Appendix K: Supporting information for Chapter **5**

## K.1 Effective ionic mobility

Table K.1 ionic mobility and effective ionic mobility values used in effective resistivity calculations and electron balance model

|  |  |  |  |
| --- | --- | --- | --- |
| **Major ion** | **Ionic mobility, ui**  **m2 s-1 V-1** | **Effective ionic mobility, ui\***  **m2 s-1 V-1** | |
| **High-K** | **Low-K** |
| Nitrate | 7.4x10-8 | 1.3 x10-8 | 7.5 x10-9 |
| Chloride | 7.9 x10-8 | 1.3 x10-8 | 7.3 x10-9 |
| Sulphate | 8.3 x10-8 | 1.4 x10-8 | 7.6 x10-9 |
| Sodium | 5.2 x10-8 | 8.6 x10-9 | 4.8 x10-9 |
| Potassium | 7.6 x10-8 | 1.3 x10-8 | 7.0 x10-9 |

## K.2 Ion balance

These values were calculated by multiplying the molar mass for both anions and cations and dividing the difference between them by the total sum. Positive values indicate a greater abundance of cations whereas negative values indicate an abundance of anions. Values are averages of ion balances for individual experiments across all eight time points. Samples include ion mass within the electrode chambers.

Figure K.1 Ion balance for homogenous and heterogeneous experiments.

## K.3 Mass flux per sampling event

Table K.2. Mass flux associated with sampling pore fluid from control experiments where no EK is applied (C-HOM\_3 and C-HET\_1) compared to mass flux by EK and pore fluid sampling.

|  |  |  |  |
| --- | --- | --- | --- |
| **Experiment** | **Heterogeneous sediment**  **(mg per sample round)** | | **Homogeneous sediment**  **(mg per sample round)** |
| **High-K** | **Low-K** | **Low-K** |
| C-HOM\_3 | - | - | 4.5 (±2.7) |
| C-HET\_1 | 56.4 (±11.3) | 22.6 (±12.1 ) | - |
| HOM\_3.1 | - | - | 455.3 (±115.7) |
| HOM\_3.2 | - | - | 456.5 (±165.0) |
| HET\_3.1 | 465.3 (±37.7) | 547.2 (±54.9) | - |
| HET\_3.2 | 518.1 (±52.6) | 482.7 (±66.6) | - |

## K.4 Electron balance model

Table K.3. Electron balance model calculations and numbered according to the Figure 9 in the main text

|  |  |
| --- | --- |
| **Equation** | **Inputs / outputs** |
| 1.  Nitrate mass flux (kg/m2/s) | J1 = mass flux 1 (kg m-2 s-1)  Ccath = concentration of nitrate, cathode (kg m-3)  u\*high-K = effective ionic mobility, high-K (m2 V-1 s-1)  EE = voltage difference between electrodes (V)  xE = distance between electrodes (m) |
| 2.  Nitrate mass flux (kg/m2/s) | J2 = mass flux 1 (kg m-2 s-1)  Chigh-K = concentration of solute, high-K (kg m-3)  u\*low-K = effective ionic mobility, high-K (m2 V-1 s-1)  EE = voltage difference between electrodes (V)  xE = distance between electrodes (m) |
| 3.  Nitrate mass flux (kg/m2/s) | J3 = mass flux 1 (kg m-2 s-1)  Chigh-K = concentration of solute, high-K (kg m-3)  u\*low-K = effective ionic mobility, high-K (m2 V-1 s-1)  Elow-K = voltage difference layers (V)  xlow-K = distance between centre and edge of the low-K zone (m) |
| 4.  Nitrate mass flux (kg/m2/s) | J4 = mass flux 1 (kg m-2 s-1)  Chigh-K = concentration of solute, high-K (kg m-3)  u\*high-K = effective ionic mobility, high-K (m2 V-1 s-1)  EE = voltage difference between electrodes (V)  xE = distance between electrodes (m) |
| 5.  Treatment time (hours) | t = time (hours)  L = distance between electrodes (m)  EE = voltage difference between electrodes (V)  xE = distance between electrodes (m) |

Table K.4. High-K material properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Hydraulic gradient, i (-) | 0.0055 | Representative field data from confidential source |
| Hydraulic conductivity, K (m s-1) | 2.20x10-4 | Experimental data |
| Porosity, n (-) | 0.3 |
| Tortuosity, τ (-) | 0.56 |
| Groundwater flow velocity, v (m s-1) | 9.7x10-5 | Calculated based on: |
| Domain height (m) | 3 | Model setting |
| Domain width (m) | 1 |
| Domain length (m) | 10 |

Table K.5. High-K chemical properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Dissolved oxygen (g m-3) | 10 | Representative field data from confidential source |
| Nitrate (g m-3) | 42 |
| Sulphate (g m-3) | 63 |
| Effective diffusion coefficient – dissolved oxygen (m2 s-1) | 4.1 x10-9 | Calculated based on:  Where:  D\*i = effective diffusion coefficient of solute, i  Di= diffusion coefficient of solute, i |
| Effective diffusion coefficient – nitrate (m2 s-1) | 3.2 x10-10 |
| Effective diffusion coefficient – sulphate (m2 s-1) | 3.6 x10-10 |

Table K.6. High-K electrokinetic properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Voltage gradient between electrodes (V m-1) | 50 | Representative based on experimental data |
| Effective ionic mobilities, see Table K.1 | - | - |

Table K.7. Low-K zone properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Hydraulic gradient, i (-) | 0.0055 | Representative field data from confidential source |
| Hydraulic conductivity, K (m s-1) | 1.2x10-7 | Experimental data |
| Porosity, n (-) | 0.34 |
| Tortuosity, τ (-) | 0.3 |
| Groundwater flow velocity, v (m s-1) | 4.5x10-8 | Calculated based on: |
| Domain height (m) | 1 | Model setting |
| Domain width (m) | 1 |
| Domain length (m) | 9 |

Table K.8. Low-K chemical properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Benzene (g m-3) | 70 | Representative field data from confidential source |
| Toluene (g m-3) | 65 |
| Ethylbenzene (g m-3) | 50 |
| Xylene (g m-3) | 60 |

Table K.9. Low-K electrokinetic properties

|  |  |  |
| --- | --- | --- |
| **Description** | **Value** | **Source/ Comment** |
| Voltage gradient between layers – no amendment (V m-1) | 2.5 | Experimental data |
| Voltage gradient between layers – 5 g L-1 nitrate amendment (V m-1) | 8.2 |
| Distance between centre and edge of low K zone (m) | 1.5 | Model setting |
| Effective ionic mobilities, see Table K.1 | - | - |