Application Of Reactive Transport Modelling To Growth And

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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.
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.
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.

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.

Growth of Sparingly-soluble AB-type Minerals as a Function of Their A:B Ratio Jacquelyn N. Bracco 2015 A fundamental understanding of mineral growth kinetics is necessary to predict mineral reactivity in geologic environments. We use hydrothermal atomic force microscopy (HAFM) to measure step advance speeds and morphological evolution of the sparingly-soluble minerals magnesite ($MgCO_3$), barite ($BaSO_4$) and celestite ($SrSO_4$) while systematically varying the concentrations of their constituent cations and anions in solution. For all three minerals, a maximum step velocity is reached at an aqueous cation:anion concentration (r) near unity and decreases with extreme r despite order of magnitude differences in the water exchange rate for the cations comprising the minerals. Affinity based models fail to reproduce the observed trends in which step velocities vary with changes in the cation-to-anion ratio. A process based model developed by Zhang and Nancollas (1990, 1998) does not fit the peak shape in experimental measurements of step speed versus r and underestimates step velocities which may arise from the model assumption that the forward reaction is tied to the back reaction through the solubility product. Step velocities as a function of r on all three minerals can be modeled well using the Stack and Grantham (2010) kink site nucleation + propagation model. While the growth of the minerals as a function of r can be described using the same model, there are some significant differences in the behavior of the three minerals. First, model derived detachment rates of ions from a step to propagate kink sites is zero for barite and celestite, but nonzero for magnesite. Significant morphological changes are also observed for barite as a function of r, but not for celestite and magnesite. Finally, step velocities on celestite are non-linear as a function of saturation

state, whereas they are linear for barite and magnesite. Together, these results suggest that current models which are utilized to predict mineral reactivity in environmental settings (e.g. reactive transport models) are missing a key parameter necessary to accurately predict mineral growth.

Microbial Biodegradation and Bioremediation Surajit Das 2014-07-01 Microbial Biodegradation and Bioremediation brings together experts in relevant fields to describe the successful application of microbes and their derivatives for bioremediation of potentially toxic and relatively novel compounds. This single-source reference encompasses all categories of pollutants and their applications in a convenient, comprehensive package. Our natural biodiversity and environment is in danger due to the release of continuously emerging potential pollutants by anthropogenic activities. Though many attempts have been made to eradicate and remediate these noxious elements, every day thousands of xenobiotics of relatively new entities emerge, thus worsening the situation. Primitive microorganisms are highly adaptable to toxic environments, and can reduce the load of toxic elements by their successful transformation and remediation. Describes many novel approaches of microbial bioremediation including genetic engineering, metagenomics, microbial fuel cell technology, biosurfactants and biofilm-based bioremediation Introduces relatively new hazardous elements and their bioremediation practices including oil spills, military waste water, greenhouse gases, polythene wastes, and more Provides the most advanced techniques in the field of bioremediation, including insilico approach, microbes as pollution indicators, use of bioreactors, techniques of pollution monitoring, and more

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.

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

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. *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.

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.

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+, Ca2+, Mg2+, SO42− 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-CO2 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-CO2 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, CO2 solubilization in water, and dissolution)

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.

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.

Advanced Methods and Mathematical Modeling of Biofilm Mojtaba Aghajani Delavar 2022-05-27 Advanced Mathematical Modelling of Biofilms and its Applications covers the concepts and fundamentals of biofilms, including sections on numerical discrete and numerical continuum models and different biofilms methods, e.g., the lattice Boltzmann method (LBM) and cellular automata (CA) and integrated LBM and individual-based model (iBM). Other sections focus on design, problem-solving and state-of-the-art modelling methods. Addressing the needs to upgrade and update information and knowledge for students, researchers and engineers on biofilms in health care, medicine, food, aquaculture and industry, this book also covers areas of uncertainty and future needs for advancing the use of biofilm models. Over the past 25-30 years, there have been rapid advances in various areas of computer technologies, applications and methods (e.g. complex programming and algorithms, lattice Boltzmann method, high resolution visualization and high-performance computation). These new and emerging technologies are providing unprecedented opportunities to develop modeling frameworks of biofilms and their applications. Introduces state-of-the-art methods of biofilm modeling, such as integrated lattice Boltzmann method (LBM) and cellular automata (CA) and integrated LBM and individual-based model (iBM) Provides recent progress in more powerful tools for a deeper understanding of biofilm complexity by implementing state-of-the art biofilm modeling programs Compares advantages and disadvantages of different biofilm models and analyzes some specific problems for model selection Evaluates novel process designs without the cost, time and risk of building a physical prototype of the process to identify the most promising designs for experimental testing

Reactive Transport Modeling Yitian Xiao 2018-03-14 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. Fast Reactions Kenneth Kustin 1969 The critically acclaimed laboratory standard, Methods in Enzymology, is one of the most highly respected publications in the field of biochemistry. Since 1955, each volume has been eagerly awaited, frequently consulted, and praised by researchers and reviewers alike. The series contains much material still relevant today - truly an essential publication for researchers in all fields of life sciences. **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.

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.

Changing Course Asian Development Bank 2009-10-01 Most Asian cities have grown more congested, more sprawling, and less livable in recent years; and statistics suggest that this trend will continue. Rather than mitigate the problems, transport policies have often exacerbated them. In this book, the Asian Development Bank outlines a new paradigm for sustainable urban transport that gives Asian cities a workable, step-by-step blueprint for reversing the trend and moving toward safer, cleaner, more sustainable cities, and a better quality of urban life.

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

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/.

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.

Modeling Groundwater Flow and Contaminant Transport Jacob Bear 2010-01-18 In many parts of the world, groundwater resources are under increasing threat from growing demands, wasteful use, and contamination. To face the challenge, good planning and management practices are needed. A key to the management of groundwater is the ability to model the movement of fluids and contaminants in the subsurface. The purpose of this book is to construct conceptual and mathematical models that can provide the information required for making decisions associated with the management of groundwater resources, and the remediation of contaminated aquifers. The basic approach of this book is to accurately describe the underlying physics of groundwater flow and solute transport in heterogeneous porous media, starting at the microscopic level, and to rigorously derive their mathematical representation at the macroscopic levels. The well-posed, macroscopic mathematical models are formulated for saturated, single phase flow, as well as for unsaturated and multiphase flow, and for the transport of single and multiple chemical species. Numerical models are presented and computer codes are reviewed, as tools for solving the models. The problem of seawater intrusion into coastal aquifers is examined and modeled. The issues of uncertainty in model input data and output are addressed. The book concludes with a chapter on the management of groundwater resources. Although one of the main objectives of this book is to construct mathematical models, the amount of mathematics required is kept minimal.

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.

Applied Contaminant Transport Modeling Chunmiao Zheng 2002-02-05 The challenges facing groundwater scientists and engineers today demand expertise in a wide variety of disciplines–geology, hydraulics, geochemistry, geophysics, and biology. As the number of the subdisciplines has increased and as each has become more complex and quantitative, the problem of integrating their concepts and contributions into a coherent overall interpretation has become progressively more difficult. To an increasing degree transport simulation has emerged as an answer to this problem, and the transport model has become a vehicle for integrating the vast amount of field data from a variety of sources and for understanding the relationship of various physical, chemical, and biological processes. Applied Contaminant Transport Modeling is the first resource designed to provide coverage of the discipline’s basic principles, including the theories behind solute transport in groundwater, common numerical techniques for solving transport equations, and step-by-step guidance on the development and use of field-scale modeling. The Second Edition incorporates recent advances in contaminant transport theory and simulation techniques, adding the following to the original text: -An expanded discussion of the role of aquifer heterogeneity in controlling solute transport -A new section on the dual-domain mass transfer approach as an alternative to the classical advection-dispersion model -Additional chemical processes and reactions in the discussion of reactive

transport -A discussion of the TVD (total-variation-diminishing) approach to transport solution -An entirely new Part III containing two chapters on simulation of flow and transport under variable water density and under variable saturation, respectively, and a third chapter on the use of the simulation-optimization approach in remediation system design Applied Contaminant Transport Modeling, Second Edition remains the premier reference for practicing hydrogeologists, environmental scientists, engineers, and graduate students in the field. In 1998, in recognition of their work on the first edition, the authors were honored with the John Hem Excellence in Science and Engineering Award of the National Ground Water Association

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.

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.

Water-Rock Interaction, Two Volume Set Richard B. Wanty 2004-09-02 The interaction of the lithosphere and hydrosphere sets the boundary conditions for life, as water and the nutrients extracted from rocks are essential to all known life-forms. Water-rock interaction also affects the fate and transport of pollutants, mediates the long-term cycling of fluids and metals in the earth's crust, impacts the migration and

Lattice Boltzmann Modeling of Complex Flows for Engineering Applications Andrea Montessori 2018-02-20 Nature continuously presents a huge number of complex and multi-scale phenomena, which in many cases, involve the presence of one or more fluids flowing, merging and evolving around us. Since its appearance on the surface of Earth, Mankind has tried to exploit and tame fluids for their purposes, probably starting with Hero's machinery to open the doors of the Temple of Serapis in Alexandria to arrive to modern propulsion systems and actuators. Today we know that fluid mechanics lies at the basis of countless scientific and technical applications from the smallest physical scales (nanofluidics, bacterial motility, and diffusive flows in porous media), to the largest (from energy production in

power plants to oceanography and meteorology). It is essential to deepen the understanding of fluid behaviour across scales for the progress of Mankind and for a more sustainable and efficient future. Since the very first years of the Third Millennium, the Lattice Boltzmann Method (LBM) has seen an exponential growth of applications, especially in the fields connected with the simulation of complex and soft matter flows. LBM, in fact, has shown a remarkable versatility in different fields of applications from nanoactive materials, free surface flows, and multiphase and reactive flows to the simulation of the processes inside engines and fluid machinery. LBM is based on an optimized formulation of Boltzmann's Kinetic Equation, which allows for the simulation of fluid particles, or rather quasi-particles, from a mesoscopic point of view thus allowing the inclusion of more fundamental physical interactions in respect to the standard schemes adopted with Navier-Stokes solvers, based on the continuum assumption. In this book, the authors present the most recent advances of the application of the LBM to complex flow phenomena of scientific and technical interest with particular focus on the multi-scale modeling of heterogeneous catalysis within nano-porous media and multiphase, multicomponent flows.

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.

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.

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.

Discontinuous Galerkin Methods Bernardo Cockburn 2012-12-06 A class of finite element methods, the Discontinuous Galerkin Methods (DGM), has been under rapid development recently and has found its use very quickly in such diverse applications as aeroacoustics, semi-conductor device simula tion, turbomachinery, turbulent flows, materials processing, MHD and plasma simulations, and image processing. While there has been a lot of interest from mathematicians, physicists and engineers in DGM, only scattered information is available and there has been no prior effort in organizing and publishing the existing volume of

knowledge on this subject. In May 24-26, 1999 we organized in Newport (Rhode Island, USA), the first international symposium on DGM with equal emphasis on the theory, numerical implementation, and applications. Eighteen invited speakers, lead ers in the field, and thirty-two contributors presented various aspects and addressed open issues on DGM. In this volume we include forty-nine papers presented in the Symposium as well as a survey paper written by the organiz ers. All papers were peer-reviewed. A summary of these papers is included in the survey paper, which also provides a historical perspective of the evolution of DGM and its relation to other numerical methods. We hope this volume will become a major reference in this topic. It is intended for students and researchers who work in theory and application of numerical solution of convection dominated partial differential equations. The papers were written with the assumption that the reader has some knowledge of classical finite elements and finite volume methods.

The Reactive Transport of Suspended Particles Richard Steven Mercier 1985

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.

Reactive Transport Modeling of Cap Rock Integrity During Natural and Engineered CO2 Storage 2004 Long-term cap rock integrity represents the single most important constraint on the long-term isolation performance of natural and engineered CO2 storage sites. CO2 influx that forms natural accumulations and CO2 injection for EOR/sequestration or saline-aquifer disposal both lead to concomitant geochemical alteration and geomechanical deformation of the cap rock, enhancing or degrading its seal integrity depending on the relative effectiveness of these interdependent processes. Using our reactive transport simulator (NUFT), supporting geochemical databases and software (GEMBOCHS, SUPCRT92), and distinct-element geomechanical model (LDEC), we have shown that influx-triggered mineral dissolution/precipitation reactions within typical shale cap rocks continuously reduce microfracture apertures, while pressure and effective-stress evolution first rapidly increase then slowly constrict them. For a given shale composition, the extent of geochemical enhancement is nearly independent of key reservoir properties (permeability and lateral continuity) that distinguish EOR/sequestration and saline-aquifer settings and CO2 influx parameters (rate, focality, and duration) that distinguish engineered disposal sites and natural accumulations, because these characteristics and parameters have negligible (indirect) impact on mineral

dissolution/precipitation rates. In contrast, the extent of geomechanical degradation is highly dependent on these reservoir properties and influx parameters because they effectively dictate magnitude of the pressure perturbation; specifically, initial geomechanical degradation has been shown inversely proportional to reservoir permeability and lateral continuity and proportional to influx rate. Hence, while the extent of geochemical alteration is nearly independent of filling mode, that of geomechanical deformation is significantly more pronounced during engineered injection. This distinction limits the extent to which naturally-occurring CO2 reservoirs and engineered storage sites can be considered analogous. In addition, the pressure increase associated with CO2 accumulation in any compartmentalized system invariably results in net geomechanical aperture widening of cap-rock microfractures. This suggests that ultimate restoration of pre-influx hydrodynamic seal integrity--in both EOR/sequestration and natural accumulation settings--hinges on ultimate geochemical counterbalancing of this geomechanical effect. To explore this hypothesis, we have introduced a new conceptual framework that depicts such counterbalancing as a function of effective diffusion distance and reaction progress. This framework reveals that ultimate counterbalancing of geochemical and geomechanical effects is feasible, which suggests that shale cap rocks may in fact evolve into effective seals in both natural and engineered storage sites.

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.

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.

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).