Hierarchical Parcel-Swapping: An efficient mixing model for turbulent reactive flows

Tommy Starick and Heiko Schmidt

1 Lehrstuhl Numerische Strömungs- und Gasdynamik, Brandenburgische Technische Universität Cottbus-Senftenberg, Siemens-Halske-Ring 14, D-03046 Cottbus, Germany

Hierarchical Parcel-Swapping (HiPS) developed by A.R. Kerstein [J. Stat. Phys. 153, 142-161 (2013)] is a computationally efficient and novel model for the effects of turbulence on time-evolving, diffusive scalar fields. The characteristic feature of HiPS is the interpretation of the one-dimensional flow domain or a state space as a binary tree structure. Every tree level corresponds to a specific length and time scale, which is based on a turbulence inertial range scaling. The state variables reside at the base of the tree and are interpreted 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. In this work, we investigate the influence of turbulent time scale variations on an isothermal series-parallel reaction scheme. The production of a desired chemical species is evaluated by means of a defined selectivity and is strongly affected by the underlying mixing time scales.

1 Introduction and HiPS model

Turbulent flow simulations are challenging due to the wide range of length and time scales. This imposes high resolution requirements. For Direct Numerical Simulations (DNS) that resolve all scales of the flow, the effort rises with at least the cube of the Reynolds number. Additionally, an immense supplementary effort is required for a proper resolution of the detailed chemistry. In respect to the currently available computational power, DNS simulations of most of the engineering applications are not feasible. Large Eddy Simulations (LES) overcome this limitation by only resolving large and intermediate scale effects and a complete modelling of the small scales. Hereby, the key challenge is to develop an accurate sub-grid scale model.

At this point, the Hierarchical Parcel-Swapping (HiPS) [1,2] model represents an attractive and computationally efficient ansatz for sub-grid scale modelling and combustion closure [5]. HiPS belongs to the family of one-dimensional, fully scale-resolved, stochastic turbulence models like the Linear Eddy Model (LEM) [3] and the One-Dimensional Turbulence (ODT) [4] model.

In comparison to LEM and ODT, HiPS uses a binary tree structure rather than a physical domain. Every level of the tree is associated with a specific length and time scale. The determination of the length scale $L$ and time scale $\tau$ is based on a turbulence inertial range scaling using $\tau = \tau_0 (L/L_0)^{2/3}$.

![Schematic illustration of the binary tree used in HiPS (left) and the reaction rates for the investigated series-parallel reaction scheme (right)](image)

$\frac{dY_A}{dt} = M - EE - Da_1 Y_A Y_B - Da_2 Y_A Y_R$ (1)

$\frac{dY_B}{dt} = M - EE - Da_1 Y_A Y_B$ (2)

$\frac{dY_R}{dt} = M - EE + Da_1 Y_A Y_B - Da_2 Y_A Y_R$ (3)

$\frac{dY_P}{dt} = M - EE + Da_2 Y_A Y_R$ (4)
The binary tree spans from the integral time scale $\tau_0$ and length scale $L_0$ (root of tree) down to the Kolmogorov or Batchelor scale (base of the tree). On the left side of Fig. 1, an exemplary four level binary tree is illustrated. The state variables reside only at the base of the tree and are considered as fluid parcels.

Turbulent advection is implemented by swapping pairs of sub-trees randomly sampled from a Poisson process at rates determined by the associated turbulent time scale. These rearrangement events are termed eddy events (EE). On the left side of Fig. 1, two exemplary eddy events are shown. The first eddy event is a swap at base node 0 (blue nodes). After selecting the base node, a grandparent node two levels below the base node is randomly sampled in each sub-tree. In this example, node 3 and 6 are selected and the sub-trees associated with the grandparent nodes are subsequently swapped. The second eddy event is a swap at base node 2 with randomly sampled grandparent nodes 11 and 13 (red node numbers).

In HiPS, molecular mixing is represented by intermixing the contents of two adjacent fluid parcels (constituting a node-joined pair). These mixing processes only occur if the proximity within a fluid parcel pair changes and is termed mixing event (ME) in HiPS. Mixing events can be implemented either instantaneously or at rates consistent with the prevailing diffusion time scales. In the binary tree in Fig. 1, an instantaneous mixing event is illustrated after the second eddy event. The second eddy event changes the proximity of the adjacent parcel pairs and requires a subsequent mixing event.

2 Results

Fig. 2 shows results of stand-alone HiPS simulations of an isothermal series-parallel reaction scheme with two parallel competitive reactions and four species: $A + B \to R, A + R \to P$. Hereby, species R is taken as desired product. A selectivity $S$ can be formulated based on the ratio between mass fraction of species P and the sum of the mass fractions of species R and P: $S = 2Y_P / (Y_R + 2Y_P)$ [6]. On the right side of Fig. 1, the governing equations for the investigated series-parallel reaction scheme are shown, whereby the Damköhler number $Da = \tau / \tau_{\text{reaction}}$ stands for the ratio of the prevailing turbulent time scale to the prevailing chemical time scale as in [6]. The molecular weights for A and B are assumed to unity. All HiPS simulations start with initially segregated reactants at either half of the domain. In Fig. 2, the temporal evolution of the mean and RMS selectivity profile is shown for HiPS simulations with a ten level binary tree and varying Damköhler numbers. For $Da_1 > Da_2$, more R is produced than consumed by the second reaction. This leads to a better selectivity. For a fixed value of $Da_2$, the selectivity is not significantly affected by a change of the value of $Da_1$ as in [6]. This work has qualitatively shown the capabilities in using HiPS as a stand-alone model for reactive flow simulations. Since HiPS is a very new model, further research is required before it can be used as a sub-grid scale model in LES.

References

[1] A. Kerstein, Hierarchical Parcel Swapping Representation of Turbulent Mixing. Part 1. Formulation and Scaling Properties, Journal of Statistical Physics 153, 142-161 (2013).
[2] A. Kerstein, Hierarchical parcel-swapping representation of turbulent mixing. Part 2. Application to channel flow, Journal of Fluid Mechanics 750, 421-463 (2014).
[3] A. Kerstein, A Linear Eddy Model of Turbulent Scalar Transport and Mixing, Combustion Science and Technology 60, 391-421 (1988).
[4] A. Kerstein, One-dimensional turbulence: model formulation and application to homogeneous turbulence, shear flows, and buoyant stratified flows, Journal of Fluid Mechanics 392, 277-334 (1999).
[5] D. Lignell, A. Kerstein, A. Perego, T. Starick, J. Frei and H. Schmidt, Application of the Hierarchical Parcel Swapping (HiPS) Model to Turbulent Reacting Flows, 11th U.S. National Combustion Meeting (2019).
[6] S. H. Frankel, P. A. McMurtry and P. Givi; Linear Eddy Modeling of Reactant Conversion and Selectivity in Turbulent Flows, AIChE Journal 41, 258-266 (1995).