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**Abstract**

# Multiscale simulation of transport phenomenon across a reactive interface

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Multiscale simulation is a powerful tool to model transport phenomenon across an interface that bridges both microscopic and macroscopic domains. The breakage of the continuity and non-slippery assumptions at or close to the interface renders molecular simulation particularly instructive to reveal what happens locally. Consequently intensive research has been conducted in the last two decades on multiscale simulation via the molecular dynamics (MD) and computational fluid dynamics (CFD) approach. Different coupling strategies, such as MD derived peripteries coupling, heterogeneous multiscale modelling (HMM) and domain decomposition (DD) have been developed. For thermophysical properties predictions, equilibrium molecular dynamics (EMD) has been widely used, which allows the predication of size-dependent properties, hence the prediction of transport phenomenon near or across an interface under quasi-equilibrium conditions possible.

For an interface involving complex chemical reactions under highly non-equilibrium conditions, however, the traditional MD-CFD coupling approach becomes unsuitable. One of these examples is the thermal protection materials (TPM), which have to be able to withstand high heat and stress under extreme conditions. The strong aero-heating associated with hypersonic flow leads to various complicated physiochemical phenomena. The fluid flow and heat transfer close to the interface exhibits strong thermal/mechanical/chemical multi-fields coupling effects in a highly non-equilibrium environment.This talk reports our progress in the multiscale RMD-CFD coupling and simulation of transport phenomenon across interfaces where strong chemical reactions occurs. Examples studies of heat and mass transfer across an interface where surface catalysis, surface oxidation and ablation occurs under highly non-equilibrium conditions for different types of TPM are illustrated. The limitation, and challenges of our multiscale approach, as well as pespective outlook of future research is discussed.

**About the speaker:**

Prof. Dongshegn Wen is the 8th Chair of the Institute of Thermodynamics, Technical University of Munich. He received BEng in Aeronautics from Beihang University, MSc in Thermophysics from Tsinghua University and DPhil in Engineering Science from the University of Oxford. Prior to his current position, he was the Chair Professor at the University of Leeds and Beihang University, and had he worked in various academic positions at the Queen Mary University of London.

His research is focused on heat: namely, how heat is produced, transported, stored and utilized across different scales via nanomaterials / nano-surfaces with targeted applications in energy and aerospace engineering. He has taken a multiscale approach, both experimentally and numerically from nanoscale to bulk scale, to investigate fundamentals of flow, heat transfer and reactions across scales, and apply these fundamentals cross-disciplinarily into different sectors. His research has produced over 20 patents, ~350 referred journal publications, with total citation of ~23000 and current H-index = 68. He is a member of the Academia of Europaea (MAE), an elected Fellow of the Royal Society of Chemistry (FRSC) and the Energy Institute (FEI), the Editor-in-Chief of <Advance in Aerodynamics>, and Associate Editor/Subject Editor in Transfer Processes of <Applied Thermal Engineering>

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