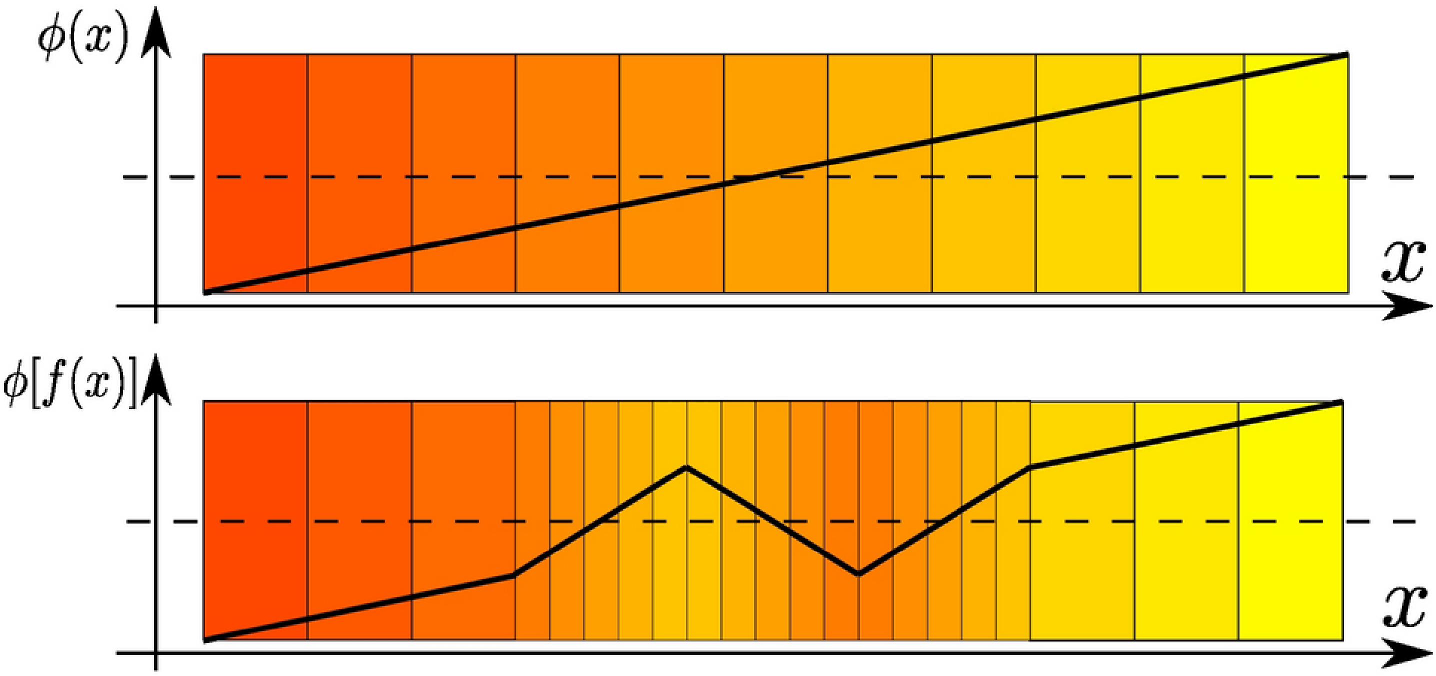

MS80

Reduced order modeling and simulation of multiphysical turbulent flows

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Online Workshop

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Cottbus - Senftenberg

MS80:
Reduced order modeling and simulation of multiphysical turbulent flows

(An online workshop in substitution of cancelled minisymposium at ECCOMAS2022)

Workshop organizers:

- **David Lignell (BYU)**
- **Marten Klein (BTU)**
- **Juan Medina (BTU)**

A Pressure coupled Representative Interactive Linear Eddy Model (RILEM) for heavy duty truck engine combustion simulations

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Key Words: *multiple Representative Interactive Linear Eddy Models, Pressure coupling, Turbulence chemistry interaction, Mixed-mode combustion.*

Running engines in nonstandard conditions, such as low-temperature ranges or using partially premixed mixtures helps with reducing harmful emissions. The Linear Eddy Model (LEM) is a candidate to simulate these scenarios. LEM is a regime and mode independent mixing model for reactive flows [1], it advances finite rate chemistry and captures turbulence chemistry interaction which is important for pollutants prediction. Coupling LEM to a CFD code that simulates the spray chamber geometry is referred to as the Representative Interactive LEM (RILEM). A previous version based on volume coupling has been successfully validated against experiment [2]. A recent version of RILEM is proposed with a pressure coupling schem where the key advantage is the intrinsic inclusion of latent heat of evaporation effects and wall heat losses in the pressure trace which is communicated from the CFD, wherein separate modelling is needed in the previous version. Enforcing the CFD pressure will break the representative nature of RILEM because of volume modifications. The spherical formulation of LEM is used to modify the line to match with the combustion chamber bore while maintaining the same LEM volume adapting the cone angle.Updating the 3D CFD chemical state from a unidimensional line will present limitations. A solution was to run multiple LEM lines on parallel with different turbulence statistics and average the results into one general solution. This approach has been entitled mRILEMs. It was tested for a single cylinder case of a heavy duty truck engine. The pressure trace was compared against experiment and reached good agreement. It was also possible to quantify intermediate species such as CO and OH. This work lead to the conclusion that coupling mRILEM to CFD based on pressure will make sure that the chemical state is controlled uniquely from the LEM lines.

Refrences

[1] A. R. Kerstein, “Linear-eddy modeling of turbulent transport. Part 4. Structure of diffusion flames,” *Comb Sci Tech*, vol. 81, pp. 75-96, 1992.

[2] T. Lackmann, A. R. Kerstein, and M. Oevermann, “A representative linear eddy model for simulating spray combustion in engines (RILEM),” *Combustion and Flame*, vol. 193, pp. 1-15, 2018.

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LARGE-EDDY SIMULATION WITH ONE-DIMENSIONAL TURBULENCE WALL MODEL APPLIED TO THE ATMOSPHERIC BOUNDARY LAYER

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Keywords: *Large-Eddy Simulation, One-Dimensional Turbulence, Atmospheric Boundary Layer*

In this study, a large-eddy simulation (LES) code with the one-dimensional turbulence (ODT) wall model is tested for the simulation of the atmospheric boundary layer under neutral, stable, unstable and free-convection conditions. The ODT model provides a vertically refined flow field near the wall, which has small-scale fluctuations from the ODT stochastic turbulence model and an extension of the LES large-scale coherent structures. From this additional field, the lower boundary conditions needed by LES can be extracted. Results are compared to the LES using the classical algebraic wall model based on the Monin–Obukhov similarity theory (MOST), showing similar results in most of the domain with improvements in horizontal velocity and temperature spectra in the near-wall region for simulations of the neutral/stable/unstable cases. For the free-convection test, spectra from the ODT part of the flow were directly compared to spectra generated by LES-MOST at the same height, showing similar behaviour despite some degradation. Furthermore, the additional flow field improved the near-wall vertical velocity skewness for the unstable/free-convection cases. The tool is demonstrated to provide adequate results without the need of any case-specific parameter tuning. Future studies involving complex physicochemical processes at the surface (such as the presence of vertically distributed sources and sinks of matter and energy) within a large domain are likely to benefit from this tool. [1]

References

[1] L. S. Freire. Large-eddy simulation of the atmospheric boundary layer with near-wall resolved turbulence. *Boundary-Layer Meteorology*, pages –, 2022.

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On the modifications to the spatial formulation of the One-Dimensional Turbulence model for internal flows

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Keywords: *Internal flows, ODT, spatial, constant property flows*

For flows of practical relevance, numerical simulations generally incorporate a turbulence model which relaxes otherwise expensive resolution requirements. These are set by a power-law scaling in terms of the Reynolds number of the flow. Turbulence models involve a compromise set by a cutoff in the spectrum of physical length and time scales. In 1999, Kerstein postulated the One-Dimensional Turbulence model [1], as a way to resolve the full range of physical scales by modeling the effects of the dynamical drivers of the turbulent kinetic energy cascade in three-dimensional flows, i.e., the turbulent eddies. The original ODT formulation conceptualizes a line of sight drawn through the turbulent flow, the latter assumed solenoidal and of constant properties, along which fully resolved discrete scalar profiles are represented and time-advanced. The dynamical change of the profiles is due to the model representation of the advective transport (triplet maps), as well as the incorporation of the numerically resolved 1-D viscous transport in accordance with a formulated partial differential equation (PDE). A relevant extension of ODT is the spatial formulation (S-ODT) [2], which ultimately aims to enable direct 2-D simulations of statistically steady flows. S-ODT advects the 1-D numerical domain in streamwise direction according to conservation laws of 2-D steady flows. S-ODT was originally postulated for flows in unconfined 1-D domains. The advection of the ODT line yields accurate results for flows of dominant parabolic character. The solution to the demanded constancy of the streamwise mass-flux on top of the implied 2-D momentum conservation PDE is also easily solvable given the ability of the domain to accomodate line-oriented fluxes in the resolved direction by considerations on a deforming Lagrangian volume. However, in confined domains, such solution in the reduced 1-D setting is not straightforward. This issue is the equivalent of the calculation of the numerical solution of a highly coupled 2-D pressure Poisson equation. Thus, a new model extension is required. The intended extension is presented here for planar and cylindrical 2-D statistically steady flows, e.g., constant property channel and pipe flows. A discussion on the balance of physical and numerical fluxes in the model is also presented in order to address the conservative features of the model.

REFERENCES

[1] A. R. Kerstein, One-dimensional turbulence: model formulation and application to homogeneous turbulence, shear flows, and buoyant stratified flows, *J. Fluid Mech.* **392** (1999) 277-334.

[2] W. T. Ashurst and A. R. Kerstein, One-dimensional turbulence: Variable-density formulation and application to mixing layers, *Phys. Fluids* **17(2)** (2005) 025107.

High-fidelity modeling and simulation of multiple scalar mixing in a coaxial jet using one-dimensional turbulence

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Keywords: concentric coaxial jet, multiple passive scalars, one-dimensional turbulence, stochastic modeling, turbulent mixing

Representation of turbulent mixing of passive scalars in spatially developing shear flows is a standing challenge for many applications in chemical, mechanical, and environmental engineering. Key problems are related to simultaneous scalar and momentum transport for differentially-diffusing scalars [1]. Here, the turbulent mixing of multiple passive scalars in a three-stream coaxial jet is investigated as a canonical problem. Reduced-order numerical simulations capturing small-scale cross-stream (radial) transport processes are performed with the one-dimensional turbulence (ODT) model [2] as stand-alone tool. Schmidt numbers are close to one as we focus on the spatial variability of turbulent mixing in gases. Model predictions for the scalar mixing are in satisfactory agreement with reference data [3] for various radial and downstream locations. One-point correlations and detailed state-space statistics are discussed. In particular, two-scalar joint probability density functions are reproduced as model prediction which is not possible with traditional averaged and filter-based models.

References

[1] M. Klein, C. Zenker and H. Schmidt. Small-scale resolving simulations of the turbulent mixing in confined jets using one-dimensional turbulence. *Chem. Eng. Sci.*, Vol. **204**, pp. 186–202, 2019.

[2] D.O. Lignell, V.B. Lansinger, J. Medina, M. Klein, A.R. Kerstein, H. Schmidt, M. Fistler and M. Oevermann. One-dimensional turbulence modeling for cylindrical and spherical flows: model formulation and application. *Theor. Comput. Fluid Dyn.*, Vol. **32**, pp. 495–520, 2018.

[3] J. Cai, M.J. Dinger, W. Li, C.D. Carter, M.D. Ryan and C. Tong. Experimental study of three-scalar mixing in a turbulent coaxial jet. *J. Fluid Mech.*, Vol. **685**, pp. 495-531, 2011.

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Towards the evaluation of heat and mass transfer in pipe flows with cocurrent falling films using One-Dimensional Turbulence

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Keywords: *ODT, cocurrent, falling film, multiphase, evaporator*

The process engineering branch of air-liquid system applications is vast and comprises relevant topics of research ranging from the influence of (liquid) surface wave dynamics, to classical laminar and turbulent flow dynamics concerning heat and mass transfer. Seminal works such as those of Yan et al. [1], and Feddauoi et al. [2] have already ellucidated important issues in the physical interactions between momentum, mass, and heat transfer of air-water systems. For such systems, an industrial application of practical relevance is the falling film evaporator. Heat and mass transfer related issues in this device are mainly concerned with the evaporative cooling of the liquid falling film, and the potential component concentration increase in the liquid. Direct Numerical Simulations (DNSs) of falling films are mostly focused on the immediate surroundings of the film. The transition dynamics of the (inner) gas stream, particularly for turbulent flows, and the effect that such dynamics could have on the interfacial shear stress at the liquid film, is an issue that should be addressed by DNS investigations. However, to the best of our knowledge, no DNS has yet been able to address a dynamically similar case to that of a full falling film evaporator. In the meanwhile, this study could be the first stepping stone to bridge the DNS gap utilizing a stochastic turbulence model which allows full scale resolution in a reduced dimensional setting, in comparison to traditional filter-based turbulence models. We use a novel numerical solver implementing the One-Dimensional Turbulence (ODT) model [3] in a cylindrical turbulent heated air flow which is surrounded by a laminar cocurrent water falling film. The solver utilizes the ODT model in order to evaluate the effects of turbulent advection and turbulent heat flux in the (inner) gas side, while the liquid side is assumed laminar. The simulation results are compared to the numerical Reynolds-Averaged Navier-Stokes (RANS) study performed by [2] for a cocurrent water falling film evaporator.

REFERENCES

[1] W.-M. Yan, Binary diffusion and heat transfer in mixed convection pipe flows with film evaporation, *Int. J. Heat Mass Transfer*, **36(8)** (1993) 2115-2123.

[2] M. Feddaoui, A. Mir and E. Belahmidi, Cocurrent turbulent mixed convection heat and mass transfer in falling film of water inside a vertical heated tube in *Int. J. Heat Mass Transfer*, **46(18)** (2003) 3497-3509.

[3] W. T. Ashurst and A. R. Kerstein, One-dimensional turbulence: Variable-density formulation and application to mixing layers, *Phys. Fluids* **17(2)** (2005) 025107.

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Super-grid Linear Eddy Model as chemical closure for turbulent combustion

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Keywords: Large Eddy Simulation, Linear Eddy Model, non-premixed, turbulent combustion.

Linear Eddy Model (LEM) has been used successfully in previous years as sub-grid chemical closure for Large Eddy Simulation (LES) in turbulent combustion [1]. Here, every CFD cell contains a highly resolved one dimensional LEM line where diffusion and reaction equations are time advanced, the leading principle being that in a sufficiently turbulent flame region, the fluctuations of scalars such as temperature and mass fraction along a given line of sight are independent of orientation owing to isotropy of the small scales. LEM, by itself, is mode independent and accounts for the influence of turbulent mixing by locally applied mapping functions. Advection between the CFD cells is realized on the LEM level using a mass conservative splicing scheme in which resolved CFD fluxes determine the transport of LEM fragments between the CFD cells in a Lagrangian way.

The current implementation aims to reduce the computational expense of LES-LEM using CFD cell agglomeration to form a coarse level *super-grid*. Each cell cluster then contains a single LEM line, thereby reducing the total number of lines and splicing operations.The filtered chemical state variables for any CFD cell in a cluster are determined using joint integration of the conditioned averages (with respect to mixture fraction, Z, and/or progress variable, c) of state variables over the associated LEM line, weighted by the Probability Density Functions (PDFs) for Z and/or c. PDF parameters are obtained by CFD-level time advancement of transport equations for mixture fraction mean, its variance and a mean progress variable. This flexible representative mapping strategy allows for either a premixed or non-premixed formulation.

LEM provides on-the-fly local flame statistics which should capture finite rate chemistry effects and the super-grid approach shows considerable speed-up compared to LES-LEM. A pressure based super-grid solver was implemented using the OpenFOAM library and tested with a premixed acetylene flame setup over backward facing step.

References

[1] V. Sankaran, "Sub-grid combustion modelling for compressible two-phase reacting flows," PhD thesis, Georgia Institute of Technology, 2003.