Tagungsbericht 9/1996

Porous Media

25.02.-2.03.1996

The meeting was organized by *Jim Douglas* (West Lafayette), *Ulrich Hornung* (Neubiberg) and *Peter Knabner* (Erlangen). Each presentation was 35 minutes long followed by 10 minutes for questions and discussion. The meeting was very much of workshop character.
The topics discussed during the meeting were:

- **Modeling** M. Celia has presented a pore-scale model for two-phase flow in porous media. M. F. Wheeler and R. Ewing gave their talks about simulating multiphase flow and transport. F. Keil's talk was about modeling of diffusion and reaction with general kinetics in three-dimensional random networks. A multicomponent model of reactive transport in heterogeneous porous media was presented by R. Liedl (mathematical aspects) and G. Teutsch (basic concepts and parametrization). M. Murad spoke about multiscale flow and deformation in hydrophilic swelling porous media. A microstructure model for microbial growth in aggregated soils was presented by E. Priesack. The talk of M. Quintard was concerned with the process of dissolution of hydrocarbon phases trapped in aquifers (NAPL). A. Schuppert has presented models for elasticity and creeps in highly anisotropic media with defects.

- **Homogenization** A. Bourgeat has presented a justification of the double porosity model for two-phase flow using periodic modulation. H. I. Ene gave a proof for convergence of the homogenization process which in the case of heat conduction leads to a two-temperature model. W. Jäger established the effective equations for flow through a filter. A. Mikelić has studied a problem with inertial effects for a stationary viscous incompressible flow in a porous medium; he has proved well-posedness of the homogenized problem and convergence of the homogenization process. B. Vernescu has presented elektrokinetic phenomena in modeling of clays.

- **Numerics** T. Arbogast presented mixed finite element methods for approximating elliptic equations posed in multi-block domains. C. Dawson studied the large time behavior of the solution to a transport model using asymptotic balancing and numerical simulation. P. Frolkovič proposed a new formulation of consistent velocity approximation for density driven flows. A framework for the numerical solution of nonlinear parabolic equations was discussed by J. Fuhrmann. J. Jaffré presented a method of generalized cell-centered finite volumes for two-phase flow in a heterogeneous porous medium. H. Molenaar spoke about multigrid and second-order upwind schemes for multiphase flow. A comparison between standard and mixed finite elements and applications in hydrology are discussed by M. Slodička. G. Wittum spoke about multigrid methods for porous media.

- **Inverse problems** A general method for solving a class of inverse problems in which the unknown ingredients to be identified are functions of the state variable only and do not depend explicitly on position or on time was presented by P. DuChateau. B. Igler studied identification of nonlinear isotherms in reactive flow through porous media. Identification of eletromagnetic parameters for media with microstructure was presented by J. Gottlieb.

- **Stochastics** J. H. Cushman has studied convection and diffusion in random media and derived nonlocal equations for the effective behavior of concentrations. G. Dagan showed the significance of heterogeneity of evolving scales to transport in porous formations. J. Glimm has investigated anomalous diffusion in media with infinite correlation lengths. A new method for generating random velocity fields in 3D was presented by Y. Rubin. T. Russel has developed a practical tool for generating upscaled dispersivity coefficients in simulations of passive solute transport in heterogeneous media.

The subjects discussed covered a large variety of aspects from the mathematical theory of flow and transport thorugh porous media.

VORTRAGSAUSZÜGE

Todd **Arbogast**, L.C. Cowsar, M.F. Wheeler, I. Yotov:

Mixed Finite Element Methods on Multi-block Domains

We present 3 numerical schemes for approximating elliptic equations posed in multi-block domains. These are domains divided into nonoverlapping sub-domains or blocks. A discretization grid is defined on each block, but these grids may not match across the subdomain interfaces. We use a mixed finite element method in each block combined with conditions on the block interfaces to control the pressure and flux discrepencies. Each of our schemes conserves mass element-by-element; in fact, across all element faces except those on the block interfaces. The first scheme approximates the interface pressure in a "mortar" finite element space defined on the block interfaces. A symmetric, positive definite, bilinear interface can be defined. It can be used to control discretization errors on the interface. The scheme therefore converges optimally; moreover, computational results show that superconvergence is achieved at the nodal points. The second scheme is similar, but it approximates the flux in a mortar space rather than the pressure. The third scheme uses no mortar space. It is based on matching Robin boundary conditions on the interface. A priori estimates show that the pressure and the flux discrepencies are controlled directly. Therefore, the scheme converges optimally, as well.

Alain **Bourgeat**:

Convergence of the Homogenization Process for Establishing the Double Porosity Model for Immiscible Two-Phase Flow

We justify rigorously by periodic homogenization the double porosity model for immiscible incompressible two-phase flow. The scaling is such that, in the final homogenized equations, the less permeable part of the matrix contributes as a nonlinear memory term. We prove the convergence of the total velocity and of the "reduced" pressure by means of two-scale convergence. But to get the homogenized equation, due to a degenerated nonlinear term, we have to use the periodic modulation tool.

Michael A. **Celia**:

Pore-Scale Models for Two-Phase Flow in Porous Media

Pore-scale models may be used to simulate capillary-dominated displacement in porous media, based on a description of the pore space as an interconnected lattice of pore bodies and pore throats. Through use of these computational models, continuum-scale constitutive relationships may be derived, including the traditional Pc - S and Kr - S relations as well as relationships between dispersivity and saturation and between mass-transfer coefficient and saturation. In addition, these models may be used to predict interfacial areas between phases. Such predictions may then be used to test recent theoretical developments that relate interfacial areas to capillary pressure and saturation. This talk shows the relationships between Pc, S, and interfacial areas, and illustrates how sphere-pack models may be used to calculate required pore-size distributions for the pore-scale network models.

John H. **Cushman**, Fei-Wen Deng, and Bill X. Hu:

Nonlocal Theories of Reactive Chemical Transport in Porous Media

A shift in paradigm is required to adequately simulate transport under uncertainty within an Eulerian framework. The new paradigm, which is discussed in detail, requires Eulerian constitutive theories for mean concentration be nonlocal. Various first and second order nonlocal models are developed for reactive transport under nonequilibrium linear adsorption with random or deterministic forward and backward rate constants. If the rate constants are deterministic and if local dispersion is neglected in the Eulerian framework, then the nonlocal Eulerian models exactly reproduce the expected moments derived via Lagrangian theory. However if local dispersion is included in the Eulerian model substantial disagreement exists between the Eulerian and Lagrangian moments. Under appropriate limiting conditions the nonlocal models reproduce results of Naff, Gelhar, Neuman, and Dagan and Cvetkovic.

Gedeon **Dagan**:

The Significance of Heterogeneity of Evolving Scales to Transport in Porous Formations

Flow takes place in a heterogeneous formation of spatially variable conductivity, which is modeled as a stationary space random function. To model the variability at the regional scale, the formation is viewed as one of a two-dimensional, horizontal structure. A constant head gradient is applied on the formation boundary such that the flow is uniform in the mean. A plume of inert solute is injected at $t = 0$ in a volume V_0. Under ergodic conditions the plume centroid moves with the constant, mean flow velocity U, and a longitudinal macrodispersion coefficient d_L may be defined as half of the time rate of change of the plume second spatial moment with respect to the centroid. For a log-conductivity covariance C_Y of finite integral scale I, at first order in the variance σ_Y^2 and for a travel distance $L = Ut \gg I, d_L \to \sigma_Y^2 UI$ and transport is coined as Fickian. Ergodicity of the moments is ensured if $l \gg I$, where l is the initial plume scale. Some field observations have suggested that heterogeneity may be of evolving scales and the macrodispersion coefficient may grow with L without reaching a constant limit (anomalous diffusion). To model such a behavior, previous studies have assumed that C_Y is stationary but of unbounded integral scale with $C_Y \sim ar^\beta(-1 < \beta < 0)$ for large lag r. Under ergodic conditions, it was found that asymptotically $d_L \sim aUL^{1+\beta}$, i.e., non-Fickian behavior and anomalous dispersion. The present study claims that an ergodic behavior is not possible for a given finite plume of initial size l, since the basic requirement that $l \gg I$ cannot be satisfied for C_Y of unbounded scale. For instance, the centroid does not move any more with U but is random, owing to the large-scale heterogeneity. In such a situation the actual effective dispersion coefficient D_L is defined as half the rate of change of the mean second spatial moment with respect to the plume centroid in each realization. This is the accessible entity in a given experiment. We show that in contrast with d_L, the behavior of D_L is controlled by l and it has the Fickian limit $D_L \sim aUl^{1+\beta}$. We also discuss the case in which Y is of stationary increments and is characterized by its variogram γ_Y. Then U and d_L can be defined only if γ_Y is truncated (equivalently, an "infrared cutof" is carried out in the spectrum of Y). However, for a bounded U it is shown that D_L depends only on γ_Y. Furthermore, for $\gamma_Y = ar^\beta, D_L \sim aUl^2L^{\beta-1}$; i.e., dispersion is Fickian for $0 < \beta < 1$, whereas for $1 < \beta < 2$, transport is non-Fickian. Since $\beta < 2, D_L$ cannot grow faster than $L = Ut$. This is in contrast with a recently proposed model (Neuman, 1990) in which the dispersion coefficient is independent of the plume size and it grows approximately like $L^{1.5}$.

Clint **Dawson**:

Asymptotic Profiles in Contaminant Transport

The large time behavior of the solution to a transport model

$$(\theta c + \rho s)_t + \nabla \cdot (qc - D\nabla c) = g(c, s)$$

$$s_t = Kc^p, p > 0$$

is studied using asymptotic balancing and numerical simulation. The numerical scheme is based on a higher-order Godunov method for advection combined with a mixed finite element method for diffusion. The numerical solutions for large time are compared to the limiting profiles derived by asymptotic balancing for several choices of p and $g(c, s) = -K(\lambda_1\theta c + \lambda_2 \rho s), \lambda_1, \lambda_2 \geq 0$, in one and two space dimensions. On all cases, the numerical solution compares well with the predicted asymptotic limit.

Paul **DuChateau** :

A Uniform Method for a Class of Structural Identification Problems

A general method is presented for solving a class of inverse problems in which the unknown ingredients to be identified are functions of the state variable only and do not depend explicitly on position or on time.

The method is based on integral identities that relate changes in the unknown ingredients and the corresponding changes in the measured outputs from which the ingredients are to be identified. The method is illustrated using the following examples:

- simultaneous identification of the hydraulic properties of a porous medium,
- identification of an unknown source term in a heat equation,
- identification of an unknown diffusivity in a non-linear diffusion equation.

Using the method it is possible to answer such questions as (a) in what sense can the output measurements distinguish between unknown ingredients (b) if the inverse problem is reformulated as an output least square problem, does the solution to the OLS problem necessarily solve the inverse problem (c) how is existence to be interpreted (d) what is the best way to design the identification experiment?

Horia I. **Ene**:

On Heat Transport in Porous Media

Using the homogenization method it is possible to obtain different models for heat transport at the macroscale. Following the order of magnitude of the interfacial thermal resistance, one can obtain a model with one-temperature equation or with two-temperature equations. The proof of the homogenization process which leads to a two-temperature equations is made in the case of the heat conduction.

Richard **Ewing** :

Simulation of Multiphase Flow and Transport

The ability to numerically simulate both single- and multiphase flow of fluids in porous media is extremely important in deve'oping an understanding of the complex phenomena governing the flow. The flow is complicated by the presence of heterogeneities in the reservoir at many length scales and by phenomena such as diffusion, dispersion, and viscous fingering. We first discuss the modeling process on both the microscopic and macroscopic scales, including issues of scale-up. The processes are modeled by terms in coupled nonlinear time-dependent partial differential equations, which form the basis of the simulator. The simulator must be able to model both single- and multiphase flow regimes and the transition betwen the two. The need for modeling a dispersive/diffusive process for multiphase flows that incorporates effects of heterogeneities will be discussed. Several models for multiphase flow will be developed and contrasted. Three-dimensional field simulations of multiphase processes will be presented together with a discussion of directions for future work.

Peter **Frolkovič**:

Consistent Velocity Approximation for Density Driven Flows

Artificial velocities can appear in the numerical simulation of density driven flow problems due to the variable density if a standard finite element or finite volume method is formally applied. To avoid this numerical artifact an algorithm was proposed by Voss & Sonza [1987]. It can be validated only by verifying hydrostatic conditions and only for linearly variable density. The new formulation of consistent velocity approximation is proposed that is validated for general conditions with nonlinear density for an arbitrary reference element of finite element or finite volume method.

Jürgen **Fuhrmann**:

A Framework for the Solution of Nonlinear Parabolic Equations

A framework for the numerical solution of nonlinear parabolic equations, e.g. the porous media equation, Richards' equation or the equation describing the movement of a viscous compressible fluid in a porous medium, is discussed. The solution scheme is based on an implicit time discretization combined with finite volume method for space discretization and an affine invariant Newton's method to solve the time step problems.

For the solution of the linear problems, iterative methods are used. The usage of algebraic multilevel preconditioners on structured and unstructured meshes is possible.

James **Glimm**:

Heterogeneities at the Pore and Field Scale

In this talk, we consider three separate topics, each related to heterogeneities: (1) statistics of pore geometry, (2) residual saturations for the problem of resin-phase filling in the manufacture of fiber reinforced plaster resin composite materials, land (3) hyperbolic vs. parabolic renormalization for the scale up of flow in heterogeneous porous media.

For pore scale statistics, we report on work of Lindquist and Venkatarangen. Data come from BNL light source, giving μm level resolution of the rock geometry pore space. Two sandstone samples and a glass bead sample were analyzed. Distribution of grain and pore-throat diameters were analyzed. The latter was observed to be exponential for the rock samples. The distribution by volume of the disconnected components of the pore space was also analyzed.

For the manufacture of composite materials, the residual air saturation (voids) is an important consideration. Our main conclusion is that residual saturation is governed by compression of pore scale microvoids. Thus the pressure ration P_{loc}/P_{init} is the key variable to control residual saturation. Here P_{loc} is the local pressure and P_{init} is the pressure at the filling front at the time and space point of the void formation.

For the upscale problem, we consider two phase immiscible displacements, with the Backley-Leverett equations. The permeability in Darcy's law is given by a lognormal random field. This problem is weakly nonlinear, and we find the degree of layering, or length range geostatistical correlation is the important factor governing the upscaling renormalization.

We consider fractal, or power law nonlocal correlations in the log permeability correlation. Cases which are regular at infinity lead to parabolic regularization (upscaling) of the flow, with an anomalous dispersion term in the upscaled equations. Cases with geostatistics singular at large distances give stronger layering and a different renormalization. Here upscaling occurs in the hyperbolic part of the flow equations.

Johannes **Gottlieb**, S.I. Kabanikhia, V.G. Romanov, S.I. Martakov, S. Schlaeger:

Identification of Eletromagnetic Parameters for Media with Microstructure

During the last time several methods of describing soil contamination from electomagnetic surface measurements are investigated.

In our paper we consider a corresponding inverse problem for the Maxwell-Hopkinson system. The latter arises from a homogenization approach to a periodic medium. We solve the inverse problem (existence and uniqueness) of ground penetrating radar for a layered medium in the case of Jonscher's dispersion model.

Finally, we discuss the numerical solution by nonlinear cg-methods and present a new method of automatic optimization of parallel programs.

Bodo **Igler**, Paul DuChateau, Peter Knabner:

Identification of Nonlinear Isotherms in Reactive Flow through Porous Media

Nonlinear isotherms are identified by soil column breakthrough experiments, which are modelled in one space dimension. The inflow concentration essentially influences the experimental design. The necessary overdetermination is given by outflow measurements.

Integral identities involving the solution of the adjoint problem are crucial in the analysis of the inverse problem. It can be shown that isotherms can be recovered uniquely (in an appropriate sense) by breakthrough measurements. The output least squares method is proven to solve the inverse problem.

The discrete output least squares method was implemented. The isotherms are parametrized as piecewise linear functions. A multigrid concept provides good start values. The gradient can be approximated at reasonable costs by solving the discrete adjoint problem. Promising identification results are obtained for realistic measurement errors.

Jérôme **Jaffré**:

Generalized Cell-Centered Finite Volumes for Two-Phase Flow in a Heterogeneous Porous Medium

This is a presentation of a numerical method which follows the finite volume methodology - approximation spaces are defined and equations are written cell per cell, interactions between cells are written out explicitly following the physics - while borrowing from mixed-hybrid finite elements the approximation spaces. The advantages of the method are shown for two-phase flow in a porous medium with several rock types.

W. **Jäger**, A. Mikelić:

Effective Equations for Flow through a Filter

Consider a pipe, separated by a porous filter into two parts. The pores of the filter are cylindrical channels distributed periodically with a period of order ε and connecting the two parts of the pipe. Assume inflow of a fluid on one end of the pipe and outflow on the other end, caused by a pressure difference. The flow is assumed to be incompressible and modelled by Navier-Stokes equation and no-slip boundary condition. The smallness of the scale ε guarantees the existence of smooth solutions.

The asymptotic behaviour for $\varepsilon \to 0$ of the flow is determined in the first order term. The expansion for the velocity starts with a term of order ε^2 which can be computed by solving Stokes systems with appropriate boundary conditions on both sides of the filter. The necessary estimates use constructions of appropriate boundary layers at the interfaces of the filter. The asymptotic analysis is similar to the approach used in a recent paper dealing with the transmission conditions on the interface between a free fluid and a flow through a porous medium.

F.J. **Keil**, C. Rieckmann:

Modeling of Diffusion and Reaction of General Kinetics in Three-Dimensional Random Networks

Three-dimensional random network models have advantages as follows: the connectivity is taken into account; any type of network, any pore size distribution, any type of pore shape (cylindrical, slit-like, etc.) can be used; and nonuniform distribution of reactants throughout the pore space can be investigated. Especially nonuniform distribution of reactants in pore space cannot be described by the continuum equation of diffusion and reaction. The same holds for phenomena close to the percolation threshold.

We have taken the dusty-gas model as a basis for the diffusion and reaction in a single pore. The pores were then assembled to a random three-dimensional network. At each node of the network the system of differential equations describing the diffusion/reaction processes were solved. At the outer surface of the network boundary conditions have to be fulfilled. The problem has been solved by a finite-difference method. Very large systems of equations are obtained. The computed values may be compared to experimental results.

Rudolf **Liedl**:

A Multicomponent Model of Reactive Transport in Heterogeneous Porous Media: Some Mathematical Aspects

This talk focuses on two mathematical aspects of a multicomponent model which is being developed in order to simulate reactive transport of solutes in heterogeneous aquifers.

First an analytical solution of modelling retarded intraparticle diffusion is presented which can be applied to heterogeneous aquifer material (different lithological components and grain sizes). Additionally, it is possible to consider non-stationary boundary conditions so that this solution can be directly coupled with numerical models for solute movement in columns or at field scale.

Second, it is shown how the 1D version of the multicomponent model could be used to simulate 3D transport. This may be achieved by employing the stochastic approach of Dagan/Cvetkovic which is based upon the Lagrangian representation of solute transport.

Andro **Mikelić**:

Inertial Effects for a Stationary Viscous Incompressible Flow in a Porous Medium

We consider the stationary viscous incompressible fluid flow through a rigid porous medium. If the geometric structure of the porous part is periodic with the period ε and if the Reynolds number and inverse of Froude's number are of order ε^{-1} then the formal asymptotic expansion established by E. Sanchez-Palencia and J.-L. Lions gives a homogenized problem called "Navier-Stokes system with two pressures". Supposing that the data are not too large, we prove the well-posedness of the homogenized problem and the convergence of the homogenization process.

Hans **Molenaar**:

Multigrid and Second-Order Upwind Schemes for Multiphase Flow

Second-order upwind schemes are widely used to avoid excessive numerical diffusion in multiphase flow computations. In many cases (like gravity driven flow or strong capillary effects) implicit time integration schemes are necessary for stability reasons. We consider the use of multigrid for the iterative solution of the discretized equations. Some preliminary results show the feasability of this approach.

Márcio A. **Murad**, John Cushman:

Multiscale Flow and Deformation in Hydrophilic Swelling Porous Media

A three-scale theory of swelling porous media is developed where the colloids and vicinal water (water next to the colloids) are considered on the microscale and hybrid mixture theory is used to upscale them to form mesoscale swelling particles. The mesoscale particles and bulk phase water (water next to the swelling particles) are then homogenized via an asymptotic expansion technique to form a swelling mixture on the macroscale. The solid phase on the macroscale can be viewed as a porous matrix consisting of swelling porous particles. Two Darcy type laws are developed on the macroscale, each corresponding to a different bulk water connectivity. One in which the bulk water is entrapped by the particles, forming a disconnected system, and the other in which the bulk water is connected and flows between particles. In the latter case the homogenized equations give rise to a distributed model with microstructure in which the vicinal water is represented by source/sinks at the macroscale. The theory is used to construct a three-dimensional model for consolidation of swelling clay soils and new constitutive relations for the stress tensor of the swelling particles are developed. Several heuristic modifications to the classical Terzaghi effective stress principle for granular (non-swelling) media which account for the hydration forces in swelling clay soils recently appeared in the literature. A notable consequence of the theory developed herein is that it provides a rational basis for these modified Terzaghi stresses.

E. **Priesack**:

A Microstructure Model for Microbial Growth in Aggregated Soils

A dual porosity model is derived for solute transport and microbial growth in unsaturated aggregated soils. Experimental results showing diffusion and degradation of ^{13}C-glucose in a singe aggregate are presented. Since the partial differential equations are of the linear diffusion-convection type, for the simulations presented a finite difference scheme is used with respect to space and a fully implicit scheme with respect to time. The nonlinear sink term is dealt with using a Newton-type iteration. Finally the solutions of the equations for macro- and micro-scale are approximated simultaneously by an alternating iteration scheme. Break-through curves and distributions of microbial bio-mass at macro- and micro-scale are compared for cases with different types of aggregation. Existence, uniqueness and L^1-estimate for weak solutions for the system of ordinary and degenerate partial differential equations are proved.

Yoram **Rubin**:

Stochastic Modeling of Flow and Transport in Heterogeneous Aquifers

A new method for generating random velocity fields in 3D is presented. The method is based on geostatistical concepts and on stochastic representation of the flow and transport processes. The method allows an extensive Monte-Carlo analysis in 3D due to its numerical efficiency. The principles of the method will be presented and some numerical results, emphasizing the statistics of the concentration field. The scale dependence of the concentration is investigated.

Tom **Russell**, David Dean, Tissa Illangasekare, R. Mapa, J. Garcia:

Upscaling of Dispersivity in Solute Transport in Heterogeneous Media

Our objective is to develop a practical tool for generation of upscaled dispersivity coefficients in simulations of passive solute transport in heterogeneous media. To be practical, restrictive assumptions such as ergodicity, periodicity, small perturbations of a uniform flow, small variance, and single-scale or continuous-scale (fractal) correlation structure should be avoided. To obtain the desired flexibility we work in the framework of a Lagrangian stochastic dispersion model developed by G. Dagan, which can yield variable coefficients on numerical grid blocks. Instead of analytical models we compute with a numerical discretization, allowing local assumptions to replace traditional global theoretical assumptions, and proceeding directly from conductivity statistics without needing velocity statistics. Lagrangian particles are tracked with an accurate analytical scheme that is exact for lowest-order Raviart-Thomas velocity fields. Non-local time- and scale-dependent dispersivities are computed for conductivity data from two-dimensional heterogeneous laboratory experiments.

Michel **Quintard**:

Active Dispersion in Porous Media: Local Non-Equilibrium Models

This paper is concerned by the process of dissolution of hydrocarbon phases trapped in aquifer (NAPL). The dispersion of the pollutant in the water is affected by the mass flux at the NAPL-Water interfaces, hence the word active dispersion by opposition to passive dispersion occurring when there is no exchange at the fluid-fluid and fluid-solid interfaces. Active dispersion in porous media can be described macroscopically by a local non-equilibrium model involving a modified dispersion tensor, and a mass exchange coefficient. Results obtained through a volume averaging technique are discussed. Examples of direct calculations of macroscopic coefficients are provided in the case of two- and three-dimensional unit cells, and for more complex, random porous media. The application of these models to the interpretation of experiments is emphasized on the basis of new core-laboratory displacements.

Andreas **Schuppert**:

Models for Elasticity and Creeps in Highly Anisotropic Media with Defects

Highly anisotripc media with defects are typically realized in highly oriented polymer fibers with stiff molecules. They have a scalable fibrillary structure where rigid rods are " glued " together by weak forces in a lamellar structure. Therefore the shear properties are much lower than tensile properties and the void concentration is comparably high causing special macroscopic effects.

By asymptotic analysis for very low and very high shear moduli it could be shown that the critical value determining the transition from a shear dominated to a tension dominated elongation mode under pure tension load can be efficiently controlled by the length of the rigid rods.

The irreversible creep elongation under constant load shows a logarithmic time law over many time scales together with an annihilation of defects. A model is presented describing the stress induced transport of defects in anisotropic fibrillary structures leading generically to the observed logarithmic time law. Due to the Saint-Venant principle, this behavior has been shown to be a typical property of fibrillary structures with a high concentration of voids.

M. **Slodička**, E. Holban, U. Hornung, Y. Kelanemer:

Standard and Mixed Finite Elements. A Comparison and Applications in Hydrology

The goal of this talk is to compare the standard and the mixed hybrid finite element methods (FEMs).The relative L_2 errors for pressure and flux are computed with respect to the CPU time which each method needs for solving the corresponding linear algebraic system. Several examples of linear elliptic partial differential equations (PDEs) related to the transport in porous media are presented.

Georg **Teutsch**:

A Multicomponent Model of Reactive Transport in Heterogeneous Porous Media: Basic Concepts and Parametrization

Abandoned gasworks sites pose a threat to the environment by the release of PAM-compounds. In the talk a model concept is developed for the transport of multiple PAM-compounds and the effect of surfactants. The model takes into account the differential advection occurring in a heterogeneous aquifer as well as surface sorption and intraparticle diffusion. Based on a so called 'parcel-tracking' technique consisting of a chain of advective reactors, we were able to simulate sorption kinetic experiments conducted in the laboratory.

Furthermore, soil column experiments were simulated including the application of surfactants below and above the CMC (critical unicell concentration). The upscaling concept is based on the stochastic streamtube approach presented by Cvetkovic & Dagan in 1994. There the reaction function can either be solved analytically for simple conditions or using our multicomponent parcel-tracking model.

Validation of the model at bench- and field-scale is presently under way.

Bogdan **Vernescu**:

Elektrokinetic Phenomena in the Modeling of Clays

We study the influence of surface charge distribution of the macroscopic behaviour of clays. At the interface between phases a double layer is formed. That is of order of magnitude of Debye's charateristic length. Due to the double layer a slip velocity condition is imposed. In the framework of the homogenization method the macroscopic behaviour of such clays is obtained. At the microscopic level the flow of a univalent electrolyte and an elastic skeleton are considered. The homogenized flow is modeled by a Darcy law and a visco-elastic type law in which the coefficients depend on the surface and bulk charge distribution.

Mary F. **Wheeler**:

Multiphase and Geochemical Modeling in Porous Media

A major problem in the numerical simulation of multiphase flow and transport with biological and chemical kinetics is the accurate and efficient modeling of a large number of chemical species in one to four fluid phases interacting with multiple solid mineral phases making up the permeable media.

In this presentation a summary of equations with N_C components, N_P flowing phases and Π solid phases (minerals) was given. It was noted that the mass transfer of components between phases is analogous to the transfer of components between species within a phase.

A new numerical algorithm for minimizing Gibbs free energy, the interior point method, was introduced. Computational examples for a multiphase case, aqueous and on mineral phases, were presented to illustrate the effectiveness and robustness of this procedure. A radionuclide (strontium) kinetic case study was also described. The problem here involved modeling the flow and transport with adsorption of a multicomponent system. Calculations provide explanation of field experiments. Collaborators: S. Bryant, G. Pope, F. Scaf.

Gabriel **Wittum**:

Multigrid methods for porous media flow

Berichterstatter: E. Holban

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