ANALYTICAL AND NUMERICAL MODELLING OF COLLOIDAL SILICA TRANSPORT THROUGH SATURATED GRANULAR SOILS

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ABSTRACT

Following injection of colloidal silica (CS) solutions in saturated granular soil, the viscosity of the solution increases until gelation is achieved. Depending on the application, this grout can improve the mechanical properties of the soil (e.g. enhanced resistance to liquefaction) or act as a barrier for contaminant containment. The time-dependent permeation potential of the CS solution was experimentally investigated by conducting one-dimensional tests in vertical soil columns, where the CS solution flowed upwardly displacing water. The experimental results were then compared to analytical and numerical solutions. The analytical approach for representing flow of the CS solution is based on the generalized form of Darcy's law for varying density, properly modified in order to account for varying viscosity as well. In addition, we used the one-dimensional advection-dispersion equation to investigate the adequacy of the assumption that advection and dispersion control CS transport. Finally, the gelation module of the TOUGH2 numerical code was used to model the vertical upward permeation of CS solutions.

The comparisons of observed and analytical values revealed that the existing analytical solution, as modified herein for varying viscosity, can describe satisfactorily the pattern of decreasing flow rates of the CS solution within the soil column. In contrast, the advection-dispersion equation failed to adequately predict CS transport. Although the dispersive component of CS transport was in agreement with the observations, the use of mean seepage velocities over-predicted the arrival time of the CS front. In the numerical simulations, we implicitly modelled the gelation process by: (a) successfully fitting an exponential curve to measurements of the viscosity of the CS solution, which increased with time, and (b) employing a simple linear mixing rule to calculate the viscosity of the liquid phase, i.e. the mixture of water-CS solution. The numerical approximations reproduced the arrival of the CS front with adequate accuracy. The effect of numerical dispersion (i.e. the spreading of the solute due to the discretization of the numerical scheme) was also investigated: despite the application of finer spatial and time discretization schemes, numerical dispersion remained greater than its experimental counterpart. More specifically, the numerically calculated zone of dispersion was two times broader than the observed one. For the application of interest, this is a conservative result, considering that CS concentrations near the target (i.e. close to the injected concentrations) are predicted to arrive later compared to the observations. Hence, the results overall corroborate the numerical modelling approach and offer the confidence required before advancing to modelling two-dimensional problems of colloidal silica permeation.

Keywords: Grouting, Modelling, Transport, Colloidal silica, Gel barrier, TOUGH2

1. Introduction

Colloidal silica (CS), as a non-toxic and inert gelling liquid, can be used safely as grouting material. Depending on the application, in-situ gelation of CS can improve the mechanical properties of the soil (e.g. mitigating liquefaction risk) or act as an impermeable barrier and reduce the potential for spreading of contaminants. Controlled injection of the CS solution relies on the permeation potential of colloidal silica. Herein, the permeation potential has been investigated experimentally by conducting one-dimensional permeation tests in columns of saturated granular soil. These tests were performed in columns with different heights and using different CS solutions and hydraulic gradients.

The main objective of this study is to model one-dimensional CS flow and transport in saturated granular soils. To this end, we investigated whether observed CS flow rates and concentrations can be reproduced by (a) simple analytical relationships, and (b) a suitable module of the TOUGH2 numerical code (Pruess 1991). Gallagher and Lin (2009) performed permeation tests under similar laboratory conditions and with comparable hydraulic gradients. They reported that advection and the increasing viscosity of CS grout were the dominant factors controlling CS transport. Consequently, in addition to modelling CS flow (i.e. advection), we aimed to implicitly model the gelation process of CS grouts. Apart from the advective component of transport, we also investigated the significance of the dispersive component, whether hydrodynamic (in the analytical approach) or numerical (in the numerical approach). This work is an effort to confirm the aforementioned distinctive modelling approaches with observed data and is a prerequisite before progressing to the modelling of two-dimensional CS permeation problems.

2. Column tests

The goal of the experiments was to observe the one-dimensional vertical upward permeation of CS solutions (the percentage per weight of CS in the solution is 10%). To this end, five tests were performed in columns filled with fully saturated sand. Table 1 gives the characteristics of these tests.

Table 1: Characteristics of the one-dimensional column tests

Property	Test 1	Test 2	Test 3	Test 4	Test 5
Column height, m	0.20	0.20	0.40	1.00	0.20
Porosity	0.38	0.38	0.38	0.39	0.38
Hydraulic conductivity, m/s	2.84×10^{-4}	3.17×10^{-4}	3.40×10^{-4}	3.10×10^{-4}	2.84×10^{-4}
CS solution pH	5.53	5.48	7.00	5.50	10.00
Ionic strength, N	0.10	0.10	0.10	0.10	0.00
Initial hydraulic gradient, i	0.05	0.05	0.05	0.25	0.05

The flow rate was measured in each test. The time-dependent viscosities of CS solutions were measured independently. The location of the CS solution front was tracked visually, as the CS solution was colored with blue food dye. Furthermore, pore water samples were extracted at time intervals from sampling ports, which were located every 10 cm along the column starting from an elevation of 5 cm from the bottom. From these samples, the evolution of CS concentration was specified at each sampling port and, consequently, the corresponding experimental breakthrough curves were estimated. Test duration ranged from three to eight hours. At the end of the tests, the viscosity of the injected CS solution was about 6×10^{-3} Pa s, apart from Test 5, during which CS viscosity remained equal to its initial value (1.47×10^{-3} Pa s).

3. Modelling colloidal silica flow and transport

As the CS solution is delivered in the soil column from the inlet, it moves upwards displacing water. The injection of a CS solution into a saturated porous medium constitutes a flow problem under viscosity and density varying conditions. As shown schematically in Figure 1, at time t, the CS solution occupies a region of the soil column with height equal to L_g. In this region, pore space is filled with the CS solution, which is heavier (CS solution density, ρ_g, is approximately equal to 1050 kg/m^3) and more viscous than water (CS solution viscosity, μ_g, is greater than 1.3×10^{-3} Pa s at the beginning of each test and increases with time).

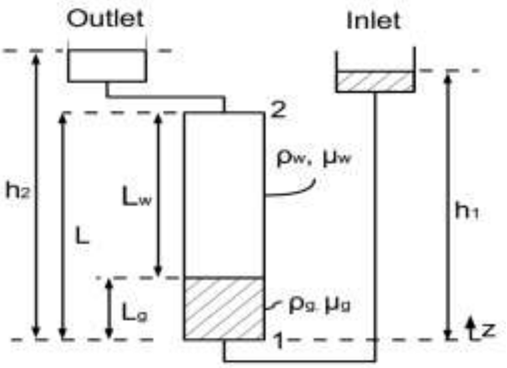

Figure 1: Schematic representation of the one-dimensional permeation tests

3.1. Analytical modelling of CS flow

For the assessment of variable-density flow, Post *et al.* (2007) suggest the application of the more general form of Darcy's law for fluid flow in a porous medium with an average fluid density, ρ_α and liquid phase viscosity μ:

$$Q_{calc}=\frac{k\rho_w g}{\mu}\left[\left(\frac{\rho_g}{\rho_w}\right)h_1-h_2-\left(\frac{\rho_\alpha}{\rho_w}-1\right)L\right]\frac{A}{L} \tag{1}$$

where k is intrinsic permeability (m^2), ρ_w is fresh water density (kg/m^3), L is the column height (m), A is the cross-sectional area perpendicular to the flow direction (m^2) and h_1 and h_2 are the measured hydraulic heads (m) corresponding to the bottom and the top of the column, respectively.

Based on the liquid phase occupying its pore space, the soil column is divided in two distinctive regions: (a) a region with height L_g and liquid phase density ρ_g occupied by the CS grout, and (b) a region with height L_w and liquid phase density ρ_w occupied by water. As a result, the average fluid density along the column is equal to:

$$\rho_\alpha=\frac{1}{(z_1-z_2)}\int_{z_1}^{z_2}\rho(z)dz=\frac{(\rho_g L_g+\rho_w L_w)}{L} \tag{2}$$

where z_1 and z_2 are the elevations (m) of the bottom and the top of the soil column, respectively. If we substitute Equation (2) in Equation (1), the flow rate can be estimated by the following analytical equation:

$$Q_{calc}=\frac{k\rho_w g}{\mu}\left\{\left[\left(\frac{\rho_g}{\rho_w}\right)h_1-h_2\right]-\left[\left(\frac{\rho_g}{\rho_w}\right)-1\right]L_g\right\}\frac{A}{L} \tag{3}$$

However, in the case of CS flow, the spatial variation of viscosity cannot be neglected. To this end, the calculation of an average viscosity term, μ_α, is recommended:

$$\mu_\alpha=\frac{1}{(z_1-z_2)}\int_{z_1}^{z_2}\mu(z)dz=\frac{(\mu_g L_g+\mu_w L_w)}{L} \tag{4}$$

where μ_w is fresh water viscosity (Pa s). Equation (3) can now be modified to the following expression:

$$Q_{calc}=\frac{k\rho_w g}{[\mu_g L_g+\mu_w(L-L_g)]}\left\{\left[\left(\frac{\rho_g}{\rho_w}\right)h_1-h_2\right]-\left[\left(\frac{\rho_g}{\rho_w}\right)-1\right]L_g\right\}A\,. \tag{5}$$

3.2. Analytical modelling of CS transport

Assuming that the CS solution is a miscible aqueous solution, we modelled CS transport using the Ogata and Banks (1961) solution for the one-dimensional advection-dispersion equation, with a constant CS concentration of C_o equal to 10% per weight at the source (i.e. the inlet):

$$\frac{C_{gel}}{C_o}=\frac{1}{2}\left[erfc\left(\frac{z-u_s t}{2\sqrt{Dt}}\right)+\exp\left(\frac{u_s z}{D}\right)erfc\left(\frac{z+u_s t}{2\sqrt{Dt}}\right)\right] \qquad (6)$$

where C_{gel} is CS concentration, z is the elevation from the bottom of the column, u_s is the seepage velocity and D is the hydrodynamic dispersion coefficient. The hydrodynamic dispersion coefficient is expressed as:

$$D=D_L=\alpha_L u_s \qquad (7)$$

where D_L is the longitudinal dispersion coefficient and α_L is the longitudinal dispersivity, taken equal to 0.042 cm (Saiers *et al.*, 1994). Diffusion was neglected. Finally, u_s was taken as the mean value of the seepage velocities calculated by the measured flow rates during each test. Thus, we implicitly accounted for density and viscosity variations in the analytical solution of CS transport.

3.3. Numerical modelling of CS flow

The numerical approach followed herein considers that advection and the gelation of the CS solution are the key mechanisms dominating transport. The flow of CS grout was simulated as a miscible gel displacement problem using the gelation module (Finsterle *et al.*, 1994) of the TOUGH2 numerical code. Two major assumptions are made: (a) the grout is treated as a miscible aqueous solution and (b) the chemical process of gelation is not explicitly modelled.

The gelation process is implicitly described by a gel-time curve and a mixing rule. More specifically, the viscosity of pure grout was simulated as a function of time by an exponential gel-time curve:

$$\mu_g=\alpha_1+\alpha_2\exp(\alpha_3 t) \qquad (8)$$

where α_1, α_2 and α_3 are fitting parameters. In addition, liquid phase viscosity was estimated as a function of grout concentration by two candidate mixing rules (Finsterle *et al.*, 1994). First, a power-law rule was implemented:

$$\mu=\left(\frac{X_{gel}}{\mu_g^{0.25}}+\frac{1-X_{gel}}{\mu_w^{0.25}}\right)^{-1/0.25} \qquad (9)$$

where X_{gel} is the mass fraction of CS in the liquid phase. Then, the following simpler linear mixing rule was evaluated also:

$$\mu=X_{gel}\mu_g+(1-X_{gel})\mu_w \qquad (10)$$

4. Results

4.1. Analytical modelling of CS flow

As shown in Figure 2, the analytical solution reproduced satisfactorily the pattern of flow rate reduction over time due to gravity and viscosity. The discrepancy between experimental and analytical values may be attributed to the difficulty in accurately locating the CS front (i.e. L_g) by visual observation and to the uncertainty accompanying the independently measured CS viscosity values. During Test 5, when CS gelation was inhibited and, hence, CS viscosity remained constant over time, the analytical solution reproduced accurately the observed flow rates.

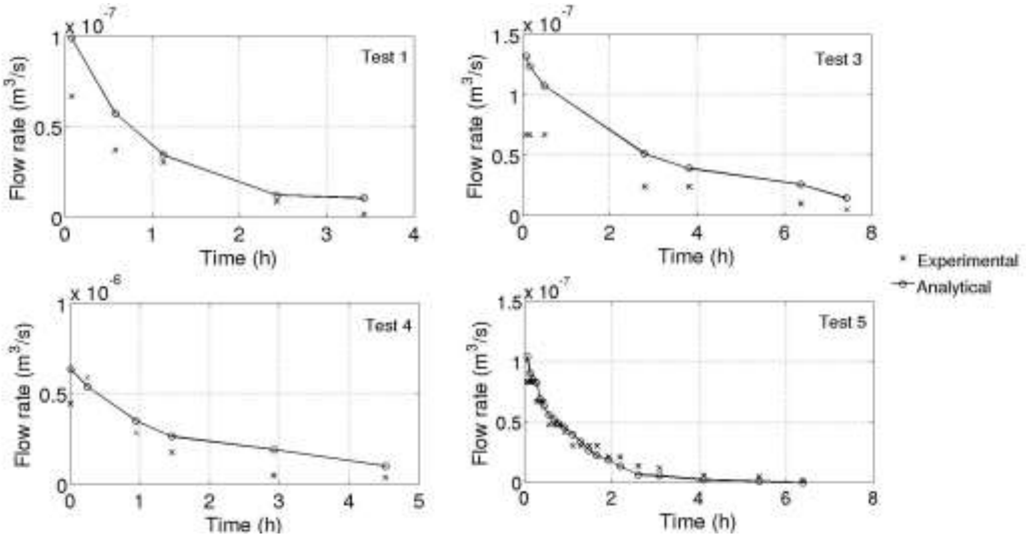

Figure 2: Observed and analytically calculated flow rates for Tests 1, 3, 4 and 5.

4.2. Analytical modelling of CS transport

The one-dimensional advection-dispersion equation failed to reproduce the observed CS breakthrough curves, as the advective arrival time was overestimated in all simulated tests (Figure 3). Nevertheless, the resulting dispersive component of transport was in agreement with the observations. Gallagher and Lin (2009) achieved a closer fit to their experimental breakthrough curves by also employing the one-dimensional advection-dispersion equation with a mean uniform seepage velocity. However, in their experimental results, CS viscosity remained relatively low (μ_g was doubled by the end of the test) and the observed seepage velocities demonstrated a smooth reduction over time. Therefore, the mean seepage velocity employed in Equation 6 deviated less from the observed minimum and maximum velocity values. The comparison between observations and analytical results indicates that the complexity of CS transport under density and viscosity varying conditions cannot be successfully simulated by employing a mean seepage velocity value.

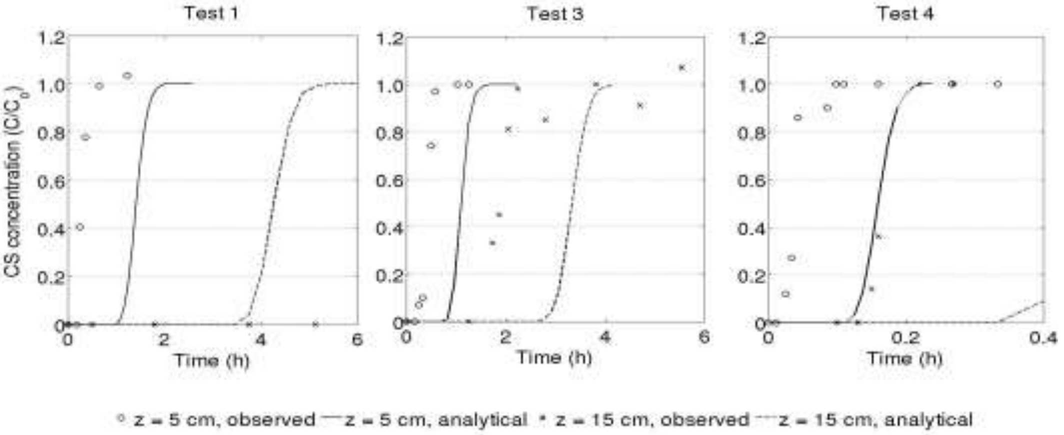

Figure 3: Observed CS concentrations and analytically calculated breakthrough curves at the two sampling ports (z = 5 cm and z = 15 cm) for Tests 1, 3 and 4.

4.3. Numerical modelling of CS flow

For the modelling of the gelation process, we had to define distinctive gel-time curves for each test by fitting Equation (8) to the independently observed CS viscosity values. The exponential gel-time curve was sufficiently fitted to the experimental values (the coefficient of determination, R^2, was at least equal to 0.60) and the parameters α_1, α_2 and α_3 were inversely estimated with reasonable accuracy. Regarding the mixing rule, for the range of measured viscosity values (from 1.3×10^{-3} Pa s to about 6×10^{-3} Pa s) both mixing rules were equivalent. Therefore, we used the simple linear equation described by Equation (10).

The gel-time curve and the mixing rule control implicitly the gelation process. Therefore, after specifying these expressions and the boundary conditions, we could model CS flow with the TOUGH2 numerical code. The comparisons between experimental data and numerical approximations demonstrated that the numerical approach simulated CS flow with adequate accuracy (Figure 4). The decrease of flow rates due to gravity and viscosity effects was successfully reproduced.

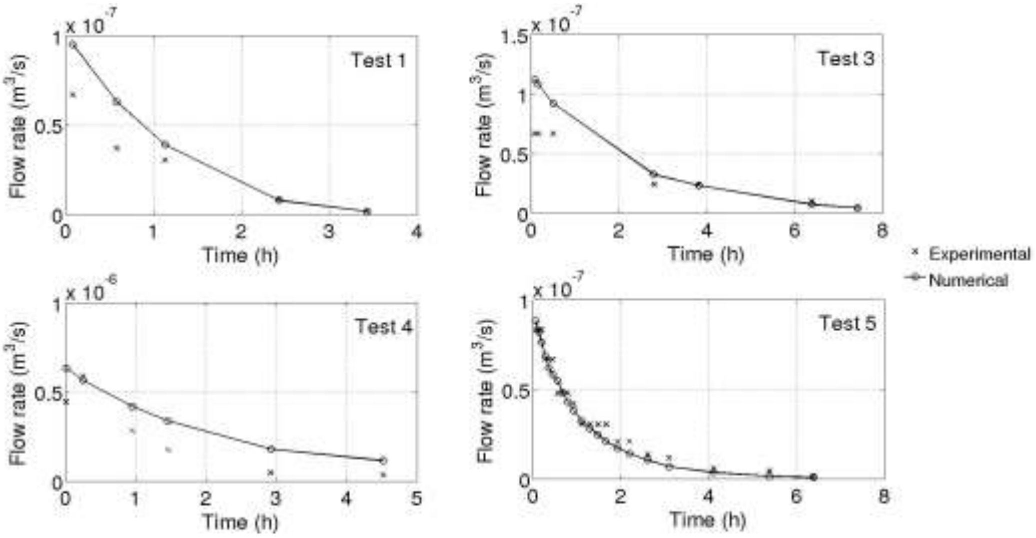

Figure 4: Observed and numerically calculated flow rates for Tests 1, 3, 4 and 5.

Due to discretization errors, numerical solutions are accompanied by an artificial dispersion term called numerical dispersion. In order to mitigate numerical dispersion, we employed small time and space steps (dt = 0.05 s, dx = 0.25 cm) in our simulations. In Figure 5, normalized CS concentrations are plotted versus the sampling point distance from the CS front. Regarding the numerical approximations, the CS front is defined as the location where CS concentration is half the concentration of the source solution, i.e. $0.5C_o$.

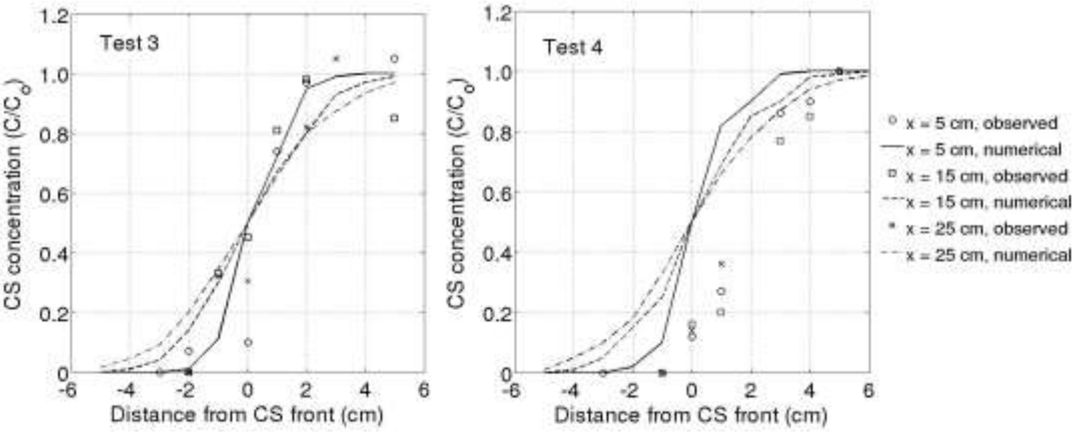

Figure 5: Observed and numerically calculated CS concentrations before and after the CS front for Tests 3 and 4.

As shown in Figure 5, the discretization scheme employed herein resulted in a dispersive component of transport greater than the observed. The observed zone of dispersion (i.e. the zone along which CS concentration varies from zero to C_o) was approximately equal to 4 cm, while the numerically calculated zone of dispersion was twice as large. Nevertheless, due to the issue of numerical dispersion we err on the side of caution for CS concentrations greater than $0.5C_o$: simulated concentrations are expected to arrive later than their experimental counterparts. Further, reduction of time or spatial steps resulted in significantly greater computational burden without any obvious reduction of numerical dispersion.

5. Conclusions

Comparisons between laboratory observations and the two modelling approaches for one-dimensional CS transport through saturated sand lead to the following conclusions:

1. The CS flow rate may be satisfactorily simulated by a simple analytical equation based on the generalized Darcy's law after appropriate adjustments for the variations in viscosity and density.
2. Analytical solutions of the one-dimensional advection-dispersion equation give poor estimates of the CS transport for sizable reductions of seepage velocity.
3. The gelation module of the TOUGH2 numerical code was capable of reproducing the decreasing trend in flow rates attributed to gravitational and viscosity effects.
4. The numerical solution of flow is accompanied by numerical dispersion greater than the experimentally observed hydrodynamic dispersion, despite the application of fine time and spatial discretization.
5. The comparison between laboratory data and numerical results provides confidence to proceed with modelling of two-dimensional problems and developing design tools for field applications of CS injection.

ACKNOWLEDGEMENTS

The advice for running TOUGH2 provided by Dr Stefan Finsterle is gratefully acknowledged. This research has been co-financed by the European Union (European Social Fund, SF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) – Research Funding Program: Thales, investing in knowledge society through the European Social Fund.

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