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<td>Azita Ahmadi</td>
<td>Krishna M. Pillai</td>
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<td>In vitro cartilage culture: coupled flow, transport and reaction in fibrous media</td>
<td>Flow modelling/transport in random, woven or stitched fibre mats used as reinforcement in the manufacture of polymer composites</td>
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<td>12:40-16:30</td>
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<td>Workshop outing: Visit to the Open Air Museum, Arnhem</td>
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<td>Paper pulp dewatering</td>
<td>Streamline methods for computing transport in fractured media</td>
<td>Influence of connected structures for two-phase flow and transport processes in heterogeneous porous</td>
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<td>18:00-19:00</td>
<td>Dinner</td>
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<td>19:00-20:30</td>
<td>Hassanizadeh, Bottero, Joekar-Niasar, Niessner, Berentsen</td>
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<td>Multiphase flow processes including interfaces; experiments and modelling</td>
<td>Flow in fractures coupled with deformation effects: application to sealing problems</td>
<td>Fluid flow in absorbing porous media media</td>
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<td>20:30-21:30</td>
<td>Insa Neuweiler</td>
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Workshop Program

Monday 12/11

From Bubbles to Fractures: Ultrasonics & Fluid Flow
Laura Pyrak-Nolte
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The physical properties of a material are strongly influenced by the presence of pores and pore structures. Pore structures can range from disconnected isolated holes to quasi-two-dimensional structures such as a fracture to three-dimensional pore/fracture networks. The probability and spatial distributions of pores affect both fluid flow as well as the mechanical properties of medium, i.e. affects the ability to ultrasonically delineate and characterize porous media. From our studies on food, rock and micro-fluidic systems, ultrasonic characterization of porous media requires an understanding of the relationships among physical processes that occur on multiple length and time scales. Pore structures have geometric length scales that can be altered over time through such physical processes as stress, fluid transport, geochemical interactions, etc. In addition, the effect of the measurement scale must also be considered. This paper examines the effect of the geometric length scales and the alteration of these length scales on the interpretation of physical properties from ultrasonic measurements.

Flow and transport in porous media: modelling and simulation- Water management in polymer electrolyte membranes fuel cells
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The development of alternative power sources/supplies is an important task nowadays. Polymer electrolyte membrane (PEM) fuel-cells currently are intensively investigated and improved for applications. This requires a profound understanding of the physical and electrochemical processes occurring in fuel cells. It has been found that the kinetics of the oxygen reduction at the cathode is a limiting factor for the performance of fuel-cells. The transport of oxygen to the cathode through its porous diffusion layer takes place in a predominantly diffusive manner. The generation of liquid water at the cathode-site limits this oxygen transport to the reaction layer. A crucial issue here is the wettability of the porous media. The material might consist, for example, of a carbon fibre structure hydrophobized with Teflon. Hydrophobic properties enhance the removal of the generated liquid water. However, it has been observed that, under operating conditions, at least parts of the diffusion layer become hydrophilic and retain liquid water in high residual saturations. Thus, an efficient water management in the cathode diffusion layer is necessary to improve the performance of the fuel-cell.
Multiphase multicomponent models originally developed at our working group for the simulation of non-isothermal multiphase processes in the subsurface are applied for modelling the diffusion layer of PEM fuel-cells. However, this is in an early stage. So far we have simulated processes occurring in the diffusive layer. Further research is necessary e.g. to understand the complex wettability behaviour.

The aim of this presentation is to discuss the physical and numerical model concept, the assumptions that are necessary and with numerical results the possibilities and restrictions.

**Numerical simulation of the dynamics of molten carbonate fuel cells**

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Molten carbonate fuel cells (MCFC) are especially well suited for stationary power plants and will be soon competitive compared with traditional power plants. The dynamical behaviour of the state variables of an averaged MCFC in the stack of MCFCs in stationary power plant can be modelled mathematically by a hierarchy of systems of partial differential algebraic equations in 1D or 2D. Integral terms appear and the nonlinear boundary conditions are given partly by a differential algebraic equation system. These equations are based on physical and chemical laws and describe the gas flow in the anode and cathode gas channels, the gas temperatures, the temperature of the (lumped) solid, and the molar fractions and partial pressures of the important gas substances in the gas channels and the pores. In contrast to other empirical models in the literature, the used models are based on physical and chemical laws and moreover a validated equation set is available for the MCFC stationary power plant of the Hot Module operated at the Magdeburg university hospital and produced by CFC Solution GmbH Munich-Ottobrunn.

In order to control the power plant in a save way the avoidance of material stress through high temperature gradients is essential to enlarge service life of the very expensive power plant. On the other hand a fast reaction of the power plant on common load changes is desirable. This formulates an optimal control problem subject to a partial differential equation system. This kind of problems is currently within the focus of mathematical research especially in Austria and Germany. We will conclude with numerical simulation results and optimal control results.

**Tuesday 13/11**

**Overview of Single and Multiphase Flows through Industrial and Geological Porous Media**

Goodarz Ahmadi  
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ahmadi@clarkson.edu
An overview of single and multiphase flows in industrial and natural porous media is presented. Particular attention is given to hot-gas filtration, catalytic converter, and flow cell and rock fractures for application to geological sequestration of carbon dioxide. Natural gas production form geological hydrate reservoir is also discussed. A computational model for analyzing the gas flow through porous filter is described and sample computational results for performance of filter vessel are presented. Experimental and computational modeling methods for studying multiphase flows in porous and fractured media are also discussed. The experimental setup of a laboratory-scale flow cell was described in details. It was shown that the gas-liquid flows generate fractal interfaces and the viscous and capillary fingering phenomena are discussed. Experimental data concerning the displacement of two immiscible fluids in the lattice-like flow cell are presented. The flow pattern and the residual saturation of the displaced fluid during the displacement are discussed. Numerical simulation results of the experimental flow in the cell are also presented.

Numerical simulation results for single and multiphase flows through rock fractures are also presented. Fracture geometry studied was obtained from a series of CT scan of an actual rock fracture. Computational results showed that the major losses occur in the regions with smallest apertures. An empirical expression for the fracture friction factor was also described. Applications to CO2 sequestration in underground brine fields and depleted oil reservoir stimulation are discussed. Sample results concerning natural gas production from hydrate reservoir are also presented.

**Paper pulp dewatering**

Stefan Rief

We are concerned with modelling and simulation of the pressing section of a paper machine. We state a two-dimensional model of a press nip which takes into account elasticity and flow phenomena. Nonlinear filtration laws are incorporated into the flow model. We present a numerical solution algorithm and numerically investigate the model with special focus on inertia effects.

**Flow in fractures coupled with deformation effects: application to sealing problems**

Didier Lasseux

TREFLE - Site de l’ENSA

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In many industrial applications, efficient seal between tight parts is a key issue. Whenever severe thermodynamic conditions are involved, the use of a rubber sealant is impossible and seal is performed by direct metal/metal contact between machined surfaces. The presentation will be focused on this last configuration. The objective is to contribute to the understanding of the coupled mechanisms under concern in leakage in order to first predict seal efficiency and further improve it with better surface design. This task is a very complicated one due to the fact that many parameters are involved like material of each surface, topology at different scales of observation resulting from machining processes, distribution and level of applied tightening, nature and thermodynamic state of fluids to be sealed, etc. Difficulty also arises while deriving adequate models to predict deformation (elastic and/or plastic) and flow. Validation of these models is another challenge if one is willing to obtain accurate and reliable experimental data of leak rate measurements under quasi-real but well controlled conditions.
In this presentation, an overview of many different aspects of the problem will be addressed. An experimental work will be presented in which careful liquid leak rate measurements were performed. Experimental results obtained under many different configurations involving various surface topologies, contact pressures and fluid pressures (pressure driven and diffusive conditions) will be discussed. Derivation of physical models will be also presented with an accent on flow models at the micro and macro scales, both in the viscous and diffusive regimes. Their numerical resolution will be illustrated over simple cases. Direct comparisons of predicted leak rates with experimental data will be discussed using direct surface topology measurements and surface generators. The impact of surface texture, topology description as well as scales of surface defaults will be illustrated.

**Influence of connected structures for two-phase flow and transport processes in heterogeneous porous media**

**Insa Neuweiler**  
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When modelling flow and transport in heterogeneous porous media, the heterogeneous structure of the medium is usually not known in detail. Therefore, upscaled models are often used to predict spatially averaged variables.

The upscaled models as well as their parameters depend on the structure of the porous medium. As the structure is not known in detail, it is important to use a good simplified characterization of the heterogeneous parameter fields, which takes its relevant features into account. Usually, second order stochastic properties of a parameter field, such as mean and covariance are used to quantify heterogeneity. Connected structures of the field are usually not considered. However, these structures have an important influence on flow and transport, in particular when two-phase flow processes are considered. They are crucial, for example, for the quantification of macroscopic trapping effects and for the applicability of local equilibrium conditions.

The influence of connected structures on trapping effects and equilibrium assumptions, as well as on model parameters will be discussed. For this purpose, upscaled models are derived using homogenization theory. It will also be discussed, how connected structures may be quantified and how such quantifications can be included into models.

**Wednesday 14/11**

**In vitro cartilage culture: coupled flow, transport and reaction in fibrous media**  
**Azita Ahmadi, Didier Lasseux and Samuel Letellier**  
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Flow and transport in fibrous media are encountered in a wide variety of domains ranging from biotechnology to filtration in chemical engineering. The context of this work is the in vitro cartilage cell culture on a fibrous biodegradable polymer scaffold placed in a bioreactor. A seeding process using a liquid containing cells (chondrocytes) initiates the culture and an imposed continuous flow
through the scaffold allows both the transport of nutrients necessary for cell-growth and of metabolic waste products. This work will attempt to contribute to the study of the hydrodynamics and transport through the fibrous scaffold at different stages of growth, both having a key role in the process of cell growth and on the final quality of the cultured cartilage.

The hydrodynamics in the scaffold and in particular the relationship between macroscopic experimentally accessible properties such as the permeability and the porosity have first been studied. For this purpose, the formalism of volume averaging is employed and the associated closure problem is solved numerically with an artificial compressibility algorithm on the basis of a finite volume scheme on a Marker and Cell type of grid. Fibrous media with different microscopic structures are studied.

Through a theoretical study, assuming local mass equilibrium, a macroscopic one-equation model describing the reactive transport (advection/diffusion/reaction) of the two species in a three-phase system composed of the cell-phase, a fluid phase and a solid phase is proposed. The volume averaging method is used to develop macroscopic transport equations and associated closure problems. Resolution of the latter over a unit cell representative of a pseudo-periodic medium allows the determination of effective macroscopic properties without any adjustable parameters. The dimensionless form of the closure problems involving advective, diffusive and reactive terms are numerically solved for any 3D geometrical configuration using a finite volume formulation using appropriate schemes. The velocity field input to the model is obtained by the resolution of the Navier-Stokes problem using a modified QUICK scheme and an Artificial Compressibility algorithm.

The numerical tool is then validated by comparing its results to those presented in the literature for 2-D unit cells and under-classes of our model (namely, diffusion, diffusion/reaction and diffusion/advection problems). The complete problem involving convection, diffusion and reaction in the three phase system is then studied for different parameters. More precisely, the influence of a cell Peclet number and the solid and cell volume fractions on the dispersion tensor has been studied.

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**Fluid Flow in Absorbing Porous Media**

**Mattias Schmidt**  
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*D-65824 Schwalbach am Taunus, Germany*  
*schmidt.mt@pg.com*

Understanding and optimizing fluid flow in absorbing porous media is critical for developing superior consumer hygiene products such as paper towels, wipes, feminine pads and baby diapers. This talk will provide an introduction into fluid flow in hygiene consumer products with the focus on baby diapers including experimental as well as theoretical aspects. Unlike in geosciences where the pore structure is typically relatively stable during fluid flow, the materials used for consumer products are soft and can deform due to wet collapse or external conditions; and adjacent materials have a large contrast of key parameters. In addition, swelling of materials such as super-absorbers leads to dimensional changes of the pore structure during the fluid transport. The talk will share advances in measuring and simulating fluid flow and outline key challenges that have not been resolved until now.

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**Thursday 15/11**
Overview of Flow through Textile and Fabrics
Goodarz Ahmadi\textsuperscript{1} and Hooman V. Tafreshi\textsuperscript{2}
\textsuperscript{1} Department of Mechanical and Aeronautical Engineering
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An overview of single and multiphase flows through woven and nonwoven fibrous materials is presented. A computational model for analyzing fluid flow through such media is described and sample computational results are presented. It is shown that by generating virtual geometries that resemble the microstructure of a fibrous material one can study the fluid and particle transport through such porous media and compute their permeability and particle capture efficiency. As an example, the modeling strategy developed for evaluating the pressure drop and nano-particle collection efficiency of light-weight nonwoven air filter medium is described in details. Comparison of the results of the micro-scale modeling with the existing analytical models as well as the experimental data in the literature is also presented. Earlier studies on modeling permeability of multi- and mono-filament woven fabrics are also reviewed.

Particular attention is given to application of the computational modelling approach to development of protective clothing for different applications. Motion of a drop through a fabric due to a wettability gradient is described. The wettability gradient is typically introduced by varying the contact angle along the staggered fibers of a fabric. The computational model for solving unsteady gas-liquid laminar flow a fixed Eulerian unstructured grid is described. The Volume of Fluid Model (VOF) is used to account for tracking the gas-liquid interface. The motion of a water drop with a given initial velocity through the fabric is studied. Several sample computer simulations results under different conditions for different fiber concentrations, contact angle distribution, and drop initial velocity are presented. In order to verify the accuracy of the computational model, the motion of a drop on a surface due to a wettability gradient is simulated as a benchmark and compared with experimental data.

Streamline methods for computing transport in fractured media
H. Haegland, H.Dahle\textsuperscript{*}, G.T. Eigestad, R. Helmig
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Dept. of Math, University of Bergen, Norway
helge.dahle@math.uib.no

The physical and numerical description of fractured systems remain one of the great challenges in porous media modelling. This is due to the great importance of understanding such systems in many practical applications: Fractures and faults may often control the displacement processes in petroleum reservoirs; they may form conduits of leakage which are important to understand in the context of waste disposal problems or for transport of contaminants; They are important for the recovery of geothermal heat, and so on.

Accurate statistical characterisation of fractured systems e.g. by inverse modelling, is needed to understand their flow and transport
properties. However, this type of modelling is hampered by the lack of efficiency of conventional numerical simulation techniques. An alternative to conventional finite difference techniques are sequential streamline based methods which have proved to be efficient in modelling advection dominated flow and transport.

In this presentation we will consider streamline methods for computing transport times for tracer flow. Although streamline methods typically apply to simplified physics, they usually provide extremely fast alternatives to conventional simulation techniques. This allows for simulations of multiple realisations on highly resolved grids. For example, they may be used to compute transport times of passive tracers, which are important because transport times reveal important information about fracture density and distribution.

Streamline methods are typically part of a sequential formulation of flow and transport equations. The flow or pressure equations form an elliptic operator, and require other types of solution and discretisation techniques.

In this presentation we will consider box-methods which are finite-element type schemes and MPFA-methods which are finite volume/difference type methods. Both types of methodologies are specially designed to handle irregular grids and heterogeneous permeability fields with strong anisotropy. The following issues will be of particular interest in this presentation:

* Streamline tracing on irregular grids;
* Streamline tracing through fractures;
* Modelling of fractures as N- or (N-1)-dimensional objects in N-dimensional space (N=2,3), or by double continuum approach;
* Discretisation schemes for the pressure equation;

**Friday 16/11**

**Geological Storage as a Carbon Mitigation Option**

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The most promising approach to solve the carbon problem involves widespread implementation of zero-emission power plants. These are likely to be fossil fuel-based plants with carbon capture and storage (CCS) technology. Low-emission electricity has the secondary advantage of allowing for electrification of the transportation sector, and as such can lead to very large reductions in CO2 emissions if implemented at the global scale. While a variety of storage options are being studied, geological storage appears to be most viable. Injection of captured CO2 into deep geological formations leads to a fairly complex flow system involving multiple fluid phases, a range of potential geochemical reactions, and mass transfer across phase interfaces. General models of this system are computationally demanding, with the problem made more difficult by the large range of spatial scales involved, and the importance of local features for both fluid flow and geochemical reactions. An especially important local feature involves leakage pathways, with
one example being abandoned wells associated with the century-long legacy of oil and gas exploration and production. Such pathways also have large uncertainties associated with their properties. Therefore, inclusion of leakage in the storage analysis requires resolution of multiple scales, and incorporation of large uncertainties. Taken together, these render standard numerical simulators ineffective due to their excessive computational demands. A series of simplifications to the governing equations can reduce computational demands, and ultimately render the system solvable by analytical or semi-analytical methods. These solutions, while restrictive in their assumptions, allow for large-scale analysis of leakage in a probabilistic framework. An example from Alberta, Canada will be used to demonstrate the utility of these solutions.