“Multi-Scale Analysis of Heat and Mass Transfer in Mini/Micro-Structures”

Over the last decades, the refrigeration, air conditioning and heat pump industry has been forced through major changes caused by new restrictions on refrigerant based on environmental issues. Essentially the great majority of the current synthetic fluids in the refrigeration technology derive from paraffinic hydrocarbons and they can be obtained by substituting the hydrogen atoms with atoms of other substances, like chlorine and fluorine (CFCs, HCFCs and HFCs). High concentrations of these fluids induce an enhanced global warming. In particular, the synthetic fluids involved in the refrigeration technology are the strongest greenhouse gases per molecule and they account for the 25 % of the change in the intensity of the Earth's greenhouse effect. Moreover the synthetic fluids attack the molecules of ozone in the stratosphere converting them into oxygen molecules. A severe decrease in the thickness of the ozone layer could lead to harmful effects, like an increase in the number of cases of skin cancer, a sharp increase in cataracts and sun burning, suppression of immune systems and a reduction in the growth of ocean phytoplankton.

For these reasons, an unquestionable trend exists, which aims to reduce and eventually eliminate the utilization of synthetic fluids in refrigeration technology, according to Kyoto and Montreal Protocol. For example, a gradual phase-out of refrigerant R-134a in mobile air conditioning in EU starting from 2008 has been recently approved. Among natural refrigerants, carbon dioxide is a very promising working fluid for vapor compression refrigerating systems.

This PhD thesis deals with investigating both numerically and experimentally the suitability of the transcritical refrigerating cycles based on carbon dioxide for the air conditioning of civil aircrafts, in order to reduce the energy consumption by increasing the efficiency of the current air-based devices and, at the same time, to realize a long-term solution by avoiding any future regulation constraint. This goal is particularly challenging from the technological point of view, because carbon dioxide components are not still reliably developed (the experimental results reported in this thesis refer to the first aeronautic prototype in the world), and from the theoretical point of view, because heat transfer phenomena close to the critical point involve multiple interacting scales (showing the limits of continuum based approach). This investigation was financially supported by the European Commission by the growth project G4RD-CT-2001-00601 “Power Optimised Aircraft” (POA) within the Action “New Perspectives in Aeronautics”, which is a four-year project with a budget of about 100 million euro, jointly funded by the EC and the 43-company consortium (main partners: Liebherr-Aerospace, Airbus, Hispano-Suiza, DLR, Rolls-Royce, Alenia Aeronautica, Volvo Aero Corporation).

Each chapter of the present PhD thesis relates to an article published on international journals and/or international conferences. The sequence of these chapters follows an ideal path from macroscopic to microscopic, in order to highlight the underlying connections which explain the technological difficulties at the final-user level and to prove how far (and how small) the most promising engineering approaches can bring the design of new solutions.

In Chapter 1, the right perspective for appreciating the reported results is explained: the selected technological application is just an example of how miniaturization and functional integration are widening the application context of engineering activity in order to include mini/micro structures as natural objects of the design process. Within this framework, the mesoscopic modeling appears as a promising tool for developing a simplified description of the link between macro-scale and micro-scale phenomena.

In Chapter 2, the design of an experimental test rig for characterizing the thermal performances of a refrigerating device based on a carbon dioxide transcritical cycle for airborne application is discussed[1]. This experimental test rig proves that the transcritical device can properly match the required specifications in order to be integrated with a conventional air–cycle machine and to realize in this way a hybrid air conditioning system for airborne application. Some practical solutions for managing the integration between the conventional system and the vapor cycle system

[1] P. Asinari, A. Cavallini, A. Mannini, C. Zilio, “Carbon Dioxide as a Working Fluid in Aircraft Air–Conditioning: an Experimental Assessment”, IIR (International Institute of Refrigeration) International Conferences, Vicenza, Italy, 2005.

are discussed on the basis of the experimental results. In particular, finned compact gascoolers made of flat extruded aluminum tubes with internal mini/micro-channels will be further discussed, because they constitute one of the main research goals for the development of this technology.

In Chapter 3, in order to reduce the computational demand required by the modeling of compact heat exchangers, some improvements to a recent numerical scheme for elliptic problems in complex structures are discussed[2]. These improvements were included in the development of a numerical code, which allows one to perform detailed three dimensional simulations for compact heat exchangers. In particular, the effects due to conduction in finned surfaces are analyzed in practical configurations involved in actual market devices[3]. The numerical results are effected by the low reliability of the heat transfer phenomenological correlations developed for carbon dioxide close to the critical point.

In Chapter 4, the heat and mass transfer of carbon dioxide flowing in mini/micro channels for conditions close to the critical point is analyzed[4,5]. In particular, the additional turbulence induced by the density fluctuations, which are relevant close to the critical point, is analyzed and a simple theoretical model for taking into account these additional terms in the averaged macroscopic equations is suggested. The numerical predictions show that the effects due to density fluctuations are smaller than it could have been initially supposed and that the heat transfer impairment for mini/micro channels, which some experiments seem to highlight, is not completely explained by the continuum based approach and this motivates the use of pseudo-kinetic modeling.

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[2] P. Asinari, "Finite-volume and Finite-element Hybrid Technique for the Calculation of Complex Heat Exchangers by Semiexplicit Method for Wall Temperature Linked Equations (SEWTLE)", Numerical Heat Transfer: Fundamentals, Vol. 45, pp. 221–247, 2004.

[3] P. Asinari, L. Cecchinato, E. Fornasieri, "Effects of Thermal Conduction in Microchannel Gas Coolers for Carbon Dioxide", International Journal of Refrigeration, Vol. 27, N. 6, pp. 577-586, 2004.

[4] P. Asinari, "Numerical Prediction of Turbulent Convective Heat Transfer in Mini/Micro Channels for Carbon Dioxide at Supercritical Pressure", International Journal of Heat and Mass Transfer, Vol. 48, N. 18, pp. 3864-3879, 2005.

[5] P. Asinari, "Comparison among Phenomenological Correlations for Convective Heat Transfer of Supercritical Carbon Dioxide Flowing in Mini/Micro Channels under Cooling Conditions", IIR (International Institute of Refrigeration) International Conferences, Vicenza, Italy, 2005.

In Chapter 5, the Lattice Boltzmann Method (LBM) is presented in a very general fashion including computational complexity, boundary conditions, parallelization and data structures. A new pseudo-kinetic model based on LBM was developed for describing the mesoscopic dynamics of gaseous mixtures by overcoming the limits of existing models[6]. This model has been recently further improved in terms of flexibility[7]. A proper numerical code implementing this model (up to 10,000 lines) was developed from scratch in order to simulate the fluid flow of reactive mixtures in randomly generated porous media. The numerical code has been developed in a parallel fashion for dealing with actual three dimensional topologies. This code is a powerful flexible tool for investigating mesoscopic phenomena and leading the design of new materials.

It is finally worth mentioning that the developed numerical code has been successfully used in a wide set of applications at "Virginia Tech" (VA, U.S.A.) on "System X" cluster facility (fastest super-computer at any academic institution in world based on TOP500 of 2004) and at "Old Dominion University" (VA, U.S.A) on "Zenith" cluster facility. Currently research topics include the fluid flow of reactive mixtures through porous media in both polymer electrolyte membrane[8,9] (PEMFC) and solid oxide fuel cells[10,11] (SOFC) and the direct numerical simulation (DNS) of

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[6] P. Asinari, "Viscous coupling based lattice Boltzmann model for binary mixtures", Physics of Fluids, Vol. 17, N. 067102, 2005.

[7] P. Asinari, "Effects of cross collisions in the simulation of binary mixtures by the lattice Boltzmann method", Second International Conference for Mesoscopic Methods in Engineering and Science, Hong Kong, 2005 (to appear).

[8] P. Asinari, M. Coppo, "Influence of porous electrode structure on PEM fuel cells design and performance", II International Conference on Fuel Cell Science, Engineering and Technology, Rochester NY, 2004.

[9] P. Asinari, M. Coppo, M. R. von Spakovsky, B. V. Kasula, "Numerical simulations of gaseous mixture flow in porous electrodes for PEM fuel cells by the lattice Boltzmann method", III International Conference on Fuel Cell Science, Engineering and Technology, Ypsilanti, MI, 2005.

[10] P. Asinari, M. Calì Quaglia, M. R. von Spakovsky, B. V. Kasula, "Numerical Simulations of Reactive Mixture Flow in the Anode Layer of Electrolyte Supported Solid Oxide Fuel Cells by the Lattice Boltzmann Method", First European Fuel Cell Technology and Applications Conference, Roma, 2005 (to appear).

[11] P. Asinari, M. Calì Quaglia, "Reconstruction of three dimensional microscopic structures using multiple–point statistics for porous anodes of solid oxide fuel cells", International Conference on CAE and Computational Technologies for Industry, Lecce, 2005 (to appear).

homogeneous isotropic turbulence decay for binary mixtures[12]. This proves how new material design can actually cut the edge of emerging energy technologies.

[12] L.-S. Luo, P. Asinari, S.S. Girimaji, B. Grossman, "Kinetic models of mixtures", MURI Meeting, United States Air Force Office of Science Research, University of Minnesota, 2005 (confidential).