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# ON COMPUTATIONAL PROCEDURES OF TRANSPORT PHENOMENA IN EQUIPMENT OF ENERGY SYSTEMS

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**ABSTRACT** Energy systems involve several components where fluid flow, heat and mass transfer, chemical and electrochemical reactions are the key transport processes. For design and development, performance evaluation as well as investigation of innovative ideas, computational methods are of vital importance. Computational fluid dynamics (CFD) approaches based on the continuum hypothesis have been developed since 1960s and today many commercial computer codes exist for engineering applications. Besides many in-house codes exist at universities and research institutes. Lately open source CFD codes have become available. Nevertheless research is still needed not the least for turbulence modeling, coupled processes, complex geometries and parallel computing. As equipment are becoming very small in size the important processes take place at nano- or micro-scale. Then the continuum approach needs to be relaxed and non-continuum methods based on some form of coarse-grained molecular dynamics are needed. In this paper, investigations of computational heat transfer, fluid flow and related transport phenomena are illustrated for compact heat exchangers, gas turbine heat transfer and fuel cells.

**KEYWORDS**: CFD, molecular dynamics modeling, fuel cells, compact heat exchangers, gas turbines