

*Water Resources Research*

Supporting Information for

**Nernst-Planck based description of transport, Coulombic interactions and geochemical reactions in porous media: Modeling approach and benchmark experiments**

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**Introduction**

This document provides a summary of the experimental datasets produced in this and previous studies, and used to benchmark the Nernst-Planck based approach presented in this work. The reported concentration and pH values are the average of duplicate measurements performed at the outlet of the 2-D and 3-D flow-through setups.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sampling Location**  ***z* [cm]** | **Scenario 1:** | | | **Scenario 2:** | | |
| **Mg2+ Concentration**  **[mol/L]** | **Cl- Concentration**  **[mol/L]** | **pH** | **Mg2+ Concentration**  **[mol/L]** | **Cl- Concentration**  **[mol/L]** | **pH** |
| 0.5 | 1.48E-04 | 4.32E-04 | 3.81 | 1.13E-02 | 2.29E-02 | 4.18 |
| 1.0 | 1.45E-04 | 4.17E-04 | 3.85 | 1.16E-02 | 2.28E-02 | 4.23 |
| 1.5 | 1.40E-04 | 4.14E-04 | 3.91 | 1.10E-02 | 2.22E-02 | 4.30 |
| 2.0 | 1.31E-04 | 3.80E-04 | 3.94 | 1.02E-02 | 2.06E-02 | 4.40 |
| 2.5 | 1.22E-04 | 3.58E-04 | 3.97 | 9.76E-03 | 1.90E-02 | 4.34 |
| 3.0 | 1.10E-04 | 3.22E-04 | 3.91 | 8.43E-03 | 1.68E-02 | 4.34 |
| 3.5 | 9.34E-05 | 2.83E-04 | 3.98 | 7.73E-03 | 1.49E-02 | 4.44 |
| 4.0 | 7.25E-05 | 2.35E-04 | 4.08 | 6.21E-03 | 1.21E-02 | 4.49 |
| 4.5 | 5.36E-05 | 1.88E-04 | 4.12 | 5.06E-03 | 9.08E-03 | 4.59 |
| 5.0 | 3.65E-05 | 1.46E-04 | 4.22 | 3.49E-03 | 6.37E-03 | 4.59 |
| 5.5 | 2.14E-05 | 1.04E-04 | 4.26 | 2.58E-03 | 4.37E-03 | 4.63 |
| 6.0 | 1.03E-05 | 7.16E-05 | 4.38 | 1.76E-03 | 2.78E-03 | 4.74 |
| 6.5 | 2.63E-06 | 4.54E-05 | 4.48 | 1.12E-03 | 1.67E-03 | 4.71 |
| 7.0 | 0 | 2.44E-05 | 4.68 | 6.23E-04 | 1.01E-03 | 4.72 |
| 7.5 | 0 | 1.09E-05 | 4.79 | 2.35E-04 | 5.15E-04 | 4.78 |
| 8.0 | 0 | 1.69E-06 | 5.01 | 6.63E-05 | 3.10E-04 | 4.91 |
| 8.5 | 0 | 0 | 5.23 | 0 | 1.54E-04 | 4.90 |
| 9.0 | 0 | 0 | 5.56 | 0 | 1.17E-04 | 4.96 |
| 9.5 | 0 | 0 | 5.85 | 0 | 7.99E-05 | 5.14 |
| 10.0 | 0 | 0 | 6.14 | 0 | 7.06E-05 | 5.37 |
| 10.5 | 0 | 0 | 6.18 | 0 | 6.77E-05 | 5.89 |
| 11.0 | 0 | 0 | 6.34 | 0 | 4.37E-05 | 6.00 |
| 11.5 | 0 | 0 | 6.45 | 0 | 0 | 6.09 |
|  | | | |  |  |  |
| Injected solution | 1.45E-4 | 4.55E-4 | 3.78 | 1.20E-2 | 2.41E-2 | 4.10 |

Table S1. Experimental data for the propagation of pH fronts during multicomponent ionic transport in a 2-D homogeneous domain under different solution compositions. Concentration and pH measurements were performed at the outlet of the flow-through setup [*Muniruzzaman and Rolle*, 2015]. These concentration and pH values are used in the benchmark of Figure 5.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sampling Location**  **z [cm]** | **Transport of NaCl in pure water** | | **Transport of MgCl2 in a buffer electrolyte (NaBr) solution** | |
| **Normalized Na+ Concentration (C/Cin)**  **[-]** | **Normalized Cl- Concentration (C/Cin)**  **[-]** | **Normalized Mg2+ Concentration (C/Cin)**  **[-]** | **Normalized Cl- Concentration (C/Cin)**  **[-]** |
| 0.5 | 0.001 | 0.002 | 0.004 | 0.004 |
| 1.0 | 0.000 | 0.005 | 0.005 | 0.007 |
| 1.5 | 0.007 | 0.009 | 0.009 | 0.015 |
| 2.0 | 0.015 | 0.022 | 0.021 | 0.029 |
| 2.5 | 0.041 | 0.044 | 0.041 | 0.049 |
| 3.0 | 0.058 | 0.064 | 0.060 | 0.070 |
| 3.5 | 0.081 | 0.083 | 0.081 | 0.088 |
| 4.0 | 0.101 | 0.105 | 0.106 | 0.114 |
| 4.5 | 0.138 | 0.136 | 0.146 | 0.151 |
| 5.0 | 0.179 | 0.175 | 0.204 | 0.182 |
| 5.5 | 0.210 | 0.208 | 0.245 | 0.209 |
| 6.0 | 0.217 | 0.215 | 0.247 | 0.216 |
| 6.5 | 0.204 | 0.202 | 0.220 | 0.198 |
| 7.0 | 0.182 | 0.184 | 0.194 | 0.176 |
| 7.5 | 0.151 | 0.148 | 0.165 | 0.159 |
| 8.0 | 0.129 | 0.127 | 0.138 | 0.136 |
| 8.5 | 0.108 | 0.106 | 0.104 | 0.109 |
| 9.0 | 0.084 | 0.083 | 0.077 | 0.082 |
| 9.5 | 0.050 | 0.050 | 0.039 | 0.046 |
| 10.0 | 0.028 | 0.028 | 0.017 | 0.026 |
| 10.5 | 0.010 | 0.011 | 0.007 | 0.014 |
| 11.0 | 0.005 | 0.004 | 0.008 | 0.009 |
| 11.5 | 0.007 | 0.003 | 0.010 | 0.005 |
| 12.0 | 0.005 | 0.000 | 0.012 | 0.004 |

Table S2. Experimental data for the transport of electrolytes in a 2-D heterogeneous flow-through domain, where ionic concentration measurements were performed at the outlet of the flow-through setup [*Muniruzzaman et al*., 2014]. Concentration values are normalized by the inflow boundary and these values are used in the benchmark of Figure 7.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Horizontal Cross-section** | | | **Vertical Cross-section** | | |
| **y [m]** | **Normalized Mg2+ Concentration (C/Cin)**  **[-]** | **Normalized Cl- Concentration (C/Cin)**  **[-]** | **z [m]** | **Normalized Mg2+ Concentration (C/Cin)**  **[-]** | **Normalized Cl- Concentration (C/Cin)**  **[-]** |
| **Transport of MgCl2 in Pure Water** | | | | | |
| 0.010 | 0.022 | 0.020 | 0.013 | 0.010 | 0.048 |
| 0.021 | 0.073 | 0.087 | 0.024 | 0.116 | 0.138 |
| 0.032 | 0.208 | 0.208 | 0.035 | 0.209 | 0.208 |
| 0.043 | 0.223 | 0.216 | 0.046 | 0.208 | 0.147 |
| 0.054 | 0.086 | 0.111 | 0.057 | 0.085 | 0.045 |
| 0.065 | 0.031 | 0.038 | 0.068 | 0.013 | 0.015 |
| 0.076 | 0.012 | 0.014 | 0.079 | 0.010 | 0.000 |
| **Transport of MgCl2 in a Background Electrolyte (NaBr) Solution** | | | | | |
| 0.010 | 0.032 | 0.027 | 0.017 | 0.010 | 0.086 |
| 0.021 | 0.123 | 0.086 | 0.028 | 0.280 | 0.161 |
| 0.032 | 0.269 | 0.151 | 0.039 | 0.321 | 0.184 |
| 0.043 | 0.321 | 0.161 | 0.050 | 0.170 | 0.113 |
| 0.054 | 0.157 | 0.098 | 0.061 | 0.051 | 0.045 |
| 0.065 | 0.041 | 0.028 | 0.072 | 0.021 | 0.025 |
| 0.076 | 0.016 | 0.014 | 0.083 | 0.000 | 0.000 |

Table S3. Experimental data for the transport of electrolytes in a 3-D homogeneous flow-through setup. Measurements of different ions’ concentrations were performed at the outlet of the flow-through chamber. These concentration values are used in Figure 9.