“Could it be that some place out there in the computational universe, we might find our physical universe?”
- Stephen Wolfram

A chapterwise summary of the major results and the models that have been formulated, implemented and the validation method is provided below:

- In chapter 2, the cascade continuum micromechanics model has been proposed to estimate the effective elastic properties of porous materials. The model predictions coincide with existing homogenization schemes depending on the level of recursion. At the self-similar limit, the model predicts a threshold value for the porosity as 0.5 beyond which the material loses its load carrying capacity typical for porous materials characterized by sintered granular particles. The model is explicit and allows for an easy computational implementation. The model predictions have been validated with experimental data for a wide range of materials ranging from foam, biomaterials, cementitious materials and ceramics.

- In chapter 3, the cascade continuum micromechanics model is applied for the case of molecular diffusion in a fully saturated disordered porous material. At the self-similar limit, in contrast to the elastic case, for the diffusion problem, the model predicts a threshold value of 0.333. Two sub models depending on the interaction characteristics have been formulated. Model predictions have been validated with experimental data. A generalized cascade continuum micromechanics model is also formulated that provides insight into a pore-volume distribution that is intrinsic in the cascade process. For completeness, the range of applicability of the existing classical homogenization schemes are also discussed.

- In chapter 4, the influence of an anisotropic and isotropic distribution of microcracks on the overall effective diffusivity is estimated using the cascade micromechanics model. To validate the model predictions, a high-resolution pixel finite element method is used to simulate
the effective diffusivity for a wide range of crack densities. The model predicts universal behavior for the effective diffusivity independent of the size distribution of the microcracks for the case of disordered microcrack distribution. An anomalous result has been observed when comparing the effective diffusivity of an anisotropic and an isotropic microcracked material for a particular range of microcrack densities where an anisotropic distribution of microcracks parallel to the direction of molecular flux is smaller than that of the isotropic case.

- In chapter 5, a novel lattice based micromechanics model have been formulated and validated against a computational pore/microcrack network model. Lattice micromechanical formulations of selected classical schemes have also been derived. The co-ordinations number and lattice type influences the threshold microcrack probability below which the material is effectively impermeable.

- In chapter 6, the influence of a porous region surrounding a microcrack on the fluid flow characteristics in the microcrack is investigated using analytical and an extended Lattice Boltzmann method. The investigation shows that the ratio of the length scales of the microcrack and the pore must be taken into account when neglecting explicitly the influence of the porous region on the fluid flow properties in microcrack.

- In chapter 7, the effective permeability of a microcracked solid is evaluated within a continuum framework where the cracks are allowed to overlap. The critical microcrack densities are estimated. Using image analysis, the structure of the microcrack network is studied.

**Outlook**

The effective elastic properties can be used to derive the effective poroelastic coefficients within the framework of linear poroelasticity using appropriate localization tensors. Evidently, these poroelastic coefficients are also characterized by a threshold porosity beyond which for e.g. the Biot coefficient $b = 1$, where the pore pressure is completely transferred to the REV stress in confined conditions. With respect to the effective diffusivity, the influence of the pore-size must be explicitly taken into account for pore-sizes close to the dimensions of the diffusing molecule. While the microcrack geometries have been assumed to be elliptic cylindrical, a 3D extension of the pixel finite element method to a voxel finite element method should allow to also validate the micromechanical model predictions with computational simulations for penny shaped microcracks.

Fig. 8.1 shows the first results of a 3D extension of the network model introduced in chapter 5 coupled to image analysis (convolution) based percolation algorithm presented in chapter 7 that is able to simulate the experimentally observed hysteresis effect in the saturation-capillary pressure curves in imbibition and drainage for a given pore-size distribution and the effective relative permeability. Evidently, the only additional assumption in this analysis is the YOUNG-LAPLACE condition $p_c \propto \frac{1}{d}$. Furthermore, as we have seen that the percolation threshold can be associated with geometrical phase transition in chapter 5, any state of a material characterized by a physical
Figure 8.1: A connectivity based approach to model the (saturation-capillary pressure) $S - P_c$ characteristics of a porous material. Top: Drainage of a fully saturated porous material (blue: fluid, Red: gas). Bottom left: The pore size distribution and right: the predicted saturation - capillary pressure curves for fluid imbibition and drainage showing hysteresis phenomena that shows a naturally spatial diffuse transition zone between two homogeneous material states should exhibit fractality. To investigate this hypothesis, the computational microcrack network model introduced in 5 can be coupled to a crack growth rule that converts a crack with a smaller width to one with a larger width when the pressure in the crack exceeds a particular critical pressure. The strength of the material can be assumed to be drawn from an extreme value distribution. First results of the simulation (see Fig.8.2) as expected shows the development of a transition zone of high disorder with fractal structures between two homogeneous regions that is formed between that of the smaller cracks and that of the larger cracks. An important consequence of this observation is in geothermal energy extraction where a highly complex crack network would actually enhance the energy production.
Figure 8.2: Isolines of the fluid velocity for zero pressure on the left boundary and increasing pressures on the right boundary. Observed is the emergence of a complex flux isoline that forms a diffuse transition zone between the two homogeneous networks of different crack widths. Top and bottom surfaces are impermeable.