compared to the orange curve ($5\tau_0$). After a time of $>30\tau_0$ (not shown here), everything is completely mixed and fluctuations can no longer be seen.

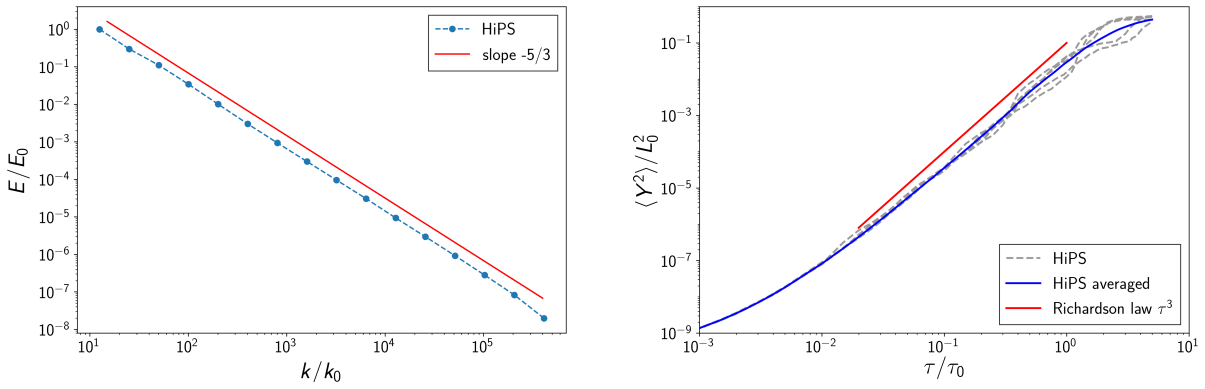
3. RESULTS

The following section shows preliminary results of a passive scalar mixing HiPS simulation. For all shown results, the same settings were used. The binary tree spans 16 levels with an associated Reynolds numbers of approximately one million. The represented Schmidt number is unity. This causes that the momentum and mass diffusivity is equal and the Kolmogorov and Batchelor length scales are located on the same level. In the Outlook, the treatment of variable Schmidt numbers is described. The scalar profile is initialized with a step function profile. All scalar values in the parcels at the left-hand sub-tree of the root node 0 are set to the value of 0 and all scalar values in the parcels at the right-hand sub-tree of the the root node 0 are set to the value of 1. The simulation considers turbulent forcing, which means that each time there is a top-level swapping event (swapping at grandparent node 0), a constant is added to the parcels in a given half of the domain so that their average is either 0 (left half) or 1 (right half). This turbulent forcing procedure doesn't change the overall mean and leaves the statistical variance of the subtrees unaffected.

3.1. Scalar spectrum

In HiPS, the generation of a scalar spectrum is not obvious and is reviewed in [10]. The tree structure induces a reduction of the length scales L_i with increasing levels i of the tree. Every step towards to the base of the tree results in an increase in the implied wavenumber $k_i = \frac{2\pi}{L_i}$. The mean variance across all sub-trees 2^i at a given level i is defined as $var_i\phi$, where ϕ denotes the scalar field. The HiPS analog of a scalar power spectrum can be calculated by $E(k) \sim \frac{1}{k_i}(var_{i-1}\phi - var_i\phi)$. In this context, $E(k)$ can be interpreted as scalar energy.

In Fig. 3a, the scalar power spectrum for passive scalar mixing with forced turbulence is shown. The dotted line marks the HiPS generated scalar power spectrum averaged over a time range of $100\tau_0$. The markers indicate the scalar $E(k)$ and the associated wavenumber k_i for the levels of the tree. A normalization with the maximum scalar energy E_0 and maximum wavenumber k_0 is carried out. For comparison purposes, the red line indicates a slope of -5/3 which represents the inertial power spectrum scaling



(a) **(b)**

Figure 3. (a) Scalar power spectrum of a passive scalar mixing HiPS simulation with forced turbulence using a step function initial condition (scalar value of 1 in all parcels at left-hand sub-tree and scalar value of 0 in all parcels of right-hand sub-tree). The dotted line shows the scalar power spectrum averaged over a time range of $100\tau_0$. The solid red line demonstrates -5/3 slope for comparison. (b) Mean square displacement of a passive scalar mixing HiPS simulation with forced turbulence. The blue solid line shows ensemble averaged HiPS results for the mean square displacement with a sample size of 100 realizations. The 5 gray dotted lines mark the mean square displacement for 5 independent HiPS realizations. The red solid line shows the Richardson-scaling law of τ^3 for comparison.

$E(k) \sim k^{-5/3}$. Fig. 3a demonstrates Kolmogorov's inertial range scaling law that is one of the core principles of HiPS. Additionally, the fundamental scaling relation in Kolmogorov turbulence of $E(k) \sim k^{-5/3}$ in the inertial range can be reproduced.

3.2. Richardson dispersion

The dispersion of particles under the influence of turbulence still poses challenges in fluid dynamics [15]. The dispersion describes how far initially adjacent particles are spatially separated from each other. Predictions for the dispersion under the influence of turbulence of particle pairs dates back to 1926 when Richardson [16] published an empirical approach where the mean square dispersion grows in time as τ^3.

In Fig. 3b, the mean square displacement $\langle Y^2\rangle$ versus time τ is presented for passive scalar HiPS simulations. A simple procedure to determine the dispersion Y of a parcel pair in HiPS is based on the length scale of the nearest shared parent. As in Fig. 1a shown, for the fluid parcels at nodes 9 and 10, the nearest shared parent has a length scale of L_2 (length scale of level 2). Similar to this procedure, for the fluid parcels at nodes 8 and 10, the nearest shared parent has a length scale of L_1 and for the fluid parcels at nodes 7 and 13, the nearest shared parent has length scale L_0.

In Fig. 3b, the mean square displacement $\langle Y^2\rangle$ is normalized by the square of the integral length scale L_0 and the time τ is normalized by the integral time scale τ_0. The blue solid line shows ensemble averaged HiPS results for the mean square displacement with a sample size of 100 realizations. The 5 gray dotted lines mark the mean square displacement for 5 different and independent HiPS realizations. The deviations of the gray lines from the blue line shows the randomness of the swapping events which is also influencing the mean square displacement. The red solid lines shows the Richardson-scaling law of τ^3 for comparison. It can be seen after a sufficiently long time the mean square displacement follows Richardsons dispersion law. Batchelor [17] predicted that the mean square displacement for times shorter than a characteristic timescale grows as τ^2. The characteristic timescale depends on the initial separation of the considered parcel pair. An investigation of the τ^2-scaling in HiPS is planned next. A finer temporal resolution of the initial phase and a wider range of length and time scales may be necessary for a detailed consideration of the Batchelor scaling. All in all, it is remarkable that such a simple and efficient mixing model is able to reproduce the Richardson dispersion law for the mean square displacement.

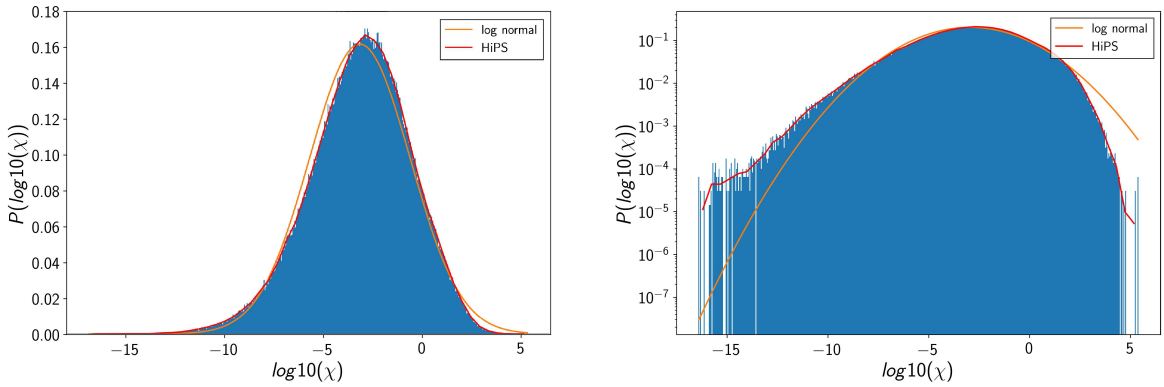
3.3. Scalar dissipation rate

The mixing of scalars in turbulent flows is a very interesting problem which provides a fundamental understanding of the basic processes involved. A key quantity in turbulent mixing that directly indicates the rate of decay of scalar fluctuations is the scalar dissipation rate χ.

The scalar dissipation rate is defined by [2],

$$\chi = \left\langle 2\Gamma \frac{\partial \phi'}{\partial x_i} \frac{\partial \phi'}{\partial x_i} \right\rangle \tag{4}$$

In Eq. 4, Γ is the diffusion coefficient of the scalar and $\frac{\partial \phi'}{\partial x_i}$ is the fluctuating scalar gradient. In



(a) **(b)**

Figure 4. (a) Probability Density Function (PDF) of the logarithmic scalar dissipation rate for a passive scalar mixing simulation in HiPS with a linear y-axis. The orange curve presents a normal distribution with the mean and standard deviation calculated from the HiPS results. (b) PDF of the logarithmic scalar dissipation rate for a passive scalar mixing simulation in HiPS with a logarithmic y-axis.

this context, ϕ is often taken as the mixture fraction. Since HiPS uses fluid parcels with proximities defined by the binary tree structure, a suitable formulation of the scalar dissipation rate in HiPS is needed. The definition of the scalar dissipation rate in HiPS is based on a similar scaling approach as in Eq. 1. For the diffusion coefficient $\Gamma \sim L^2/\tau$. The analogy to the fluctuating scalar gradient is given by the changes of the scalar field by the occurrence of swapping events. $\Delta\phi$ is computed by $\Delta\phi = \phi^{**} - \phi^{*}$. ϕ^{**} is the mixture fraction of the scalar before a swapping event and ϕ^{*} is the mixture fraction of the scalar after a swapping event.

This results in following relationship for the definition of the scalar dissipation rate in HiPS.

$$\chi = 2\frac{(\Delta\phi)^2}{\tau_{mix}} \tag{5}$$

In Eq. 5, τ_{mix} is the time since the last occurrence of a mixing process at the fluid parcel.

In Fig. 4a and 4b, the PDF of the log of the scalar dissipation rate is shown. For comparison purposes, a normal distribution with the mean and standard deviation calculated from the HiPS results is illustrated. Figs. 4a and 4b indicates that the commonly accepted log-normal distribution of the scalar dissipation rate χ is preserved. Additionally, HiPS exhibits a negative skewness in Fig. 4b, which is also seen in experiments and DNS [18].

4. OUTLOOK

In the current HiPS formulation, only unity Schmidt number passive scalars can be considered. This means that the Kolmogorov and Batchelor length scales are located on the same level. Arbitrary Schmidt number effects can be incorporated in the model by modifying the micromixing and swapping procedure, effectively allowing the creation of additional and intermediate levels in the binary tree. For the case of $Sc < 1$, the scalar has a very high diffusivity and the Batchelor length scale is larger than the Kolmogorov length scale. In this case, the mixing process can take place on levels above the leaf level (above the Kolmogorov scale).

The contrary is the case if $Sc > 1$. The diffusivity of the scalar is low and the Batchelor length scale is smaller than the Kolmogorov length scale. For the binary tree representation, this implies the existence of additional tree levels below the existing leaf level, which are turbulently advected, but only by swapping events with grandchildren on Kolmogorov or larger length scales. This implies that the nodes at these levels may be swapped as a consequence of a swapping event on upper tree nodes, but they can not be selected as children nodes themselves. Mixing processes, nonetheless, given by the set of mixing rules implied in the model, may still take place at these nodes below the leaf level.

The model extension for the treatment of variable Schmidt numbers opens the door for the investigation of differential diffusion effects, i.e., simultaneous mixing of scalars with different Schmidt numbers. Differential diffusion effects could be simulated in practice by specifying different mixing rules for each scalar in the binary tree. This allows investigation of multi-parcel correlations and scaling laws at very large or small Reynolds and Schmidt numbers.

5. SUMMARY

HiPS is a novel, computationally efficient and physics-based mixing model which at the same time fulfills constraints for good mixing models and several desirable properties of mixing models like locality of mixing in composition space, dependence of the mixing rate on scalar length scales and the incorporation of parametric dependencies such as Reynolds and Schmidt number dependencies. Additionally, the possibility to consider a large range of scales

while being computationally tractable is a significant advantage.

The results show noticeable agreement with known theories in passive scalar mixing. Given the simplicity of the model, a reproduction of the Richardson dispersion in passive scalar mixing and the preservation of a log-normal distribution of the PDF of the scalar dissipation rate are remarkable results. The extension to variable Schmidt numbers as described in the outlook is a necessary next step in the stand-alone HiPS formulation to investigate multi-parcel correlations and scaling laws at very large or small Reynolds and Schmidt numbers.

It is noted that HiPS has also been formulated as a turbulence model in [14], by means of the incorporation of momentum equations, and the use of a stochastic sampling procedure for swapping events analogous to the implementation of eddy events in the One-Dimensional Turbulence model [19]. A future application of HiPS could be the coupling with LES or RANS in a top-down or bottom-up approach, or by means of a sub-grid mixing model in PDF transport methods.

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