POLITECNICO DI TORINO
DOCTORAL PROGRAM IN ENERGETICS
Ph. D. THESIS PROPOSAL

Subject
Mesoscopic numerical simulation of reactive mixtures in porous media applied to solid oxide fuel cells by means of the Lattice Boltzmann Method

List of proponents (with e-mail address of the responsible person)		
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Description of the international background of the proposal

Among the new technologies under development for energy conversion, the *high-temperature solid oxide fuel cells* (SOFCs) are the leading candidates for stationary distributed power generation. Fuel-cell systems are seen as more environmentally friendly and energy efficient than their primary fossil-fuel counterparts and unlike renewables have a high potential for playing a significant role in the energy economy. Central to these systems are the fuel cell stack and the individual components which comprise each of the cells which make up the stack. It is the proper and optimal synthesis and design and manufacture of these components which will be key to the future success or failure of this technology.

At present the synthesis and design of these materials and structures is a rather ad hoc process of making trial-and-error changes in order to see if such changes improve the performance of the fuel cell. This approach can be quite expensive both in terms of time and resources. The 3D *macroscopic* models and simulation tools [1–4], which have been developed in order to predict fuel cell performance, cannot completely overcome the problem. In fact, the *macroscopic* approach always involves some phenomenological coefficients which are used into the constitutive correlations for simplifying the analysis of the microscopic phenomena. For example, many models are based on the mean transport pore assumption (MTPA), which means that the structure of the porous medium is considered isotropic so that it can be described by three structural parameters (the ratio of porosity to tortuosity, the mean value and the standard deviation of the pore radii) [5]. Unfortunately all the previous parameters are difficult to measure accurately and, since they are characterised by strong statistical scattering around the average values, the reliability of results due to *macroscopic* models becomes somehow ambiguous. Even the experimental validation reduces its effectiveness because an averaged index of performance for the whole fuel cell, like the polarization curve, can be satisfied by tuning the microscopic parameters according to multiple strategies, which are all equivalent in principle. This situation shows that the analysis of reactive multi-component mixtures of gases in porous solids needs additional investigation tools, in order to be truly accurate [6].

A much more systematic approach is needed, which applies a fundamental understanding at a *microscopic* scale of the selective transport of molecules, atoms, and ions in electrolytes and electrode layers [7]. A systematic approach would be guided by models which can predict the behaviour and the properties of these components with each change in material and structure. Such models can, for example, in the electrode-electrolyte layer, be used to describe the competition effect between neighbouring particles, describe diffusion limitations, predict the geometric characteristics of the porous medium (i.e. layer thickness, active area to geometrical area, mean inter-particle distance, pore size and agglomerate thickness), and suggest ways of

improving layer structure.
Unfortunately the conventional *microscopic* tools are limited to computational domains much smaller than those required by practical design purposes. For this reason, during the last years some methods have been suggested which try to recover the hydrodynamic information by starting from a pseudo kinetic description of the phenomena. These techniques are called *mesoscopic* approaches and in particular the Lattice Boltzmann Methods (LBMs) are very popular examples [8,9]. The LBMs are essentially based on the single-relaxation-time collision model originally proposed by Bhatnagar, Gross, and Krook (BGK) in order to simplify the Boltzmann equation. Further modifications to deal with the various phenomena occurring in the fuel cell components under investigation (e.g. reactive flows, current transport and electrochemistry) will also be required. The advantage of LBMs as numerical tools is that they are very efficient for investigating transport phenomena in highly complex geometries such as porous media. Even though traditional computational fluid dynamics (CFD) solvers could be used to describe transport in porous media as is done in the 3D *macroscopic* models mentioned above, LB methods do not require pressure-velocity decoupling or the resolution of a large system of algebraic equations [10]. They solve a simplified Boltzmann equation for an ensemble-averaged distribution of moving, interacting particles on a discrete lattice. The macroscopic quantities that describe the fluid flow can be calculated as integrals of this distribution. Since the motion of particles is limited to fixed paths connecting lattice nodes, the resolution process needs only information about the nearest neighbouring nodes. In this way, fluid flow through complex geometries can be analysed by means of this *mesoscopic* approach.
During the last years, a numerical code based on the Lattice Boltzmann Method has been developed from scratch for describing the fluid flow of gasses in porous media [11-13]. The original code has been modified in order to include multi-component mixtures by means of an explicit discrete version of the kinetic model due to Hamel [12]. This activity is part of the ongoing effort of the proponent group to modify the Lattice Boltzmann models in order to include the phenomena involved into the fuel cells [14-16]. The proponent group shares this goal and actively collaborates with the Center for Energy Systems Research at Virginia Tech (VA, U.S.A.). In particular the parallel version of the code is under development in order to use the System X facility, which is the new cluster computing facility at Virginia Tech and it is one of the biggest super-computers in the world.

Research program objectives (intermediate and final) and expected results

The objectives for the proposed project are the following.

1) To develop 3D *mesoscopic* models based on Lattice Boltzmann Method in order to charge transport and electrochemistry in the solid oxide fuel cell components.
2) To improve the numerical algorithm and the parallel features of the existing numerical code in order to better benefit from the cluster computing facilities.
3) To tie these 3D *mesoscopic* models into the 3D *macroscopic* models which the group has already developed for the heat, mass, and charge transport as well as electrochemistry of solid oxide fuel cells.
4) Connect a number of *mesoscopic* kinetic and structural parameters to such *macroscopic* parameters as porosity, tortuosity, diffusivity, Darcy's constant for advective flow, electrical conductivity, thermal conductivity, cinematic viscosity, etc. with the purpose of being able to better predict these essential macroscopic parameters. Currently, these parameters are partially based on experiment or are used as fudge factors to make the overall model fit experimental data.

5) To predict how the structures of electrodes and electrolyte layers can be synthesized and designed in order to improve their performance.
6) To investigate whether or not *mesoscopic* models can be developed which are able to predict how the performance electrode/electrolyte layers may degrade in time.
7) To validate the developed models where appropriate with experimental data published in the literature as well as generated in-house. The last option is due to the fact that the proponent group is involved in the design of an experimental test facility with a solid oxide fuel cell.

The expected results for the proposed project are the following.

1) To develop a reliable 3D *mesoscopic* code based on the Lattice Boltzmann Method which can properly take advantage of the parallel cluster computing.
2) To proof that the *mesoscopic* models can be suitably applied in the analysis of the fundamental phenomena involved into the solid oxide fuel cell components.

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