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Mineral Solubility and Free Energy Controls on Microbial Reaction Kinetics 2016 Recent developments in the theoretical treatment of geomicrobial reaction processes have resulted in the formulation of kinetic models that directly link the rates of microbial respiration and growth to the corresponding thermodynamic driving forces. The overall objective of this project was to verify and calibrate these kinetic models for the microbial reduction of uranium(VI) in geochemical conditions that mimic as much as possible field conditions. The approach combined modeling of bacterial processes using new bioenergetic rate laws, laboratory experiments to determine the bioavailability of uranium during uranium bioreduction, evaluation of microbial growth yield under energy-limited conditions using bioreactor experiments, competition experiments between metabolic processes in environmentally relevant conditions, and model applications at the field scale. The new kinetic descriptions of microbial U(VI) and Fe(III) reduction should replace those currently used in reactive transport models that couple catabolic energy generation and growth of microbial populations to the rates of biogeochemical redox processes. The above work was carried out in collaboration between the groups of Taillefert (batch reactor experiments and reaction modeling) at Georgia Tech and Van Cappellen (retentostat experiments and reactive transport modeling) at University of Waterloo (Canada).
The Individual Microbe: Single-Cell Analysis and Agent-Based Modelling Johan H. J. Leveau 2019-02-19 Recent technological advances in single-cell microbiology, using flow cytometry, microfluidics, x-ray fluorescence microprobes, and single-cell -omics, allow for the observation of individuals within populations. Simultaneously, individual-based models (or more generally agent-based models) allow for individual microbes to be simulated. Bridging these techniques forms the foundation of individual-based ecology of microbes (µIBE). µIBE has elucidated genetic and phenotypic heterogeneity that has important consequences for a number of human interests, including antibiotic or biocide resistance, the productivity and stability of industrial fermentations, the efficacy of food preservatives, and the potential of pathogens to cause disease. Individual-based models can help us to understand how these sets of traits of individual microbes influence the above. This eBook compiles all publications from a recent Research Topic in Frontiers in Microbiology. It features recent research where individual observational and/or modelling techniques are applied to gain unique insights into the ecology of microorganisms. The Research Topic “The Individual Microbe: Single-Cell Analysis and Agent-Based Modelling” arose from the 2016 @ASM conference of the same name hosted by the American Society for Microbiology at its headquarters in Washington, D.C. We are grateful to ASM for funding and hosting this conference.
Microbial Community Modeling: Prediction of Microbial Interactions and Community Dynamics Hyun-Seob Song 2018-07-04 This book is a printed edition of the Special Issue "Microbial Community Modeling: Prediction of Microbial Interactions and Community Dynamics" that was published in Processes
The Rock Physics Handbook Gary Mavko 2019-12-31 Brings together widely scattered theoretical and laboratory rock physics relations critical for modelling and interpretation of geophysical data.
Growth and Transport in Nanostructured Materials Angel Yanguas-Gil 2016-11-30 This book will address the application of gas phase thin film methods, including techniques such as evaporation, sputtering, CVD, and ALD to the synthesis of materials on nanostructured and high aspect-ratio high surface area materials. We have chosen to introduce these topics and the different application fields from a chronological perspective: we start with the early concepts of step coverage and later conformality in semiconductor manufacturing, and how later on the range of application branched out to include others such as energy storage, catalysis, and more broadly nanomaterials synthesis. The book will describe the ballistic and continuum descriptions of gas transport on nanostructured materials and then will move on to incorporate the impact of precursor-surface interaction. We will finally conclude approaching the subjects of feature shape evolution and the connection between nano and reactor scales and will briefly present different advanced algorithms that can be used to effectively compute particle transport, in some cases borrowing from other disciplines such as radiative heat transfer. The book gathers in a single place information scattered over thirty years of scientific research, including the most recent results in the field of Atomic Layer Deposition. Besides a mathematical description of the fundamentals of thin film growth in nanostructured materials, it includes analytic expressions and plots that can be used to predict the growth using gas phase synthesis methods in a number of ideal approximations. The focus on the fundamental aspects over particular processes will broaden the appeal and the shelf lifetime of this book. The reader of this book will gain a thorough understanding on the coating of high surface area and nanostructured materials using gas phase thin film deposition methods, including the limitations of each technique. Those coming from the theoretical side will gain the knowledge required to model the growth process, while those readers more interested in the process development will gain the theoretical understanding will be useful for process optimization.
The Reactive Transport of Suspended Particles Richard Steven Mercier 1985
EuroCVD 17/CVD 17 M. T. Swihart 2009-09 This issue of ECS Transactions includes papers presented at the 2009 EuroCVD-17 and CVD 17 symposium. Topical areas covered include fundamentals of chemical vapor deposition (CVD), chemistry of precursors for CVD, synthesis of nanomaterials by CVD and related methods, industrial applications of CVD, and novel CVD reactors and processes. This issue is sold as a two-part set and also includes a CD-ROM of the entire issue.
Groundwater Geochemistry Broder J. Merkel 2008-05-30 To understand hydrochemistry and to analyze natural as well as man-made impacts on aquatic systems, hydrogeochemical models have been used since the 1960’s and more frequently in recent times. Numerical groundwater flow, transport, and geochemical models are important tools besides classical deterministic and analytical approaches. Solving complex linear or non-linear systems of equations, commonly with hundreds of unknown parameters, is a routine task for a PC. Modeling hydrogeochemical processes requires a detailed and accurate water analysis, as well as thermodynamic and kinetic data as input. Thermodynamic data, such as complex formation constants and solubility-products, are often provided as databases within the respective programs. However, the description of surface-controlled reactions (sorption,

cation exchange, surface complexation) and kinetically controlled reactions requires additional input data. Unlike groundwater flow and transport models, thermodynamic models, in principal, do not need any calibration. However, considering surface-controlled or kinetically controlled reaction models might be subject to calibration. Typical problems for the application of geochemical models are: • speciation • determination of saturation indices • adjustment of equilibria/disequilibria for minerals or gases • mixing of different waters • modeling the effects of temperature • stoichiometric reactions (e.g. titration) • reactions with solids, fluids, and gaseous phases (in open and closed systems) • sorption (cation exchange, surface complexation) • inverse modeling • kinetically controlled reactions • reactive transport Hydrogeochemical models depend on the quality of the chemical analysis, the boundary conditions presumed by the program, theoretical concepts (e.g.

Numerical and Analytical Modeling of Gas Mixing and Bio-Reactive Transport during Underground Hydrogen Storage Birger Hagemann 2018-01-11 In this thesis the major differences between underground hydrogen storage and the conventional storage of natural gas are lined out to be bio-reactive and gas mixing phenomena. A new mathematical model was developed to describe the coupling between two-phase flow and microbial populations which consume hydrogen for their metabolism. Different analytical and numerical techniques were applied to investigate the storage of hydrogen in the geological subsurface. An analytical solution was derived for gravity-driven multi-component two-phase flow in heterogeneous porous media. Oscillating scenarios, similar to Turing instability, were detected. Storage scenarios were simulated including a field scale demonstration in a realistic geological model.

Carbonate Geochemistry Annette Summers Engel 2011-08-01 Selected papers and abstracts of the symposium held August 6 through 9, 2011, Billings, Montana

Modeling the Effect of Secondary Mineral Formation and Microbial Growth on the Hydraulic Properties of a Zero-valent Iron Barrier Eileen Marie Belding 2005

Contaminants in the Subsurface National Research Council 2005-03-23 At hundreds of thousands of commercial, industrial, and military sites across the country, subsurface materials including groundwater are contaminated with chemical waste. The last decade has seen growing interest in using aggressive source remediation technologies to remove contaminants from the subsurface, but there is limited understanding of (1) the effectiveness of these technologies and (2) the overall effect of mass removal on groundwater quality. This report reviews the suite of technologies available for source remediation and their ability to reach a variety of cleanup goals, from meeting regulatory standards for groundwater to reducing costs. The report proposes elements of a protocol for accomplishing source remediation that should enable project managers to decide whether and how to pursue source remediation at their sites.

Isotopic Constraints on Earth System Processes Kenneth W. W. Sims 2022-06-01 Using isotopes as a tool for understanding Earth processes From establishing the absolute age of the Earth to providing a stronger understanding of the nexus between geology and life, the careful measurement and quantitative interpretation of minor variations in the isotopic composition of Earth's materials has provided profound insight into the origins and workings of our planet. Isotopic Constraints on Earth System Processes presents examples of the application of numerous different isotope systems to address a wide range of topical problems in Earth system science. Volume highlights include: examination of the natural fractionation of non-traditional stable isotopes utilizing isotopes to understand the origin of magmas and evolution of volcanic systems application of isotopes to interrogate and understand Earth's Carbon and Oxygen cycles examination of the geochemical and hydrologic processes that lead to isotopic fractionation application of isotopic reactive transport models to decipher hydrologic and biogeochemical processes The American Geophysical Union promotes discovery in Earth and space science for the benefit of humanity. Its publications disseminate scientific knowledge and provide resources for researchers, students, and professionals.

Porous Media Kambiz Vafai 2010-08-24 Presenting state-of-the-art research advancements, Porous Media: Applications in Biological Systems and Biotechnology explores innovative approaches to effectively apply existing porous media technologies to biomedical applications. In each peer-reviewed chapter, world-class scientists and engineers collaborate to address significant problems and discuss exciting research in biological systems. The book begins with discussions on bioheat transfer equations for blood flows and surrounding biological tissue, the concept of electroporation, hydrodynamic modeling of tissue-engineered material, and the resistance of microbial biofilms to common modalities of antibiotic treatments. It examines how biofilms influence porous media hydrodynamics, describes the modeling of flow changes in cerebral aneurysms, and highlights recent advances in Lagrangian particles methods. The text also covers passive mass transport processes in cellular membranes and their biophysical implications, the modeling and treatment of mass transport through skin, the use of porous media in marine microbiology, the transport of large biological molecules in deforming tissues, and applications of magnetic stabilized beds for protein purification and adsorption, antibody removal, and more. The final chapters present potential in situ characterization techniques for studying porous media and conductive membranes and explain the development of bioconvection patterns generated by populations of gravitactic microorganisms in porous media. Using a common nomenclature throughout and with contributions from top experts, this cohesive book illustrates the role of porous media in addressing some of the most challenging issues in biomedical engineering and biotechnology. The book contains sophisticated porous media models that can be used to improve the accuracy of modeling a variety of biological processes.

On Some Problems in the Simulation of Flow and Transport Through Porous Media Sunil George Thomas 2009 The dynamic solution of multiphase flow through porous media is of special interest to several fields of science and engineering, such as petroleum, geology and geophysics, bio-medical, civil and environmental, chemical engineering and many other disciplines. A natural application is the modeling of the flow of two immiscible fluids (phases) in a reservoir. Others, that are broadly based and considered in this work include the hydrodynamic dispersion (as in reactive transport) of a solute or tracer chemical through a fluid phase. Reservoir properties like permeability and porosity greatly influence the flow of these phases. Often, these vary across several orders of magnitude and can be discontinuous functions. Furthermore, they are generally not known to a desired level of accuracy or detail and special inverse problems need to be solved in order to obtain their estimates. Based on the physics dominating a given sub-region of the porous medium, numerical solutions to such flow problems may require different discretization schemes or different governing equations in adjacent regions. The need to couple solutions to such schemes gives rise to challenging domain decomposition problems. Finally, on an application level, present day environment concerns have resulted in a widespread increase in CO2 capture and storage experiments across the globe. This presents a huge modeling challenge for the future. This research work is divided into sections that aim to study various inter-connected problems that are of significance in sub-surface porous media applications. The first section studies an application of mortar (as well as nonmortar, i.e., enhanced velocity) mixed finite element methods (MMFEM and EV-MFEM) to problems in porous media flow. The mortar spaces are first used to develop a multiscale approach for parabolic problems in porous media applications. The implementation of the mortar mixed method is presented for two-phase immiscible flow and some a priori error estimates are then derived for the case of slightly compressible single-phase Darcy flow. Following this, the problem of modeling flow coupled to reactive transport is studied. Applications of such problems include modeling bio-remediation of oil spills and other subsurface hazardous wastes, angiogenesis in the transition of tumors from a dormant to a malignant state, contaminant transport in groundwater flow and acid injection around well bores to increase the permeability of the surrounding rock. Several numerical results are presented that demonstrate the efficiency of the method when compared to traditional approaches. The section following this examines (non-mortar) enhanced velocity finite element methods for solving multiphase flow coupled to species transport on non-matching multiblock grids. The results from this section indicate that this is the recommended method of choice for such problems. Next, a mortar finite element method is formulated and implemented that extends the scope of the classical mortar mixed finite element method developed by Arbogast et al (12) for elliptic problems and Girault et al (62) for coupling different numerical discretization schemes. Some significant areas of application include the coupling of pore-scale network models with the classical continuum models for steady single-phase Darcy flow as well as the coupling of different numerical methods such as discontinuous Galerkin and mixed finite element methods in different sub-domains for the case of single phase flow (21, 109). These hold promise for applications where a high level of detail and accuracy is desired in one part of the domain (often associated with very small length scales as in pore-scale network models) and a much lower level of detail at other parts of the domain (at much larger length scales). Examples include modeling of the flow around well bores or through faulted reservoirs. The next section presents a parallel stochastic approximation method (68, 76) applied to inverse modeling and gives several promising results that address the problem of uncertainty associated with the parameters governing multiphase flow partial differential equations. For example, medium properties such as absolute permeability and porosity greatly influence the flow behavior, but are rarely known to even a reasonable level of accuracy and are very often upscaled to large areas or volumes based on seismic measurements at discrete points. The results in this section show that by using a few measurements of the primary unknowns in multiphase flow such as fluid pressures and concentrations as well as well-log data, one can define an objective function of the medium properties to be determined, which is then minimized to determine the properties using (as in this case) a stochastic analog of Newton's method. The last section is devoted to a significant and current application area. It presents a parallel and efficient iteratively coupled implicit pressure, explicit concentration formulation (IMPEC) (52-54) for non-isothermal compositional flow problems. The goal is to perform predictive modeling simulations for CO2 sequestration experiments. While the sections presented in this work cover a broad range of topics they are actually tied to each other and serve to achieve the unifying, ultimate goal of developing a complete and robust reservoir simulator. The major results of this work, particularly in the application of MMFEM and EV-MFEM to multiphysics couplings of multiphase flow and transport as well as in the modeling of EOS non-isothermal compositional flow applied to CO2 sequestration, suggest that multiblock/multimodel methods applied in a robust parallel computational framework is invaluable when attempting to solve problems as described in Chapter 7. As an example, one may consider a closed loop control system for managing oil production or CO2 sequestration experiments in huge formations (the "instrumented oil field"). Most of the computationally costly activity occurs around a few wells. Thus one has to be able to seamlessly connect the above components while running many forward simulations on parallel clusters in a multiblock and multimodel setting where most domains employ an isothermal single-phase flow model except a few around well bores that employ, say, a non-isothermal compositional model. Simultaneously, cheap and efficient stochastic methods as in Chapter 8, may be used to generate history matches of well and/or sensor-measured solution data, to arrive at better estimates of the medium properties on the fly. This is obviously beyond the scope of the current work but represents the over-arching goal of this research.

Reactive transport modeling of fluid-rock interactions associated with carbonate diagenesis and implications for reservoir quality prediction Ying Xiong 2022-07-26 Diagenesis research is the foundation of hydrocarbon reservoir characterization and exploration. Reactive transport modeling (RTM) is an emerging approach for diagenesis research, with unique capability of quantification and forward modeling of the coupled thermo-hydro-chemical processes of diagenesis. Using TOUGHREACT simulator, this thesis investigates the two most important fluid-rock interactions in carbonate rocks, i.e., dolomitization and karstification, based on generic model analyses and a case study in the Ordos Basin, China. In particular, this study attempts to quantitatively characterize the diagenetic processes and to reconstruct the diagenesis-porosity evolution of carbonate reservoirs. Some controversies in carbonate diagenesis research, which cannot be well explained by classical geological methods, have also been discussed. The results are helpful to better understand the spatial-temporal distribution and co-evolution of diagenesis-mineral-porosity during the complicated diagenetic processes with their potential controlling factors, and to reduce the uncertainty of reservoir quality prediction.

Distributed Hydrological Modelling Michael B. Abbott 2012-12-06 It is the task of the engineer, as of any other professional person, to do everything that is reasonably possible to analyse the difficulties with which his or her client is confronted, and on this basis to design solutions and implement these in practice. The distributed hydrological model is, correspondingly, the means for doing everything that is reasonably possible - of mobilising as much data and testing it with as much knowledge as is economically feasible - for the purpose of analysing problems and of designing and implementing remedial measures in the case of difficulties arising within the hydrological cycle. Thus the aim of distributed hydrologic modelling is to make the fullest use of cartographic data, of geological data, of satellite data, of stream discharge measurements, of borehole data, of observations of crops and other vegetation, of historical records of floods and droughts, and indeed of everything else that has ever been recorded or remembered, and then to apply to this everything that is known about meteorology, plant physiology, soil physics, hydrogeology, sediment transport and everything else that is relevant within this context. Of course, no matter how much data we have and no matter how much we know, it will never be enough to treat some problems and some situations, but still we can aim in this way to do the best that we possibly can.

Selected Water Resources Abstracts 1989

An In-situ Permeable Reactive Barrier for the Treatment of Hexavalent Chromium and Trichloroethylene in Ground Water: Multicomponent reactive transport modeling 1999

Reactive Transport Modeling Yitian Xiao 2018-06-05 Teaches the application of Reactive Transport Modeling (RTM) for subsurface systems in order to expedite the understanding of the behavior of complex geological systems This book lays out the basic principles and approaches of Reactive Transport Modeling (RTM) for surface and subsurface environments, presenting specific workflows and applications. The techniques discussed are being increasingly commonly used in a wide range of research fields, and the information provided covers fundamental theory, practical issues in running reactive transport models, and how to apply techniques in specific areas. The need for RTM in engineered facilities, such as nuclear waste repositories or CO2 storage sites, is ever increasing, because the prediction of the future evolution of these systems has become a legal obligation. With increasing recognition of the power of these approaches, and their widening adoption, comes responsibility to ensure appropriate application of available tools. This book aims to provide the requisite understanding of key aspects of RTM, and in doing so help identify and thus avoid potential pitfalls. Reactive Transport Modeling covers: the application of RTM for CO2 sequestration and geothermal energy development; reservoir quality prediction; modeling diagenesis; modeling geochemical processes in oil & gas production; modeling gas hydrate production; reactive transport in fractured and porous media; reactive transport studies for nuclear waste disposal; reactive flow modeling in hydrothermal systems; and modeling biogeochemical processes. Key features include: A comprehensive reference for scientists and practitioners entering the area of reactive transport modeling (RTM) Presented by internationally known experts in the field Covers fundamental theory, practical issues in running reactive transport models, and hands-on examples for applying techniques in specific areas Teaches readers to appreciate the power of RTM and to stimulate usage and application Reactive Transport Modeling is written for graduate students and researchers in academia, government laboratories, and industry who are interested in applying reactive transport modeling to the topic of their research. The book will also appeal to geochemists, hydrogeologists, geophysicists, earth scientists, environmental engineers, and environmental chemists.

Geochemical and Biogeochemical Reaction Modeling Craig M. Bethke 2007-12-06 This book provides a comprehensive overview of reaction processes in the Earth's crust and on its surface, both in the laboratory and in the field. A clear exposition of the underlying equations and calculation techniques is balanced by a large number of fully worked examples. The book uses The Geochemist's Workbench® modeling software, developed by the author and already installed at over 1000 universities and research facilities worldwide. Since publication of the first edition, the field of reaction modeling has continued to grow and find increasingly broad application. In particular, the description of microbial activity, surface chemistry, and redox chemistry within reaction models has become broader and more rigorous. These areas are covered in detail in this new edition, which was originally published in 2007. This text is written for graduate students and academic researchers in the fields of geochemistry, environmental engineering, contaminant hydrology, geomicrobiology, and numerical modeling.

Progress in Computational Physics Volume 3: Novel Trends in Lattice-Boltzmann Methods Matthias Ehrhardt 2013-06-18 Progress in Computational Physics is an e-book series devoted to recent research trends in computational physics. It contains chapters contributed by outstanding experts of modeling of physical problems. The series focuses on interdisciplinary computational perspectives of current physical challenges, new numerical techniques for the solution of mathematical wave equations and describes certain real-world applications. With the help of powerful computers and sophisticated methods of numerical mathematics it is possible to simulate many ultramodern devices, e.g. photonic crystals structures, semiconductor nanostructures or fuel cell stacks devices, thus preventing expensive and longstanding design and optimization in the laboratories. In this book series, research manuscripts are shortened as single chapters and focus on one hot topic per volume. Engineers, physicists, meteorologists, etc. and applied mathematicians can benefit from the series content. Readers will get a deep and active insight into state-of-the art modeling and simulation techniques of ultra-modern devices and problems. The third volume - Novel Trends in Lattice Boltzmann Methods - Reactive Flow, Physicochemical Transport and Fluid-Structure Interaction - contains 10 chapters devoted to mathematical analysis of different issues related to the lattice Boltzmann methods, advanced numerical techniques for physico-chemical flows, fluid structure interaction and practical applications of these phenomena to real world problems.

Handbook of Metal-Microbe Interactions and Bioremediation Surajit Das 2017-04-07 Around the World, metal pollution is a major problem. Conventional practices of toxic metal removal can be ineffective and/or expensive, delaying and exacerbating the crisis. Those communities dealing with contamination must be aware of the fundamentals advances of microbe-mediated metal removal practices because these methods can be easily used and require less remedial intervention. This book describes innovations and efficient applications for metal bioremediation for environments polluted by metal contaminates.

Pore Scale Geochemical Processes Carl Steefel 2015-09-25 This RiMG (Reviews in Mineralogy & Geochemistry) volume includes contributions that review experimental, characterization, and modeling advances in our understanding of pore-scale geochemical processes. The volume had its origins in a special theme session at the 2015 Goldschmidt Conference in Prague. From a diversity of pore-scale topics that ranged from multi-scale characterization to modeling, this work summarizes the state-of-the-science in this subject. Topics include: modification of thermodynamics and kinetics in small pores. chemo-mechanical processes and how they affect porosity evolution in geological media. small angle neutron scattering (SANS) techniques. how isotopic gradients across fluid–mineral boundaries can develop and how these provide insight into pore-scale processes. Information on an important class of models referred to as "pore network" and much more. The material in this book is accessible for graduate students, researchers, and professionals in the earth, material, environmental, hydrological, and biological sciences. The pore scale is readily recognizable to geochemists, and yet in the past it has not received a great deal of attention as a distinct scale or environment that is associated with its own set of questions and challenges. Is the pore scale merely an environment in which smaller scale (molecular) processes aggregate, or are there emergent phenomena unique to this scale? Is it simply a finer-grained version of the "continuum" scale that is addressed in larger-scale models and interpretations? The scale is important because it accounts for the pore architecture within which such diverse processes as multi-mineral reaction networks, microbial community interaction, and transport play out, giving rise to new geochemical behavior that might not be understood or predicted by considering smaller or larger scales alone.

The metabolic pathways and environmental controls of hydrocarbon biodegradation in marine ecosystems Joel E. Kostka 2015-05-15 Biodegradation mediated by indigenous microbial communities is the ultimate fate of the majority of oil hydrocarbon that enters the marine environment. The aim of this Research Topic is to highlight recent advances in our knowledge of the pathways and controls of microbially-catalyzed hydrocarbon degradation in marine ecosystems, with emphasis on the response of microbial communities to the Deepwater Horizon oil spill in the Gulf of Mexico. In this Research Topic, we encouraged original research and reviews on the ecology of hydrocarbon-degrading bacteria, the rates and mechanisms of biodegradation, and the bioremediation of discharged oil under situ as well as near in situ conditions.

Computational Models for CO2 Geo-sequestration & Compressed Air Energy Storage Rafid Al-Khoury 2014-04-17 A comprehensive mathematical and computational modeling of CO2 Geosequestration and Compressed Air Energy StorageEnergy and environment are two interrelated issues of great concern to modern civilization. As the world population will soon reach eight billion, the demand for energy will dramatically increase, intensifying the use of fossil fuels. Ut

Groundwater Reactive Transport Models Gour-Tsyh (George) Yeh 2012-03-15 Ground water reactive transport models are useful to assess and quantify contaminant precipitation, absorption and migration in subsurface media. Many ground water reactive transport models available today are characterized by varying complexities, strengths, and weaknesses. Selecting accurate, efficient models can be a challenging task. This book addresses the needs, issues and challenges relevant to selecting a ground water reactive transport model to evaluate natural attenuation and alternative remediation schemes. It should serve as a handy guide for water resource managers seeking to achieve economically feasible results.

Water Reclamation Technologies for Safe Managed Aquifer Recharge Christian Kazner 2012 Different treatment applications in terms of behaviour of key microbial and chemical contaminants are assessed. Engineered as well as natural treatment trains are investigated to provide guidance for sustainable MAR schemes using alternative sources such as recycled water and stormwater. The technologies considered are also well suited to the needs of developing countries, which have a growing need of supplementation of freshwater resources. A broad range of international full-scale case studies enables insights into long-term system behaviour, operational aspects, and fate of a comprehensive number of compounds and contaminants, especially microbiological hazards, organic micropollutants and bulk organics.

Reactive Transport in Porous Media Peter C. Lichtner 2018-12-17 Volume 34 of Reviews in Mineralogy focuses on methods to describe the extent and consequences of reactive flow and transport in natural subsurface systems. Since the field of reactive transport within the Earth Sciences is a highly multidisciplinary area of research, including geochemistry, geology, physics, chemistry, hydrology, and engineering, this book is an attempt to some extent bridge the gap between these different disciplines. This volume contains the contributions presented at a short course held in Golden, Colorado, October 25-27, 1996 in conjunction with the Mineralogical Society of America's (MSA) Annual Meeting with the Geological Society of America in Denver, Colorado.

Multi-mechanistic Modeling of Engineered Waterflooding in Reactive-transport Simulations Fabio Bordeaux Rego 2021 Engineered Waterflooding has gained increased attention in the past few decades as an emerging enhanced oil recovery (EOR) method. Besides the well-known waterflooding high displacement efficiency and reliable injectivity into hydrocarbon-bearing formations, the technique is very attractive because of its relatively low cost. The method consists of controlling the injected brine chemical composition aiming improved oil recovery. Laboratory and field studies indicated contradictory results, showing significant, minor, or no benefit on oil production even for similar experimental conditions. Although it is a consensus that wettability alteration is the leading cause for the improved recovery, modeling its underlying mechanisms is fundamental for successful project design and deployment. The dissertation presented here provides a comprehensive investigation of engineered waterflooding as an improved oil recovery method. It is hypothesized that changes in wettability are based on rock-fluid interactions through geochemical reactions and interfacial phenomena. Thus, a multi-mechanistic model that combines surface complexation and disjoining pressure calculations to predict contact angle and zeta-potential measurements is improved and validated. A method for determining surface complexation equilibrium constants is presented to honor several zeta-potential measurements for different ion concentrations (Na^+, Ca^{2+}, Mg^{2+}, SO_4^{2-} and H^+). In addition, a new data-driven wettability correlation is proposed to calculate contact angle based on surface complexation modeling and compared with the disjoining pressure approach. After the fundamental investigation of wettability in pore-scale, the modeling is coupled with UTCOMP-IPhreeqc, a reservoir simulator developed at The University of Texas at Austin, to study wettability alteration in core and field scale. Reactive-transport simulations are performed to history-match capillary pressure and relative permeability curves from spontaneous imbibition and coreflood experiments under controlled conditions and different lithologies (sandstone, carbonate, and shale). Geochemical calculations are conducted to study simultaneous wettability alteration mechanisms (e.g., electric double-layer expansion, multi-ion exchange, local pH increase). In addition, several physical phenomena related to changes in injected brine composition are modeled, such as clay swelling and scale deposition. Wettability and geochemical modeling are applied to investigate the synergy between engineered waterflooding and other EOR methods during reactive-transport simulations. An adsorption model for cationic surfactant is proposed based on surface complexation reactions and combined with contact angle calculations. The method is employed to match laboratory data and explore the combined effect of brine dilution and surfactant in field scale. In another study, the dissolution phenomenon, its impact on petrophysical properties, and well injectivity is investigated during water-alternating-CO_2 gas. A predictive model is proposed and validated against published coreflood data. Besides the effect of brine composition, other reservoir conditions are investigated during the water-alternating-CO_2 flood in field scale, such as mineralogy type, heterogeneity, and gravity segregation. Reactive-transport modeling has been improved significantly with recent advances in geochemical and petrophysical characterization. However, detailed simulations are usually associated with an increase in computational cost. A method is proposed to decrease the computational time during reactive-transport simulations in porous media. It is hypothesized that, if geochemical calculations can be ignored for regions under equilibrium conditions (far from the saturation front), then the computational performance would be improved without compromising simulation results. The validity of the approach is tested for three simulation cases considering different complexities (e.g., heterogeneity, wettability alteration, CO_2 solubilization in water, and dissolution)

Groundwater Reactive Transport Models Fan Zhang 2012 Ground water reactive transport models are useful to assess and quantify contaminant precipitation, absorption and migration in subsurface media. Many ground water reactive transport models available today are characterized by varying complexities, strengths, and weaknesses. Selecting accurate, efficient models can be a challenging task. This ebook addresses the needs, issues and challenges relevant to selecting a ground water reactive transport model to evaluate natural attenuation and alternative remediation schemes. It should serve as a handy guide for water resource managers seeking to ach.

Environmental Applications of Geochemical Modeling Chen Zhu 2002-05-13 An application of geochemical modeling to environmental problems, illustrated with case studies of real-world environmental investigations.

Reactive Transport in Soil and Groundwater Gunnar Nützmann 2006-02-08 In this book, the authors focus on the improvement of the scientific base for the development of environmental risk indicators measured by the presence of pollutants in water and porous media. In pursuit of a correct and complete numerical approach, they deliver insight into the understanding of integrated process, and also of modeling capabilities.

The Role of Natural and Constructed Wetlands in Nutrient Cycling and Retention on the Landscape Jan Vymazal 2014-09-26 Natural and constructed wetlands play a very important role on the landscape and their ecological services are highly valuable. In fact, some wetland types are regarded as one of the most valuable ecosystems on the Earth. Water management, including flood water retention, biomass production, carbon sequestration, wastewater treatment and biodiversity sources, are among the most important ecological services of wetlands. The book is aimed at the use of constructed wetlands for wastewater treatment and for the evaluation of various ecosystem services of natural wetlands. Special attention is paid to the role and potential use of wetlands on the agricultural landscape. The book presents up-to-date results of ongoing research and the content of the book could be used by wetland scientists, researchers, engineers, designers, regulators, decision-makers, universities teachers, landscape engineers and landscape planners as well as by water authorities, water regulatory offices or wastewater treatment research institutions.

Wastewater Re-use and Groundwater Quality J. H. A. M. Steenvoorden 2004

BIOMOC, a Multispecies Solute-transport Model with Biodegradation Hedeff I. Essaid 1997

Carbonates—Advances in Research and Application: 2012 Edition 2012-12-26 Carbonates—Advances in Research and Application: 2012 Edition is a ScholarlyEditions™ eBook that delivers timely, authoritative, and comprehensive information about Carbonates. The editors have built Carbonates—Advances in Research and Application: 2012 Edition on the vast information databases of ScholarlyNews.™ You can expect the information about Carbonates in this eBook to be deeper than what you can access anywhere else, as well as consistently reliable, authoritative, informed, and relevant. The content of Carbonates—Advances in Research and Application: 2012 Edition has been produced by the world's leading scientists, engineers, analysts, research institutions, and companies. All of the content is from peer-reviewed sources, and all of it is written, assembled, and edited by the editors at ScholarlyEditions™ and available exclusively from us. You now have a source you can cite with authority, confidence, and credibility. More information is available at http://www.ScholarlyEditions.com/.

Reactive Transport in Natural and Engineered Systems Jennifer Druhan 2020-03-04 Open system behavior is predicated on a fundamental relationship between the timescale over which mass is transported and the timescale over which it is chemically transformed. This relationship describes the basis for the multidisciplinary field of reactive transport (RT). In the 20 years since publication of Review in Mineralogy and Geochemistry volume 34: Reactive Transport in Porous Media, RT principles have expanded beyond early applications largely based in contaminant hydrology to become broadly utilized throughout the Earth Sciences. RT is now employed to address a wide variety of natural and engineered systems across diverse spatial and temporal scales, in tandem with advances in computational capability, quantitative imaging and reactive interface characterization techniques. The present volume reviews the diversity of reactive transport applications developed over the past 20 years, ranging from the understanding of basic processes at the nano- to micrometer scale to the prediction of Earth global cycling processes at the watershed scale. Key areas of RT development are highlighted to continue advancing our capabilities to predict mass and energy transfer in natural and engineered systems.

Numerical Simulation of Reactive Flow in Hot Aquifers

Christoph Clauser 2003 This book deals with the numerical simulation of reactive transport in porous media using the simulation package SHEMAT/Processing SHEMAT. SHEMAT (Simulator for HEat and MAss Transport) is an easy-to-use, general-purpose reactive transport simulation code for a wide variety of thermal and hydrogeological problems in two or three dimensions. You can download the updated version of the SHEMAT software from our Springer-Extras server: http://extras.springer.com/2003/978-3-540-43868-7. The book is a richly documented manual for users of this software which discusses in detail the coded physical and chemical equations. Thus, it provides the in-depth background required by those who want to apply the code for solving advanced technical and scientific problems. The enclosed software and data package is applicable for all of the case studies. The software includes user-friendly pre- and post-processors which make it very easy to set up a model, run it and view the results, all from one platform. Therefore, the software is also very suitable for academic or technical "hands-on" courses for simulating flow, transport of heat and mass, and chemical reactions in porous media.
Coupled Modeling of Groundwater Flow Solute Transport, Chemical Reactions and Microbial Processes in the 'SP' Island Guoxiang Zhang 2003 The Redox Zone Experiment was carried out at the Aespoe HRL in order to study the redox behavior and the hydrochemistry of an isolated vertical fracture zone disturbed by the excavation of an access tunnel. Overall results and interpretation of the Redox Zone Project were reported by /Banwart et al, 1995/. Later, /Banwart et al, 1999/ presented a summary of the hydrochemistry of the Redox Zone Experiment. Coupled groundwater flow and reactive transport models of this experiment were carried out by /Molinero, 2000/ who proposed a revised conceptual model for the hydrogeology of the Redox Zone Experiment which could explain simultaneously measured drawdown and salinity data. The numerical model was found useful to understand the natural system. Several conclusions were drawn about the redox conditions of recharge waters, cation exchange capacity of the fracture zone and the role of mineral phases such as pyrite, calcite, hematite and goethite. This model could reproduce the measured trends of dissolved species, except for bicarbonate and sulfate which are affected by microbially-mediated processes. In order to explore the role of microbial processes, a coupled numerical model has been constructed which accounts for water flow, reactive transport and microbial processes. The results of this model is presented in this report. This model accounts for groundwater flow and reactive transport in a manner similar to that of /Molinero, 2000/ and extends the preliminary microbial model of /Zhang, 2001/ by accounting for microbially-driven organic matter fermentation and organic matter oxidation. This updated microbial model considers simultaneously the fermentation of particulate organic matter by yeast and the oxidation of dissolved organic matter, a product of fermentation. Dissolved organic matter is produced by yeast and serves also as a substrate for iron-reducing bacteria. Model results reproduce the observed increase in bicarbonate and sulfate concentration, thus adding additional evidence for the possibility of organic matter oxidation as the main source of bicarbonate. Model results indicate that pH and Eh are relatively stable. The dissolution-precipitation trends of hematite, pyrite and calcite also coincide with those indicated by the conceptual model. A thorough sensitivity analysis has been performed for the most relevant microbial parameters as well as for initial and boundary POC and DOC concentrations. The results of such analysis indicate that computed concentrations of bicarbonate, sulfate and DOC are sensitive to most of the microbial parameters, including specific growth rates, half-saturation constants, proportionality coefficients and yield coefficients. Model results, however, are less sensitive to the yield coefficient of DOC to iron-reducer bacteria. The sensitivity analysis indicates that changes in fermentation microbial parameters affect the growth of the iron-reducer, thus confirming the interconnection of both microbial processes. Computed concentrations of bicarbonate and sulfate are found to be sensitive to changes in the initial concentration of POC and the boundary concentration of DOC, but they lack sensitivity to the initial concentration of DOC and the boundary concentration of POC. The explanation for such result is related to the fact that POC has a low mobility due to its large molecular weight. DOC, however, can migrate downwards. Although a coupled hydro-bio-geochemical 1-D model can reproduce the observed ''unexpected'' increase of concentrations of bicarbonate and sulfate at a depth of 70 m, further modeling work is required in order to obtain a similar conclusion under the more realistic two dimensional conditions of the fracture zone.