



Description and verification of a novel flow and transport model for silicate-gel emplacement



Marc Walther^{a,*}, Utku Solpuker^b, Norbert Böttcher^c, Olaf Kolditz^{c,d},
Rudolf Liedl^a, Frank W. Schwartz^b

^a Technische Universität Dresden, Institute for Groundwater Management, D-01062 Dresden, Germany

^b School of Earth Sciences, The Ohio State University, Columbus, OH 43210, USA

^c Helmholtz-Centre for Environmental Research – UFZ, Department of Environmental Informatics, Permoserstr. 15, D-04318 Leipzig, Germany

^d Technische Universität Dresden, Applied Environmental System Analysis, D-01062 Dresden, Germany

ARTICLE INFO

Article history:

Received 30 March 2013

Received in revised form 11 October 2013

Accepted 22 October 2013

Available online 8 November 2013

Keywords:

Gelation

Viscosity change

Density-dependent

Numerical modeling

Laboratory experiment

OpenGeoSys

ABSTRACT

We present a novel approach for the numerical simulation of the gelation of silicate solutions under density-dependent flow conditions. The method utilizes an auxiliary, not density-dependent solute that is subject to a linear decay function to provide temporal information that is used to describe the viscosity change of the fluid. By comparing the modeling results to experimental data, we are able to simulate the behavior and the gelation process of the injected solute for three different compositions, including long-term stability of the gelled area, and non-gelation of low concentrations due to hydro-dynamic dispersion. This approach can also be used for other types of solutes with this gelling property and is useful in a variety of applications in geological, civil and environmental engineering.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

Mathematical models continue to play an enormously important role in the study of problems of groundwater contamination and remediation. In theoretical applications, they have contributed to a deep understanding of the key flow and mass transport processes, the interactions of those processes, and the key parameters controlling them. In practice, hydrogeologists are able to model the physical, chemical and biological processes leading to the development of plumes of dissolved contaminants and to estimate their future patterns of spreading. In problems of remediating contaminated groundwater, flow and transport codes are now routinely used in selecting the best and most cost-efficient remedy and in designing the actual remedial systems.

Over the past 40 years, since the first simple flow and transport codes were developed, the pace of progress has been impressive. Early codes capable of simulating coupled flow and physical transport with simple reactions have given way to more powerful simulation models able to accommodate variable density flow, e.g., FEFLOW (Diersch, 1981), SUTRA (Voss, 1984), MITSU3D (Ibaraki, 1998), TOUGH (Oldenburg and Pruess, 1995), ROCKFLOW (Kolditz et al., 1998), HydroGeoSphere (Graf and Therrien, 2005), GeoSys (Beinhorn et al., 2005), and D3F (Grillo et al., 2010). More recently, codes like TOUGHREACT (Xu et al., 1999), MIN3P (Mayer et al., 2001), PHT3D (Prommer et al., 2002), HYTEC (van der Lee et al., 2003), RetrasoCodeBright (Saaltink et al., 2005), OGS (Xie et al., 2006), CrunchFlow (Steeffel, 2009), and UG (Musuuza et al., 2011) have provided capabilities to incorporate homogeneous and heterogeneous reactions within an equilibrium or kinetic framework.

Evolution in the complexity of models to a significant extent has been informed by the needs of practice in terms

* Corresponding author.

E-mail address: marc.walther@tu-dresden.de (M. Walther).

of addressing types of dissolved contaminants, and processes affecting them. In this paper, we describe a new modeling approach that originates from a need in remediation problems to consider a miscible treatment fluid with a capability of evolving to a gel. More specifically, an aqueous solution with an ordinary viscosity can experience at least a four order-of-magnitude increase in viscosity as gelation occurs.

This modeling study is part of a larger study aimed at using oxidants (e.g., KMnO_4) in remediating large, deep and dilute plumes of chlorinated solvents. The efficacy of slow release systems in passively degrading contaminants in situ has already been well established. For example, slow-release solids have been developed by mixing potassium permanganate with other matrix materials such as clay-rich slurries (Siegrist et al., 1999) or oxidation resistant waxy polymers (Lee and Schwartz, 2007; Lee et al., 2009; Ross et al., 2005). These materials can either be injected as a slurry into horizontal hydraulically-created fractures, into vertical trenches and boreholes (Murdoch et al., 1997), or installed in vertical boreholes as solid cylinder-shaped slow-release solids (Lee and Schwartz, 2007). Such slow-release systems also have constraints on their lifetime, installation depths and spacings (Lee et al., 2008).

Our basic approach is to overcome these constraints through the use of dense fluids and slow-release gels to deliver remediation chemicals to deeper plumes and less permeable units. This approach takes advantage of the unique flow and mixing properties of dense fluids, and the potential of engineered gels as a diffusion-controlled mechanism for releasing the treatment chemical. The essence of this new remediation approach is all about increasing the residence time of oxidants close to the site where they are injected, which will be determined by characteristics of the actual contaminated site.

Previously, we performed flow-tank experiments to explore the behavior of dense viscous solutions in fresh water, which provided some understanding of processes involved and the experimental data needed for validating a modeling approach (Solpuker et al., 2012). The goals of this paper here are to describe and demonstrate an approach for modeling this variable density flow/gelation problem. It also presents illustrative data from three flow-tank experiments to verify the modeling approach.

2. Validation experiments

A series of flow tank experiments was undertaken in order to help validate the new simulation concept. In order to diminish data uncertainty, these experiments were designed to be as simple as possible with a (nearly) homogeneous and isotropic medium. Convective dispersion is helpful in mixing the dense fluids.

2.1. Materials and experimental setup

Silicate solutions are widely used as chemical grouts and considered to be environmentally safe, economic and stable inorganic solutions (PQ Corp., 2012). Dilute silicate solutions are relatively dense with added benefits of a relatively low initial viscosity ($\sim 2 \cdot 10^{-3}$ Pa s) and the potential for gelling after a predetermined time period (PQ Corp., 2012).

When dilute silicate solutions are acidified, silicate anions polymerize to form an amorphous, porous gel, which is a coherent, rigid, three-dimensional network of contiguous particles of colloidal silica (Blankenship, 2002). Temperature, pH, total silica concentration and type of setting agent can affect the degree and timing of polymerization (Karol, 2003; PQ Corp., 2012).

We conducted three experiments with a small flow tank to observe the transport and gelation of three different solutions in a saturated homogeneous porous medium. To produce solutions for injection we used N-Clear sodium silicate solution (PQ Corp., 2012). The quantity of dissolved silica was 28.7 wt.% with a silica to alkali weight ratio of 3.22. The initial density and viscosity of the stock solution were 1380 kg m^{-3} and $\sim 1.8 \cdot 10^{-1}$ Pa s, respectively. The solution was then diluted with deionized water to 30% by weight with diluted sodium bicarbonate solution as the setting agent. A concentrated bicarbonate stock solution (8 g NaHCO_3 /100 mL H_2O) was diluted with deionized water to 65%, 60%, and 55% by weight. Diluted bicarbonate solutions were mixed with diluted silicate solutions with mixing proportions 50% and 50% by weight, respectively. The first, second, and third gelling solutions incorporated 65%, 60%, and 55% bicarbonate solutions, respectively, to control gelation rates in the three injection experiments (experiments 1, 2, and 3). Dense solutions were colored with 300 mg L^{-1} Rhodamine WT to facilitate visual observation of the time-delayed gelling. Density and viscosity of these three solutions were determined using a hydrometer and a u-tube calibrated Ubbelohde glass viscometer following ASTM D445-12 (2006) and ASTM D446-12 (2008) (see Tables 1 and 2).

Fluid movement in the flow tank was monitored using a digital high definition video camera recorder (Sony HDR-SR8). The processing of individual scenes involved converting information on light intensity to optical density because optical density is proportional to the concentration of the dye. The optical density was calibrated using a gray scale visible at all times during the experiments. The gray scale has 20 bars with 0.1 optical density increments ranging from 0.0 optical density (white) to 1.9 optical density (black).

The small glass flow tank is 0.45 m high, 0.97 m long and 0.17 m wide. Between the inflow and outflow chambers (0.13 m wide each) is a flow chamber filled with uniform, spherical glass beads (Potters Industries, NJ) with hydraulic conductivities ranging from $3 \cdot 10^{-3} \text{ m s}^{-1}$ (Schincariol and

Table 1
Parameters in the simulations.

Parameter	Value
Hydraulic conductivity K (m s^{-1}) ^a	$1.5 \cdot 10^{-3}$ ($\pm 15\%$)
Porosity ϕ (–) ^b	0.20
Fresh water density ρ_0 (kg m^{-3}) ^b	998.2
Fresh water viscosity μ_0 (Pa s) ^b	$1 \cdot 10^{-3}$
Viscosity coefficient α (–) ^b	0.9
Molecular diffusion coefficient D_m ($\text{m}^2 \text{s}^{-1}$) ^a	$1 \cdot 10^{-9}$
Longitudinal dispersivity α_l (m) ^a	$1.5 \cdot 10^{-3}$
Transversal dispersivity α_t (m) ^a	$1.5 \cdot 10^{-4}$
Injection time t_{inj} (s) ^b	60
Injection flow rate q ($\text{m}^2 \text{s}^{-1}$) ^b	$1.5 \cdot 10^{-5}$

^a Determined through model calibration.

^b Acquired through experimental measurement.

Download English Version:

<https://daneshyari.com/en/article/4546612>

Download Persian Version:

<https://daneshyari.com/article/4546612>

[Daneshyari.com](https://daneshyari.com)