Optimisation of water quality for sustainable irrigation with coal seam gas produced water

Dirk Mallants, Jirka Simunek, Saeed Torkzaban

December 2015
# Contents

Optimisation of water quality for sustainable irrigation with coal seam gas produced water .......................................................... i

Contents .................................................................................................................................................................................. 3
List of Figures ................................................................................................................................................................. 5
List of Tables ....................................................................................................................................................................... 6
Acknowledgments ................................................................................................................................................................ 7

## Executive summary

1 Introduction

1.1 Beneficial use of produced water for irrigation ................................................................. 9
1.2 Potential impact on soil health (soil structure, permeability) ........................................... 11
1.3 Potential impact on vegetation health ............................................................................... 14
1.4 Scope of the study .............................................................................................................. 17

## Modelling process

2 Numerical model for multi-component reactive transport modelling in saturated/unsaturated media ........................................................................................................... 22
2.1 Conceptual model .............................................................................................................. 18
2.1.1 Soil hydrological model ............................................................................................... 18
2.1.2 Soil geochemical model ........................................................................................... 20
2.2 Numerical model for multi-component reactive transport modelling in saturated/unsaturated media ........................................................................................................... 22
2.2.1 HYDRUS .................................................................................................................. 22
2.2.2 UNSATCHEM .......................................................................................................... 22
2.3 Model implementation ..................................................................................................... 24
2.3.1 Soil hydrological characteristics ................................................................................. 24
2.3.2 Soil geochemical Model ............................................................................................ 24
2.3.3 Chemical composition of the irrigation water ............................................................ 26
2.3.4 Vegetation parameters ............................................................................................... 27
2.3.5 Summary of simulation cases ..................................................................................... 29

## Detailed description of the simulation cases

3 Scenario 1: Base case ............................................................................................................. 31
3.2 Scenario 2: Major ion chemistry ..................................................................................... 34
3.3 Scenario 3: Major ion chemistry including effect of salinity on soil hydraulic properties ......................................................................................................................... 38
3.4 Scenario 4: Amended produced water ............................................................................. 41
3.5 Scenario 5: Treated produced water ............................................................................... 43
3.6 Summary of soil water balance calculations ..................................................................... 47
<table>
<thead>
<tr>
<th>4</th>
<th>Conclusions</th>
<th>49</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>References</td>
<td>51</td>
</tr>
</tbody>
</table>
List of Figures

Figure 1.1 Estimated volumes of produced water in Queensland (Source: DNRM 2012). ........................................ 10
Figure 2.1 Soil water retention curves for three soil layers (based on parameters from Table 2.1). ........... 19
Figure 2.2 Irrigation, potential transpiration and evaporation rates applied during the simulations.... 20
Figure 2.3 Finite element grid with soil layers (left) and location of four observation nodes (right). ... 24
Figure 2.4 Schematic of the plant water stress response function, α(h), as used by a) Feddes et al. (1978) and b) van Genuchten (1987). The Feddes et al. function was used in this study: for definition of parameters, see Table 2.8 (h1 = P0, h2 = POpt, h3 = P2L/P2H, h4 = P3). .................................................. 28
Figure 2.5 Plant water stress response function, α(h), for pasture and alfalfa as applied in this study.... 29
Figure 3.1 Simulated water content at three depths in the soil profile. Only first 100 days are shown. Arrows show times at which results at observation nodes are outputted for producing profile plots (at 30, 60, 90 days)........................................................................................................................................ 31
Figure 3.2 Simulated pressure head at three depths in the soil profile. Only first 100 days are shown. ... 32
Figure 3.3 Simulation of tracer movement through soil. Tracer is applied through the irrigation water. 32
Figure 3.4 Simulated solute concentration following infiltration of solute-containing irrigation water. Comparison of models including ET (solid lines), excluding T (transpiration, dashed lines) or excluding ET (evapotranspiration, symbols) (left). Comparison of simulated soil water content for models including ET, excluding T or excluding ET (right)......................................................................................................... 33
Figure 3.5 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for pasture and alfalfa (scenario 1). Cumulative potential and actual surface flux are identical. ................................................................................................................. 34
Figure 3.6 Solute tracer concentration profiles for scenario 1 (left), 2 (middle) and scenario 3 (right).... 35
Figure 3.7 Water content profiles for scenario 2 (left) and scenario 3 (right)............................................. 35
Figure 3.8 Simulated SAR (left) and electrical conductivity (right) for scenario 2. ANZECC trigger value for SAR and EC (see Table 1.3).................................................................................................................. 36
Figure 3.9 Simulated concentrations of dissolved major ions Ca, Mg, Na, K, and Cl. ANZECC trigger value for sodium (see Table 1.3).................................................................................................................. 37
Figure 3.10 Calcite concentration for scenario 2 (left). Calcite mineral volume after 365 days of irrigation (right). ..................................................................................................................................... 37
Figure 3.11 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for scenario 2. .......................................................................................... 38
Figure 3.12 Simulated SAR (left) and electrical conductivity (right) for scenario 3. ......................... 39
Figure 3.13 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for scenario 3. ......................................................... 39
Figure 3.14 Root water uptake function for scenario 1 (top left), scenario 2 (top right) and scenario 3 (bottom left). Pressure head exceeds the POpt = -25 cm threshold after 300 days (bottom right)...... 40
Figure 3.15 Simulated SAR (left) and electrical conductivity (right) for scenario 4. ANZECC trigger value for SAR and EC (see Table 1.3)........................................................................................................ 41
Figure 3.16 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for scenario 4, in comparison with scenario 3...................... 42
Figure 3.17 Simulated SAR (left) and electrical conductivity (right) for scenario 5. ANZECC trigger value for SAR (light clay) and EC (0.65 dS/m) (see Table 1.3)................................................................. 43
Figure 3.18 Simulated concentrations of dissolved major ions Ca, Mg, Na, K, and Cl. ........................................ 44
Figure 3.19 Surface species concentration versus soil depth during irrigation cycles. Total adsorbed concentration for Ca, Mg, Na, and K is constant (279 meq/kg). .................................................................................. 45
Figure 3.20 Calculated soil water content and pressure head at 10 cm depth (scenario 5; pasture). Every five days a 24-hour irrigation event takes place. POpt = pressure head below which root water uptake is optimal, and P2H = limiting pressure head below which root water uptake is no longer optimal (according to Figure 2.4). ........................................................................................................ 46

List of Tables

Table 1.1 Estimated water production rates in the main coal seam gas areas in Queensland and New South Wales........................................................................................................................................................................ 9
Table 1.2 Irrigation trials in Queensland and New South Wales using untreated and RO treated produced water. ........................................................................................................................................................................ 11
Table 1.3 Permissible levels of irrigation water quality parameters to preserve soil and plant health. ... 12
Table 1.4 SAR values for produced water for selected locations in Australia. Calculated SAR values based on reported concentrations for Na+, Ca2+, and Mg2+ expressed in milliequivalents/litre. .......................... 14
Table 1.5 Water quality parameters for Gloucester basin (Tiedeman Dam, NSW) and Surat basin (Woleebee Creek, QLD) produced water. ...................................................................................................................................................... 16
Table 2.1 van Genuchten soil hydraulic properties for Vertosols (average across the Cox’s Creak Catchment area, NSW) (source: Bennett, 2012). ........................................................................................................................................................................ 19
Table 2.2 Initial concentrations of exchangeable cations (source: Ringrose-Voase 2004). .................... 21
Table 2.3 Initial soil solution composition used to calculate initial solution in equilibrium with the cation exchange complex. Data represents composition of rainwater in Wagga-Wagga (Source: Crosbie et al. 2012). ............................................................................................................................................ 21
Table 2.4 Chemical species included in the UNSATCHEM major ion module of HYDRUS-1D. ............. 23
Table 2.5 Defined variable boundary conditions. ....................................................................................... 24
Table 2.6 Gapon Exchange Constants (Source: Jacques et al. 2012). ........................................................ 25
Table 2.7 Composition of irrigation waters. Kenya/rain water = ratio of treated produced water to rain water composition........................................................................................................................................ 26
Table 2.8 Root water uptake reduction parameters without solute stress (based on Wesseling et al. 1991). .......................................................................................................................................................... 28
Table 2.9 Root water uptake reduction parameters with solute stress for alfalfa. ................................. 29
Table 2.10 Description of scenarios used.................................................................................................... 30
Table 3.1 Water balance components for a 365 day simulation period. Negative infiltration values means inflow; negative net drainage values means outflow. ......................................................................................... 47
Table 3.2 Chemical mass fluxes (gram/m²) through upper and lower model boundary for a 365 day simulation period. For upper model boundary negative fluxes are input to the soil; for lower model boundary negative values refer to fluxes leaving the soil. For each element and each scenario, first row is flux through upper boundary; second row is flux through lower boundary......................................................... 48
Acknowledgments

The authors would like to acknowledge Sarah Bennett (formerly University of NSW) for providing detailed soil hydraulic property data on the Cox Creak Catchment (NSW). We equally acknowledge the Land and Water Business Unit for funding the strategic appropriation research project “Next generation methods and capability for multi-scale cumulative impact and management”. Professor Jirka Šimůnek (University of California Riverside) received a travel grant through this project. This report was subject to internal peer review during its production.
Executive summary

Coal seam gas production in Australia generates large volumes of so-called produced water that contains elevated concentrations of naturally occurring inorganic and organic compounds, and usually has a high salinity. Treated coal seam gas water may be utilised for beneficial or alternative uses, including agricultural uses (irrigation and stock), urban uses (town water supply) and industrial uses (construction and processing). For instance, assessment of alternative use for treated coal seam gas water for the Central Condamine Alluvium (Queensland) indicates the region has capacity to deliver 854 GL, or around 35% of the historic depletion, by 2050 to irrigators and the Chinchilla Weir water supply scheme. Most coal seam gas operators in Australia are considering some kind of agricultural uses for their coal seam gas water, including irrigation.

Coal seam gas produced water is generally high in total dissolved solids and has a high salinity which may affect soil and plant health if used untreated for irrigation. For example, waters with a high sodium absorption ratio (SAR), if used for irrigation, will result in salt accumulation in the soil profile, potentially killing off plant species that are not salt tolerant. Use of irrigation water with high SAR values may further result in dispersion of the soil clay minerals and, once dry, soils may become structureless destroying natural particle aggregation. This degrades soil properties by making the soil more dispersive and erodible, restricting water entry and reducing hydraulic conductivity.

Prior to any use of such produced water for irrigation purposes, an in-depth assessment has to be undertaken of the potential long-term effects of dissolved ions on soil and plant health. We here simulate coupled processes of variably saturated water flow, plant water uptake and coupled transport of multiple major ions in soils irrigated with produced water featuring different water qualities. By coupling major ion soil chemistry to unsaturated flow and plant water uptake, and by explicitly incorporating effects of salt concentrations on soil hydraulic properties and on root water uptake (so-called salinity stress), critical soil processes required for salinity risk assessment associated with coal seam gas produced water are effectively included in our analysis. Simulations with different irrigation water qualities provided detailed results regarding chemical indicators of soil and plant health, i.e. SAR, EC and sodium concentrations. By comparing such indicators in the soil profile with permissible ANZECC values, an assessment was made of the risk to soil and plant health. We also evaluated the effect of high salt concentrations in the soil profile on plant salinity stress, a condition which reduces the capacity for plants to uptake water causing yield reduction. Finally, the simulations also allowed to test if soil hydraulic properties, in particular the hydraulic conductivity, are negatively impacted by high salt concentrations, especially by the accumulation of the monovalent cations sodium and potassium.

Results from a base case scenario indicated that use of untreated irrigation water would cause SAR and EC values to significantly exceed the ANZECC guide values. The purpose of this what-if scenario was to provide an upper bound impact against which alternative scenarios with improved irrigation water quality would be tested. While it is highly unlikely that such highly saline water will be used for long-term irrigation, the simulations do provide useful insights in the type of coupled processes that might occur, and what the potential impacts are on soil and plant health. For example, by using highly saline irrigation water, we demonstrated that accumulation of monovalent cations occurs in the soil, resulting in a decrease in hydraulic conductivity. This in turn caused water stagnation, leading to plant water stress and reduced transpiration. Calcite precipitation in the top soil layer made the available pore space decrease by 3%.

In case amended irrigation water was used (a mixture of produced and surface water), the calculated soil SAR values were much lower and generally acceptable for sandy to sandy-loam soil. Permissible SAR values for light clay were still exceeded for most of the soil profile. Calcite formation does still occur, but only in the top of the soil profile and with a negligible impact on soil porosity. The use of treated produced water yielded an acceptable salinity profile not exceeding guide values for SAR and EC; plant water stress was limited as there was no additional salinity stress associated with the low level of salts.
1 Introduction

1.1 Beneficial use of produced water for irrigation

Production of coal seam gas requires de-pressurisation of the coal seam layers by extracting groundwater. Reducing the hydrostatic pressure on the gas in the pores allows gas to flow from high pressure areas to the area with the lowest pressure (i.e. the production well). Coal layers generally have a sufficiently high permeability (i.e. ability to transmit fluids, including gas) to facilitate water and gas flow without the need for improving the coal permeability by means of hydraulic fracturing. In the least permeable coal measures, coal seam gas operations require the use of hydraulic fracturing as a means to increase coal permeability and connectivity between naturally occurring fractures in coal beds. In Australia, coal measures in the Bowen Basin (Queensland) have much lower permeability than, for example, the Surat Basin (Queensland) and are therefore likely to require increased levels of hydraulic fracturing.

A summary of the water extraction rates in the main coal seam gas areas in Australia is provided in Table 1.1. It is acknowledged that the forecasts of water production will vary over time and geographically (QWC 2012). For example, Figure 1.1 shows estimates of expected volumes of produced water per development area and the whole-of-industry forecast in Queensland. Much of the variation is due to different assumptions about the size and rate of coal seam gas industry development over the 50-year time frame that is generally assumed for forecasting water production (DNRM 2012). By 2050, most coal seam gas areas will have reached the end of their production stage.

Table 1.1 Estimated water production rates in the main coal seam gas areas in Queensland and New South Wales.

<table>
<thead>
<tr>
<th>Water production rate</th>
<th>Area</th>
<th>Comment</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2 – 0.7 GL/year</td>
<td>Gloucester (New South Wales)</td>
<td>Average total water extraction for an estimated resource life of 14 years</td>
<td>RPS 2011</td>
</tr>
<tr>
<td>0.028 GL/year</td>
<td>Clarence-Moreton (New South Wales)</td>
<td>Average total water extraction assuming 697 ML over a 25-year period</td>
<td>RPS 2011</td>
</tr>
<tr>
<td>95 GL/year</td>
<td>Surat Basin (Queensland)</td>
<td>Average total water extraction over the life of the industry based on a regional model predictions</td>
<td>QWC 2012</td>
</tr>
<tr>
<td>75 to 98 GL/year</td>
<td>Surat Basin (Queensland)</td>
<td>Average total water extraction over the life of the industry based on predictions from industry and DNRM (2012)</td>
<td>QWC 2012</td>
</tr>
<tr>
<td>140 GL/y</td>
<td>Surat Basin (Queensland)</td>
<td>Peak water production rate around the year 2026</td>
<td>QWC 2012</td>
</tr>
<tr>
<td>140 to 281 GL/y</td>
<td>Queensland’s Surat and southern Surat Basins.</td>
<td>Peak water production rates</td>
<td>DNRM 2012; CWIMI 2008</td>
</tr>
<tr>
<td>150 to 180 GL/y</td>
<td>Surat Basin (Queensland)</td>
<td>Peak water production rate based on different scenarios for coal seam gas production and assuming operations ceased either in year 2040 or 2060</td>
<td>DNRM 2012</td>
</tr>
</tbody>
</table>
In Australia, like in the US, there is increasing use of treated and untreated produced water from the coal seam gas industry for agriculture and forestry (Table 1.2). The Gloucester Coal Seam Gas Project in NSW under the operation of Lucas Energy has used low salinity produced water for dust suppression and received approval to irrigate using this water (AGL 2008). Produced water from some of the Stratford Pilot wells with EC of about 3000 µS/cm was used for pasture irrigation at the Tiedman property, but it was not seen as a viable long-term option without improving the quality of this water (AGL 2008; Lucas 2008). AGL Energy Ltd reports pasture irrigation trials have been undertaken as part of the Gloucester Gas Project in NSW in FY2010, but not in FY2011 as the irrigation approval lapsed (AGL 2011). In June 2011, AGL commissioned a review of environmental factors for the Gloucester irrigation project (Tiedman), which recommended blending produced water with fresh river water as a contingency measure if soil salinity increased by more than 50% in the root zone (Parson Brinkerhoff 2011). The AGL (2012) report describes the proposal to irrigate pasture, using up to 70 ML of produced water blended with water from the Avon River (at a ratio of about 3 parts river water: 1 part produced water) over a maximum area of 40 ha over a three-year period at the Tiedman site. Table 1.5 provides typical water quality data for untreated surface water-amended produced water (calculated based on a 3:1 ratio of surface water:groundwater).

Assessment of alternative use for treated coal seam gas water for the Central Condamine Alluvium (Queensland) indicates the region has capacity to deliver 854 GL, or around 35% of the historic depletion, by 2050 to irrigators and the Chinchilla Weir water supply scheme (DNRM 2013).

Other irrigation projects in Australia where produced water is used include the large-scale forestry by Santos in Queensland’s Bowen Basin and the legume plantation by Origin Energy (RPS 2011). In the Bowen Basin, up to 8 ML/day of reverse osmosis (RO) treated produced water was used to irrigate 234 ha pasture crop and an 800,000 tree timber plantation in the Fairview Project Area (Santos 2009; Santos 2010). Santos also trialled hardwood drip-irrigation in the Fairview Field where a 2000 ha plantation of eucalyptus trees were irrigated with approximately 14 ML of “amended” water per day (Coordinator-General 2010). The amendment process did not involve salt removal, but rather reducing the pH level and adding calcium and magnesium to balance excess sodium (i.e. to reduce the SAR (Coordinator-General 2010)). In Spring Gully
Field, Queensland, Origin Energy irrigates 300 ha of oilseed-bearing legume tree (*Pongamia pinnata*) plantation with RO treated produced water (Parsons 2010).

### Table 1.2 Irrigation trials in Queensland and New-South Wales using untreated and RO treated produced water.

<table>
<thead>
<tr>
<th>Geographic area</th>
<th>Specifics of irrigation trials</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>NSW - Gloucester</td>
<td>Stratford project: untreated produced water from trial wells; EC = 3000 µS/cm; pasture; 0.02 ML/day</td>
<td>AGL 2008; Lucas 2008</td>
</tr>
<tr>
<td></td>
<td>Tiedman project: blending river water with produced water at a ratio of 3:1 (river:produced); EC between 1500 and 200 µS/cm; salt tolerant crops (sorghum, lucerne, cereals); 40 ha; 70 ML blended water over 3 years</td>
<td>Parson Brinkerhoff (2011); AGL (2012)</td>
</tr>
<tr>
<td>QLD – Bowen Basin</td>
<td>Fairview project: 8 ML/day RO water; 234 ha forage crops and timber trees</td>
<td>Santos 2009; Santos 2010</td>
</tr>
<tr>
<td></td>
<td>2000 ha; 14 ML of “amended” water per day; eucalyptus plantation (Chinchilla White Gum)</td>
<td>Coordinator-General 2010</td>
</tr>
<tr>
<td></td>
<td>Spring Gully Field; RO treated produced water; 300 ha of oilseed-bearing legume tree;</td>
<td>Parsons 2010</td>
</tr>
</tbody>
</table>

In a recent report to the Office of NSW Chief Scientist and Engineer the “risk of salinization of soil or destruction of flora and stream habitats if untreated or partially treated produced water is used for irrigation or surface dispersal” was highlighted as one of several community concerns over the recovery of coal seam gas in New South Wales (Fell 2014). The potential impacts on soil and plant health from use of irrigation water with a high SAR is discussed in section 1.2 and section 1.3.

### 1.2 Potential impact on soil health (soil structure, permeability)

Coal seam gas produced water is generally high in total dissolved solids and may contain organic and inorganic compounds that may affect soil and plant health if used untreated for irrigation. For example, coal seam gas waters are typically high in sodium but relatively low in calcium and magnesium, and therefore yield a high sodium absorption ratio (SAR). If such produced water is used for irrigation, it leads to sodium displacing calcium and magnesium in the soil and salt accumulation in the soil profile. This will cause a decrease in the ability of the soil to form stable aggregates and results in a loss of soil structure. This in turn will result in a decrease in infiltration leading to problems with crop production.

Prior to any use of such produced water for irrigation purposes, an in-depth assessment has to be undertaken of the long-term effects of dissolved ions on soil and plant health. In an accompanying study the effect of leaching of alkaline produced water through soil on the migration of inorganic compounds naturally present in soil is discussed (Mallants et al. 2015).

The minimum quality of irrigation water is defined by several national and state regulations. The Australian and New Zealand Guidelines for Fresh and Marine Water Quality (ANZECC 2000) provide rationale and background information on quality of irrigation and general water uses, stock drinking water, aquaculture and human consumers of aquatic foods. For instance, for different soil types, permissible levels of chloride, sodium and SAR have been defined (Table 1.3). The permissible SAR levels decrease with increasing clay content: high SAR values mean a high proportion of sodium in soil. This results in dispersion of the clay

---

1 Sodium adsorption ratio (SAR) = [Na⁺] / ([(Ca²⁺) + [Mg²⁺]) / 2]¹/² where [Na⁺], [Ca²⁺], and [Mg²⁺] are in milliequivalents/litre
minerals and, once dry, soils may become dense, cloddy and structureless, destroying natural particle aggregation. This degrades soil properties by making the soil more dispersible and erodible, restricting water entry and reducing hydraulic conductivity.

Although no trigger values have been defined for bicarbonate, elevated levels in irrigation waters can adversely affect soil structure. If the solubility of calcium carbonate is exceeded, precipitation of calcium carbonate in soil can occur. This will increase the soil SAR (when calcium carbonate precipitates, concentration of exchangeable calcium decreases) and may lead to structural issues.

Plant salt tolerances are provided in ANZECC 2000. Concentrations of metals and metalloids in irrigation water should be less than the recommended trigger values.

**Table 1.3 Permissible levels of irrigation water quality parameters to preserve soil and plant health.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Maximum (DEPH 2014)</th>
<th>ANZECC 2000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical conductivity (µS/cm)‡</td>
<td>&lt; 950¹</td>
<td>&lt; 650</td>
</tr>
<tr>
<td>SAR</td>
<td>&lt; 6⁴ for heavy soils; &lt; 12⁴ for light soils</td>
<td>&gt;20⁶; 20-8⁶; 13-6⁶; 11-5⁴</td>
</tr>
<tr>
<td>Bicarbonate (mg/L)</td>
<td>100⁴</td>
<td>No trigger value recommended</td>
</tr>
<tr>
<td>Fluoride (mg/L)</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>pH</td>
<td>6 – 8.5⁹</td>
<td>6-9</td>
</tr>
<tr>
<td>Chloride (mg/L)</td>
<td>&lt; 175⁸; 175-350¹; 350 – 700⁸; &gt; 700⁹</td>
<td></td>
</tr>
<tr>
<td>Sodium (mg/L)</td>
<td>&lt; 115⁷; 115-230¹; 230-460⁶; &gt;460¹⁰</td>
<td></td>
</tr>
<tr>
<td>Heavy metals and metalloids (trigger values in mg/L; short-term use up to 20 years)</td>
<td>Al (20); As (2); Cd (0.05); Cr (1); Co (0.1); Cu (5); Fe (10); Li (2.5); Pb (5); Mn (10); Hg (0.002); Mb (0.05); Ni (2); Zn (5)</td>
<td></td>
</tr>
</tbody>
</table>

¹95th percentile over a one-year period; ²DERM 2010; ³1000 µS/cm = 1 dS/m; a: sand-sandy loam; b: loam-silty loam; c: clay loam; d: light clay; e: sensitive crop; f: moderately sensitive crop; g: moderately tolerant crop; h: tolerant crop

Produced water is generally unsuitable for direct surface discharge or irrigation without any treatment or amendment (Stearns et al. 2005; Beletse et al. 2008; Nghiem et al. 2011). While sodium ions cause soil particles to disperse, particularly if the soils contain montmorillonite clays, most ions increase the aggregation of soil particles (Nghiem et al. 2011). Irrigation water with a high SAR can lead to a decrease in infiltration and deterioration of the soil structure. SAR values greater than 13 pose a risk to the soil ecosystem (Stearns et al. 2005), and even SAR values between 5 and 8 have been shown to cause irreversible plugging of soil pores and swelling (Mace and Amrhein 2001). Traditional treatments to mitigate saline-sodic irrigation water can be used, for example the addition of gypsum and elemental sulfur (S) (Vance et al. 2008; Šimůnek et al. 2006).

Studies have been undertaken to assess the feasibility of using sodium-rich produced water for salt-tolerant crop production (Johnston et al. 2008; Vance et al. 2008; Beletse et al. 2008). Vance et al. (2008) used saline-sodic coal seam gas produced water with a SAR between 17 and 57 for irrigating grasslands and hayfields in the Powder River Basin, Wyoming. For the use of produced water to be effective, the method
further required applications of gypsum and elemental S to provide calcium ions and an acidified soil environment to promote calcite dissolution. Water produced during the depressurisation phase of coal seam gas mining in Waterberg district, South Africa, is highly saline and dominated by sodium bicarbonate. With careful management, Beletse et al. (2008) determined that coal seam gas irrigation water with SAR values of 85 could be used to grow certain crops, but additions of gypsum and organic matter to the soil were necessary to counteract infiltration problems that arose due to the excessive sodium that had accumulated in the soil.

In Australia, the Queensland Department of Environment and Heritage Protection (DEHP) recommends that parties proposing to use produced water for irrigation purposes should seek professional advice to understand and manage site-specific soil-water interaction, agronomic, monitoring and irrigation management issues (DEHP 2014). Furthermore, among the minimum standards for using produced water for irrigation purposes, the guidelines indicate that the electrical conductivity (EC) shall be less than 950 \( \mu \text{s/cm} \) or 0.95 dS/m (95th percentile over a one-year period), and the SAR shall be less than 6 for heavy soils and less than 12 for light soils (95th percentile over a one-year period) (DEHP 2014).

There are broader requirements in Queensland regarding management of salinity risks that are relevant to use of produced water. In particular the requirement under Schedule B – Basin Salinity Management to Part 12 Schedule 1 of the Water Act 2007 (Commonwealth) to not permit the undertaking of any action that may have a significant effect on stream salinity in the Murray-Darling Basin, which supports assessment of salinity risk out to 100 years (Biggs et al. 2012).

To support the sustainable management of soil and landscapes under irrigated agriculture, Biggs et al. (2012) have developed a framework to assess the salinity risk associated with the use of coal seam gas water for irrigation in the Queensland Murray-Darling Basin (QMDB). Biggs et al. (2012) identified the description of the unsaturated zone as the key knowledge and data gap when conducting salinity risk assessments. In particular, unsaturated zone-related gaps include:

- Soil and regolith (unsaturated zone) properties, including i) studies of critical soil attributes (porosity, initial soil water content, substrate permeability/conductivity) undertaken to depths below the “root zone”, ii) defining the root zone for different crops, and iii) quantifying lateral flow processes.
- Better rainfall salinity data is required to improve the input side of the salt balance equation.
- A need for a more strategic approach to install gauging stations for various monitoring purposes that will provide long-term benefits to the assessment of cumulative risk in catchments
- Considerable research is needed to better define critical thresholds for agronomic and degradation purposes (e.g. acceptable root zone salinity) across landscapes
- Process understanding: understanding of the fate of excess water (lateral flow or drainage), deeper soil/regolith processes and properties
- Further detailed assessment is needed to delineate emerging salt expressions and to investigate existing salt expressions
- Detailed shallow groundwater monitoring is required to allow detection of drainage fluxes
- Capture past and current land management practices as these affect historic and current deep drainage/recharge rates
- Drainage rates from modelling need to be tested against measured deep drainage data to provide reliable long-term estimates of deep drainage.

The current study endeavours to address at least those knowledge gaps that relate to better process understanding (e.g. critical soil properties, critical thresholds) using the unique features of the HYDRUS-1D simulator that are relevant for salinity risk assessment (Jacques et al. 2013; Šimůnek et al. 2006, 2009).

SAR values based on cation concentration data have been compiled from a selection of CSG company reports (Table 1.4). In the Fairview project area (Surat and Bowen Basins), the coal seam gas target is the Bandanna Formation, which is not considered to be a significant regional aquifer (Santos 2010). The coal
seams within the Bandanna Formation are recognised as fractured aquifers based on the well-cleated coal, and the seams are separated by siltstone and sandstone that restrict vertical leakage between the seams and the overlying and underlying units (Santos 2010). In the Woleebee Creek block, the produced water is from the Walloon Coal Measures, which are heterogeneous formations with coal seams dispersed in an aquitard (QGC 2011). Interconnection between the Walloon Coal Measures and over- and underlying aquifers due to faulting is not apparent within the tenement (QGC 2011). The produced water data from Arrow Energy are also from the Walloon Coal Measures in its southern tenements in Queensland in the Surat Basin. These include gas production from Daandine, Tipton West, Stratheden and Kogan North near Dalby (AE 2011).

Table 1.4 SAR values for produced water for selected locations in Australia. Calculated SAR values based on reported concentrations for Na+, Ca²⁺, and Mg²⁺ expressed in milliequivalents/litre.

<table>
<thead>
<tr>
<th>Location</th>
<th>SAR</th>
<th>Comment</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fairview Project Area, Surat and Bowen Basins, Qld</td>
<td>16-567 (Q75)</td>
<td>Range reported for CSG water sampled from operations (ponds and wells)</td>
<td>Santos 2010</td>
</tr>
<tr>
<td>Fairview Project Area, Surat and Bowen Basins, Qld</td>
<td>512</td>
<td>Average reported for CSG water from operations (ponds and wells)</td>
<td>Santos 2010</td>
</tr>
<tr>
<td>Fairview Project Area, Surat and Bowen Basins, Qld</td>
<td>181</td>
<td>Calculated based on maximum cation concentrations for CSG water sampled from operations (ponds and wells)</td>
<td>Santos 2010</td>
</tr>
<tr>
<td>Woleebee Creek Block, Surat Basin, Qld</td>
<td>77</td>
<td>Calculated based on average concentrations of cations sampled from raw CSG water from ponds</td>
<td>QGC 2011</td>
</tr>
<tr>
<td>Surat Basin, Arrow Energy southern tenements, Qld</td>
<td>3</td>
<td>Calculated based on minimum cation concentrations in CSG water sampled from wells</td>
<td>AE 2011</td>
</tr>
<tr>
<td>Surat Basin, Arrow Energy southern tenements, Qld</td>
<td>61</td>
<td>Calculated based on maximum cation concentrations in CSG water sampled from wells</td>
<td>AE 2011</td>
</tr>
<tr>
<td>Surat Basin, Arrow Energy southern tenements, Qld</td>
<td>196</td>
<td>Calculated based on average concentrations of cations sampled from an aggregation pond of untreated CSG water that feeds the Daandine RO facility</td>
<td>AE 2011</td>
</tr>
</tbody>
</table>

All produced waters, except one, exceed the DEPH and ANZECCC trigger values for SAR. This indicates short-term irrigation (20 years) with untreated produced water is not a viable option to maintain soil health.

1.3 Potential impact on vegetation health

Irrigation with high SAR water will effectively killing off plant species that are not salt tolerant (Moore 2012). A key publication on soil remediation standards for salt ions is a set of technical reports by Bright and Addison (2002a; 2002b) to inform policy decisions in British Columbia, Canada. A major catalyst for this study was to develop standardised guidance to assist spill response and soil remediation in northern British Columbia at sites where salt-containing produced water is released as part of oil and gas exploration and extraction activities (Bright and Addison 2002b). Generic soil quality standards for human health, aquatic life, and soil ecological functioning, as manifested through soil invertebrate and plant responses, were developed for salt ions (Bright and Addison 2002b). Whilst the impairment of metabolic functioning of soil microbes is recognised as playing a major role in nutrient cycling and other processes important to terrestrial ecosystems, there is insufficient data available to define a threshold for salt ions; instead, a microbial functional impairment standard is used that is developed from nutrient and energy cycling data (CCME 1996; Bright and Addison 2002b). The report provides a model for predicting concentrations of chloride in soils that are protective of groundwater and surface water uses based on categories of site properties. The categorisation of site types considers soil texture (coarse versus fine grained, or low versus high Water Holding Capacity) and climatic conditions (Bright and Addison 2002a). As discussed in the
report, the major controlling influences on salt concentration enroute to the saturated groundwater zone are:

- the leachate concentration in and immediately below the soil source area
- the water flux as the driving force for migration
- the soil type as an important factor defining the amount of salt that can adsorb on the clay and silt particles.

Another potential issue when produced water is used for irrigation is the relatively high boron content. If not removed, boron can be damaging to some flora. The ANZECC guide value for long-term irrigation (up to 100 y) is 0.5 mg/L (Table 1.5). An analysis of the migration of boron in soil was beyond the scope of this study.

Overall salt concentrations do not significantly decrease while migrating through the soil because salt ions do not biodegrade, volatilise or undergo photolysis (Bright and Addison 2002b).

An investigation of soil and vegetation recovery over a ten-year period after a gas well blowout and salt release in British Columbia conducted by Leskiw et al. (2012) documents the natural recovery of salt-affected plots and discusses the advantages of allowing for natural recovery over imposing soil reclamation measures. This study analysed whether leaching of salts from natural precipitation events were sufficient to improve the soil on the basis of certain soil and vegetation parameters (i.e. sodium adsorption ratio, soil EC, pH, soluble ions, and vegetation recovery). Natural attenuation from above normal rainfall in the first few years after the blowout was effective in removing salt from the root zone and subsoil (Leskiw et al. 2012). These results are obtained for a humid climate; it is expected that natural attenuation under arid or semi-arid climates would be much less effective.

In a study conducted by Dewalle and Galeone (1990), gas well brine was applied to forest land during the dormant season to test the feasibility of wastewater disposal in forested catchments in Pennsylvania. Different loading rates for brine were applied to the ground surface on different plots and macro- and micropore soil water chemistry changes were monitored at a depth of 70 cm. Concentrations of Cl, Ba, Pb, As, Se and Cd exceeded drinking water guidelines for several months following treatment on all plots at 70 cm depth (Dewalle and Galeone 1990). High mobility of trace metals (Cd and Pb) in the soil appeared to be enhanced by complexation of these metals with chloride in the brine (see earlier discussions on the mobility enhancement of metals by several anions). These interactions between metals and inorganic complexing species may have also mobilised metals naturally present in soil profiles, leading to:

1. concentrations in the soil pore-water that were higher than acceptable
2. migration to groundwater at a faster rate.

The study suggests treating forest soil to raise soil pH, pretreating brines to remove toxic elements or using brines with lower chloride concentrations as options to reduce trace metal mobility problems (Dewalle and Galeone 1990).

Adams (2011) describes the land application of shale gas flowback water in a deciduous forest in West Virginia, which showed a 50-fold increase in concentrations of sodium and chloride in the surface soil within the treatment area that declined over time. The composition of the hydraulic fracturing fluid was not made publicly available; however, Adams (2011) surmised based on the study results that Na and Cl were the main constituents in the hydraulic fracturing fluid, and thus in the flowback water.
Table 1.5 Water quality parameters for Gloucester basin (Tiedeman Dam, NSW) and Surat basin (Woleebee Creek, QLD) produced water.

<table>
<thead>
<tr>
<th>Chemical parameter</th>
<th>Gloucester basin (NSW) water quality*</th>
<th>Surat basin (QLD) water quality**</th>
<th>ANZECC 2000 guideline for irrigation$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Site 1 produced water</td>
<td>Site 2 produced water</td>
<td>Avon river surface water</td>
</tr>
<tr>
<td>Electrical conductivity (µS/cm)</td>
<td>4180 - 4280</td>
<td>2610 - 2790</td>
<td>158-324</td>
</tr>
<tr>
<td>Total alkalinity (mg/L)</td>
<td>872-989</td>
<td>395-577</td>
<td>29-52</td>
</tr>
<tr>
<td>SO4 (mg/L)</td>
<td>&lt;5-14</td>
<td>22-29</td>
<td>11-440$^e$</td>
</tr>
<tr>
<td>Cl (mg/L)</td>
<td>569-663</td>
<td>425-489</td>
<td>24-56</td>
</tr>
<tr>
<td>Ca (mg/L)</td>
<td>&lt;1-2</td>
<td>3-5</td>
<td>5-12</td>
</tr>
<tr>
<td>Mg (mg/L)</td>
<td>&lt;1</td>
<td>1-2</td>
<td>3-8</td>
</tr>
<tr>
<td>Na (mg/L)</td>
<td>768-776</td>
<td>602-624</td>
<td>16-38</td>
</tr>
<tr>
<td>K (mg/L)</td>
<td>317-323</td>
<td>40-43</td>
<td>6-32</td>
</tr>
<tr>
<td>Al (mg/L)</td>
<td>0.13-0.48</td>
<td>0.05-0.07</td>
<td>0.02-0.22</td>
</tr>
<tr>
<td>Ba (mg/L)</td>
<td>0.086-0.228</td>
<td>0.241-0.265</td>
<td>0.043-0.08</td>
</tr>
<tr>
<td>B (mg/L)</td>
<td>0.79-0.83</td>
<td>0.70</td>
<td>0.06-0.14</td>
</tr>
</tbody>
</table>

* Parson Brinkerhoff 2011; ** raw water pond average (QGC 2011); $^a$2014 data (Parson Brinkerhoff 2015); $^b$calculated based on a 3:1 ratio of surface water:groundwater using Site 1 produced water and Avon surface water; $^c$ Dawson Valley Beneficial Use Scheme; $^d$ long-term use (up to 100 y); short-term use (up to 20 y); NG = no guideline available; $^e$bicarbonate alkalinity
1.4 Scope of the study

The aim of this study is to simulate coupled processes of variably saturated water flow, plant water uptake and coupled transport of multiple major ions in soils irrigated with produced water featuring different water qualities. By coupling major ion soil chemistry to unsaturated flow and plant water uptake, and by explicitly incorporating effects of salt concentrations on soil hydraulic properties and on root water uptake (so-called salinity stress), critical soil processes required for salinity risk assessment associated with coal seam gas produced water are effectively included in our analysis. In doing so, the current study addresses several of the knowledge gaps that are pivotal for an improved salinity risk assessment (Biggs et al. 2012).

Simulations are based on the finite element code HYDRUS-1D (Šimůnek et al. 2008). The major ion chemistry module Unsatchem is implemented to simulate the simultaneous movement of multiple ions present in irrigation water in a vegetated soil profile.

The produced water continuously emerges from the well for its life-time after a hydraulic fracturing process (Vidic et al. 2013; Ward et al. 2015). It has a high load of dissolved solutes (Batley et al. 2012; Ward et al. 2015), a high alkalinity (Ward et al. 2015) and contains organic and inorganic chemicals (Batley et al. 2012). The subject of this study are the non-metal and non-metalloid inorganic substances of the produced water that define its high salinity.
2 Modelling process

2.1 Conceptual model

2.1.1 SOIL HYDROLOGICAL MODEL

Simulation of variably saturated flow in soil requires a mathematical relationship between i) the soil water content \( \theta \) and the soil pressure head \( h \), and ii) either the water content or the pressure and the unsaturated hydraulic conductivity, respectively \( K(\theta) \) and \( K(h) \). The most commonly used mathematical expression for the soil water retention curve, \( \theta(h) \), is the van Genuchten equation (van Genuchten 1980) since it permits a relatively good description of \( \theta(h) \) for many soils using only a limited number of parameters. The van Genuchten soil moisture retention characteristic is defined as:

\[
\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |ah|^n)^m} \tag{1}
\]

where \( \theta_r \) is the residual water content [cm\(^3\)/cm\(^3\)], \( \theta_s \) is the saturated water content [cm\(^3\)/cm\(^3\)], and \( a [1/m], n [-] \) and \( m = 1 - 1/n [-] \) are curve shape parameters specifically for the van Genuchten equation.

The second important soil hydraulic property is the unsaturated hydraulic conductivity function, \( K(h) \). The hydraulic conductivity characterises the ability of a soil to transmit water, and as such is inversely related to the resistance to water flow. The hydraulic conductivity depends on many factors, including the pore-size distribution of the porous medium, and the tortuosity, shape, roughness, and degree of interconnectedness of pores. The hydraulic conductivity decreases considerably as soil becomes unsaturated and less pore space is filled with water. The unsaturated hydraulic conductivity function gives the dependency of the hydraulic conductivity on the water content, \( K(\theta) \), or pressure head, \( K(h) \). The conceptual model that views the soil as a bundle of capillaries of different radii may be used to evaluate the hydraulic conductivity function. By adding the conductivity of all capillaries that are filled with water at a particular water content or pressure head, one obtains the hydraulic conductivity of the complete set of capillaries, and consequently of the soil itself.

Similarly, as for the soil water retention curve, analytical models are often used also for the unsaturated hydraulic conductivity function, \( K(h) \). The van Genuchten (1980) retention function is coupled mostly with the model of Mualem (1976) to give

\[
K(h) = K_s S_e^l \left[ 1 - \left( 1 - S_e^{1/m} \right)^m \right]^2 \tag{2}
\]

where

\[
m = 1 - \frac{1}{n}, \quad n > 1
\]

\( K_s \) is saturated hydraulic conductivity, and \( S_e = (\theta - \theta_r)/(\theta_s - \theta_r) \) is the effective saturation. The pore-connectivity parameter \( l \) was estimated by Mualem (1976) to be about 0.5 as an average for many soils. Also in this study the \( l \) parameter was fixed at 0.5.

The soil profile is assumed 1-m deep, with three soil layers: 0-0.3 m, 0.3-0.7 m, and from 0.7-1.0 m. The van Genuchten soil hydraulic properties were taken from Bennet (2012). These soil hydraulic properties were calculated on the basis of the pedotransfer functions of Minasny and McBratney (2002) using soil data points within the Cox’s Creek catchment, NSW. For three soil horizons particle size distribution and the bulk density from the SALIS (New South Wales Soil And Land Information System) dataset were used as predictor variables in the pedotransfer functions. From six soil types (Tenosols, Dermosols, Vertosols, Chromosols, Sodosols, Kandosols), Vertosols were most prominent with 84 out of 143 soil profiles (59%).
Vertosol hydraulic properties were therefore selected here for the simulations (Table 2.1). The mean soil water retention curves together with their uncertainty bands (mean ± 2 standard deviation) are shown in Figure 2.1.

Table 2.1 van Genuchten soil hydraulic properties for Vertosols (average across the Cox’s Creak Catchment area, NSW) (source: Bennett, 2012).

<table>
<thead>
<tr>
<th>Soil layer</th>
<th>$\Theta_r$ [cm$^3$/cm$^3$]</th>
<th>$\Theta_s$ [cm$^3$/cm$^3$]</th>
<th>$\alpha$ [1/m]</th>
<th>$n$ [-]</th>
<th>$K_s$ [m/day]</th>
<th>$l$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (0-0.3 m)</td>
<td>0.059</td>
<td>0.515</td>
<td>8.3</td>
<td>1.217</td>
<td>6.04</td>
<td>0.5</td>
</tr>
<tr>
<td>2 (0.3-0.7 m)</td>
<td>0.066</td>
<td>0.538</td>
<td>7.4</td>
<td>1.190</td>
<td>4.51</td>
<td>0.5</td>
</tr>
<tr>
<td>3 (0.7-1.0 m)</td>
<td>0.07</td>
<td>0.515</td>
<td>7.9</td>
<td>1.150</td>
<td>3.35</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Figure 2.1 Soil water retention curves for three soil layers (based on parameters from Table 2.1).

In order to reach the (pseudo) steady-state concentrations profile, the following hypothetical irrigation scheme was used. The potential ET is equal to 1 cm/d (summer conditions in Queensland$^2$), divided into potential evaporation (2 mm/d) and potential transpiration (8 mm/d) (Figure 2.2). Irrigation of 6 cm is applied each 5 days, i.e., 20% above potential ET (6/5). The annual total irrigation of 438 cm is much higher than the combined rainfall and irrigation in irrigation areas of the Northern Darling Basin for crops such as cotton (up to nearly 140 cm) or sorghum (up to 110 cm) (Silburn and Montgomery 2004). However, irrigation of pasture, especially for grazing (beef and lamb), uses more water: for example, nearly 1500 mm was recorded in a flood irrigated pasture in the South East of South Australia (Horizon 2006). The application rate used in this study therefore corresponds to the equivalent applied water of two to three growing seasons. Our purpose was not to have the most realistic irrigation regime, rather did we apply a simplified water application rate that would simplify the analysis of complex coupled chemical-hydrological processes.

No precipitation was considered at this time; while this is a simplification of a soil’s hydrological balance and does not account for effects of rainfall salinity on the salt mass balance, it does allow focus on effects of irrigation only when coupled chemical-hydrological-biological processes are considered. The root zone was assumed to be 0.50 m deep and root distribution was assumed to decrease linearly with depth. The initial water content at the beginning of each simulation was assumed to be -100 cm throughout the soil profile. Top boundary condition was specified as atmospheric BC with surface runoff. At the bottom of the profile a free drainage BC was imposed. The soil water and chemical balance was calculated for one year.

2.1.2 SOIL GEOCHEMICAL MODEL

In the first scenario (Run3a), the standard Hydrus “General Solute Transport” was used, with salinity modelled as a tracer with a unit input concentration. This is the base case which serves as a yardstick against which the effects of saline irrigation water can be compared. Simulations consider effects on soil water chemical composition and on vegetation (i.e. crops). Only the effect of water stress on plant water uptake was considered (for details see section 2.3.4).

The same scenario was rerun (Run3b) using the Hydrus “Major Ion Chemistry” module and concentrations of major ions (for details see section 2.3.3). Salinity was explicitly modelled with major ions in irrigation water (Ca, Mg, Na, K, alkalinity, Cl, SO4) accounted for. In addition to effects on soil water chemical composition, this scenario further calculates the effects of both water and salinity stress on plant water uptake.

A third scenario (Run3c) uses the Hydrus “Major Ion Chemistry” module and considers the reduction of hydraulic conductivity due to the solution composition (McNeal 1968, 1974). The accumulation of monovalent cations, such as sodium and potassium, often leads to clay dispersion, swelling, flocculation and overall poor soil physico-mechanical properties. These processes have an adverse effect on the soil hydraulic properties including hydraulic conductivity, infiltration rates and soil water retention as a result of swelling and clay dispersion. These negative effects are usually explained based on the diffuse double layer theory.

Scenario four (Run3d) considers amended produced water while a final fifth scenario (Run3e) uses treated produced water (see section 2.3.3 for chemical composition of irrigation water).

The initial concentrations of soil exchangeable cations (Table 2.2) are taken from a lysimeter study by Ringrose-Voase (2004). The lysimeter is located in paddock C1 at the Australian Cotton Research Institute (ACRI) near Narrabri in northern New South Wales (30° 11.53’ South, 149° 36.31’ East). The soil is a Haplic, Self-mulching, Grey Vertosol. The bulk density for different soil depths was estimated to range between
1.32 and 1.45 (Ringrose-Voase 2004). Because the total cation exchange capacity is similar for all three soil layers, the cation exchange capacity and the concentration of exchangeable cations of the first layer was assigned to all three layers.

Table 2.2 Initial concentrations of exchangeable cations (source: Ringrose-Voase 2004).

<table>
<thead>
<tr>
<th>Soil layer</th>
<th>Bulk density (g/cm³)</th>
<th>CEC (meq/kg soil)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (0-0.3 m)</td>
<td>1.32</td>
<td>275</td>
</tr>
<tr>
<td>2 (0.3-0.7 m)</td>
<td>1.42</td>
<td>278</td>
</tr>
<tr>
<td>3 (0.7-1.0 m)</td>
<td>1.45</td>
<td>274</td>
</tr>
</tbody>
</table>

Exchangeable cations for layer 1

<table>
<thead>
<tr>
<th>Ions</th>
<th>Ca</th>
<th>Mg</th>
<th>Na</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>mmol/kg</td>
<td>86.3</td>
<td>44</td>
<td>4.6</td>
<td>9.4</td>
</tr>
<tr>
<td>meq/kg</td>
<td>173</td>
<td>88</td>
<td>4.6</td>
<td>9.4</td>
</tr>
</tbody>
</table>

The initial solution composition in the soil profile (Table 2.3) was defined using the solution composition of rainwater measured in Wagga-Wagga (Crosbie et al. 2012). Note that this solution will be automatically brought into equilibrium with the cation exchange complex.

Table 2.3 Initial soil solution composition used to calculate initial solution in equilibrium with the cation exchange complex. Data represents composition of rainwater in Wagga-Wagga (Source: Crosbie et al. 2012).

<table>
<thead>
<tr>
<th>Solution composition (meq/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
</tr>
<tr>
<td>0.012</td>
</tr>
</tbody>
</table>
2.2 Numerical model for multi-component reactive transport modelling in saturated/unsaturated media

2.2.1 HYDRUS

HYDRUS-1D (Šimůnek et al. 2008, 2009) is a public domain computer software package (www.hydrus2d.com) that simulates the one-dimensional movement of water, heat, and multiple solutes in variably saturated media. The program uses finite elements to numerically solve the Richards equation for saturated-unsaturated water flow and Fickian-based advection-dispersion equations for both heat and solute transport. The flow equation includes a sink term to account for water uptake by plant roots as a function of both water and salinity stress. The heat transport equation considers conduction as well as advection with flowing water. The solute transport equations assume advective-dispersive transport in the liquid phase, and diffusion in the gaseous phase. The transport equations also include provisions for nonlinear and/or nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one which is independent of other solutes, and one which provides the coupling between solutes involved in the sequential first-order decay reactions. The program may be used to analyse water and solute movement in unsaturated, partially saturated, or fully saturated media. The flow region itself may consist of non-uniform (layered) soils. The unsaturated soil hydraulic properties (the constitutive relationships) are described using van Genuchten (1980) or Brooks and Corey (1964, 1966) type analytical functions, or modified van Genuchten type functions that produce a better description of the hydraulic properties near saturation. HYDRUS-1D incorporates hysteresis by assuming that drying scanning curves are scaled from the main drying curve, and wetting scanning curves from the main wetting curve. Root growth is simulated by means of a logistic growth function. Water and salinity stress response functions can also be considered. HYDRUS-1D was recently modified to also allow simulations of the transport of viruses, colloids, and bacteria (Schijven and Šimůnek 2002; Bradford et al. 2003). HYDRUS-1D uses a Microsoft Windows based Graphics User Interface (GUI) to manage the input data required to run the program, as well as for nodal discretization and editing, parameter allocation, problem execution, and visualization of results. All spatially distributed parameters, such as those for various soil horizons, the root water uptake distribution, and the initial conditions for water, heat and solute movement, are specified in a graphical environment. The program offers graphs of the distributions of the pressure head, water content, water and solute fluxes, root water uptake, temperature and solute concentrations in the soil profile at pre-selected times. Also included are a small catalogue of unsaturated soil hydraulic properties (Carsel and Parish 1988), as well as pedotransfer functions based on neural networks (Schaap et al. 2001).

2.2.2 UNSATCHEM

The solute transport module of HYDRUS-1D as described above is limited to single ions, or ions subject to relatively simple first-order consecutive decay reactions (e.g., nitrification-denitrification chains, or radionuclide decay chains). As an alternative to this approach, we recently implemented into HYDRUS-1D also a major ion chemistry module based on the UNSATCHEM model (Šimůnek and Suarez 1994, 1997; Šimůnek et al. 1996, 2008). This module considers the transport of major ions and carbon dioxide in soils. CO₂ transport is assumed to be governed by diffusion in both the liquid and gas phases, and by advection in the liquid phase. The major variables of the chemical system are Ca, Mg, Na, K, SO₄, Cl, NO₃, H₂SiO₄, alkalinity, and CO₂ (Table 6). The model accounts for equilibrium chemical reactions between these components such as complexation, cation exchange and precipitation-dissolution. For the precipitation-dissolution of calcite and the dissolution of dolomite, either equilibrium or multicomponent kinetic expressions are used, including both forward and backward reactions. Other precipitation-dissolution reactions considered involve gypsum, hydromagnesite, nesquehonite, and sepiolite. Since the ionic strength of soil solutions can vary considerably in time and space and often reach high values, both the modified Debye-Hückel and Pitzer expressions were incorporated into the model, thus providing options for calculating single-ion activities. This module also considers the effects of solution composition on the
unsaturated soil hydraulic properties. The UNSATCHEM module of HYDRUS-1D enables quantitative predictions of processes involving major ions, such as simulations of the effects of salinity on plant growth and estimating the amount of water and amendment required to reclaim soil profiles to desired levels of salinity and ESP (exchangeable sodium percentage).

Table 2.4 Chemical species included in the UNSATCHEM major ion module of HYDRUS-1D.

<table>
<thead>
<tr>
<th>Category</th>
<th>Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous components</td>
<td>Ca$^{2+}$, Mg$^{2+}$, Na$^+$, K$^+$, SO$_4^{2-}$, Cl$^-$, NO$_3^-$</td>
</tr>
<tr>
<td>Complexed species</td>
<td>CaCO$_3$, CaHCO$_3^-$, CaSO$_4^{2-}$, MgCO$_3^-$, MgHCO$_3^-$, MgSO$_4^2$, NaCO$_3$, NaHCO$_3^-$, NaSO$_4^-$, KSO$_4$</td>
</tr>
<tr>
<td>Precipitated species</td>
<td>CaCO$_3$, CaSO$_4$, 2H$_2$O, MgCO$_3$, 3H$_2$O, Mg$_2$(CO$_3$)$_2$(OH)$_2$, 4H$_2$O, Mg$_2$Si$_2$O$_5$(OH)$_2$, 3H$_2$O, CaMg(CO$_3$)$_2$</td>
</tr>
<tr>
<td>Sorbed (exchangeable) species</td>
<td>Ca, Mg, Na, K</td>
</tr>
<tr>
<td>CO$_2$-H$_2$O species</td>
<td>$P_{CO_2}$, H$_2$CO$_3^-$, CO$_3^{2-}$, HCO$_3^-$, H$^+$, OH$^-$, H$_2$O</td>
</tr>
<tr>
<td>Silica species</td>
<td>H$_4$SiO$_4$, H$_2$SiO$_4^-$, H$_3$SiO$_4^{2-}$</td>
</tr>
</tbody>
</table>
2.3 Model implementation

2.3.1 SOIL HYDROLOGICAL CHARACTERISTICS

The soil water redistribution in the soil profile will be discussed for scenario 1, the base case (Run3a) against which changes in the other scenarios will be compared. Boundary conditions are summarised in Table 2.5. The following features were simulated with Hydrus:

- Time series of soil water content, matric head, and tracer concentrations
- Depth profiles of soil water content, matric head, and tracer concentrations
- Water fluxes bottom (drainage) and top (actual root water uptake) of soil profile.

Table 2.5 Defined variable boundary conditions.

<table>
<thead>
<tr>
<th>Time</th>
<th>Flux [cm/day]</th>
<th>Boundary solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Every 5 days</td>
<td>6 cm/day</td>
<td>Irrigation water</td>
</tr>
<tr>
<td>Constant</td>
<td>0.8 cm/day</td>
<td>Potential transpiration</td>
</tr>
<tr>
<td>Constant</td>
<td>0.2 cm/day</td>
<td>Potential evaporation</td>
</tr>
</tbody>
</table>

The 1-m numerical domain was discretised in 100 finite elements, each 0.01 m long. The numerical grid, the three soil layers and four observations nodes are shown in Figure 2.3.

![Figure 2.3 Finite element grid with soil layers (left) and location of four observation nodes (right).](image)

2.3.2 SOIL GEOCHEMICAL MODEL

Migration of chemicals in soil is primarily by advection (sometimes referred to as convection) and dispersion (ignoring gaseous transport). By mathematically solving the solute transport or advection-dispersion equation (ADE when advection is used, or CDE when convection is used), predictions of solute concentrations at different depths and times can be obtained (Mallants et al. 2011). For transport of inert, non-adsorbing contaminants during transient water flow the ADE is as follows (Toride et al. 1995):

\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial c}{\partial z} \right) - \nu \frac{\partial c}{\partial z}
\]

Equation 3
where \( c \) is solute concentration in the water phase (mg/L), \( t \) is time (s), \( D \) is hydrodynamic dispersion (total dispersion, which is the sum of molecular diffusion and mechanical dispersion) \( (m^2/s) \), \( z \) is soil depth (m), and \( v \) is pore-water velocity \( (m/s) \). In the unsaturated zone, advective transport usually becomes an important component of the overall transport, hence the two-component dispersion coefficient \( (D) \ (m^2/s) \) has to be used. Molecular diffusion \( (D_m) \ (m^2/s) \) is one component of the hydrodynamic dispersion, but unless water flow is extremely slow, molecular diffusion is of secondary importance\(^3\) in the migration of elements in soils and permeable aquifer sediments. The second component of hydrodynamic dispersion is mechanical dispersion, \( \alpha \times v \), as shown in the following equation:

\[
D = D_p + \alpha \times v \quad \text{Equation 4}
\]

where \( D \) is hydrodynamic dispersion, or simply dispersion, \( \alpha \) is dispersivity\(^4\) \( (m) \), and \( v \) is pore-water velocity \( (m/s) \). Water content \( \theta \) is needed to obtain pore-water velocities \( (v) \) from water fluxes \( (q) \) following:

\[
v = q/\theta \quad \text{Equation 5}
\]

Diffusion or molecular diffusion is transport of solutes from an area of higher concentration to an area of lower concentration; it occurs as long as such a concentration gradient exists, even if the water is not flowing. Mechanical dispersion is a transport process due to heterogeneous distribution of water flow velocities within and between different soil pores (Mallants et al. 2011). The result is that some solute particles will be ahead of the solute front whereas others will lag behind, leading to solute mixing and generally a bell-shaped distribution of velocities and thus of arrival times, typical of a breakthrough curve. The processes of molecular diffusion and mechanical dispersion are incorporated into one parameter, the hydrodynamic dispersion coefficient \( D \). Phenomenologically, dispersion has two effects: it increases the passage time of a complete solute pulse and it decreases the maximum concentration. In the case of a toxic contaminant for example, it leads to a longer exposure time but also to a lower maximum concentration.

Dispersivity is a transport parameter that is often obtained experimentally by fitting measured breakthrough curves with analytical solutions of the advection-dispersion equation (Seuntjens et al. 2001). In this study a dispersivity \( = 0.1 \) m was taken, or one tenth of the total travel distance from top to bottom of the soil profile.

Partitioning between the solid and solution phases is described with the Gapon equation (White and Zelazny 1986) provided in the Major Ion Chemistry module. This requires definition of the Gapon Exchange Constants for exchange of calcium and magnesium, calcium and potassium, and calcium and sodium. The Gapon Exchange Constant are taken from Jacques et al. (2012). The exchange coefficients can be interpreted as follows: for the \( \text{Ca}^{2+}/\text{Mg}^{2+} \) exchange, \( \text{Ca}^{2+} \) is the preferred ion relative to \( \text{Mg}^{2+} \). For the \( \text{Ca}^{2+}/\text{Na}^+ \) exchange, \( \text{Ca}^{2+} \) is the preferred ion relative to \( \text{Na}^+ \). Finally, for the \( \text{Ca}^{2+}/\text{K}^+ \) exchange, \( \text{K}^+ \) is the preferred ion relative to \( \text{Ca}^{2+} \).

Table 2.6 Gapon Exchange Constants (Source: Jacques et al. 2012).

<table>
<thead>
<tr>
<th>Soil layer</th>
<th>( K [\text{Ca/Mg}] )</th>
<th>( K [\text{Ca/Na}] )</th>
<th>( K [\text{Ca/K}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.2</td>
<td>2.9</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>1.2</td>
<td>2.9</td>
<td>0.2</td>
</tr>
<tr>
<td>3</td>
<td>1.2</td>
<td>2.9</td>
<td>0.2</td>
</tr>
</tbody>
</table>

\(^3\) Mechanical dispersion in most subsurface transport problems dominates molecular diffusion in the liquid phase, except when the fluid velocity becomes relatively small or is negligible. Diffusion dominated transport occurs in low permeability media, such as clays and rock matrices.

\(^4\) Longitudinal dispersivity \( (\alpha_v) \) is a term used to indicate dispersion along the main direction of flow.
Three different chemical compositions of the irrigation water were assumed; the first corresponds to untreated produced water (scenario 2 and 3), the second to surface water amended produced water (scenario 4), and the third to treated produced water (scenario 5). The first (untreated) and third (treated) compositions represent end-members that can be mixed to various degrees to obtain fit-for-purpose irrigation water. Unlike the amended and treated produced waters that are actually being tested and/or being used for irrigation, the untreated water would almost certainly not receive any permission for use as irrigation water owing to its high potassium and SAR values (Table 2.7). It is included here only to demonstrate effects of several interacting processes, such as major ion composition triggering a reduction in soil hydraulic conductivity and subsequent modification of water redistribution in the soil profile and how root water uptake responds to such changes.

It is worth noting that the treated water is still much more saline than rainfall (see Table 2.3 for rainfall composition). In other words, even irrigation with treated produced water is likely to have some effect on the soil’s chemical balance.

Table 2.7 Composition of irrigation waters. Kenya/rain water = ratio of treated produced water to rain water composition.
*site 4 from Table 1.5 (QGC 2011); † maximum values from Table 1.5; ** from SunWater 2014 (average across 3 sampling dates between July 2013 to 30 June 2014); @ calculated as $\Sigma[EC_i(S.cm^2/mol)xC_i(mmol/L)]$
(Appelo and Postma 2004 Table 1.7)

It is important to note that from all the ions considered in the simulation, only potassium (K) has an ANZECC guide value for irrigation (ANZECC 2000). For long term use (up to 100 years), the guide value for K is 0.05 mg/L. For short term use (up to 20 years), the guide value is 0.8 mg/L. The calculated SAR for the untreated produced water is 77 (Table 2.7); this is considerably higher than the DEHP maximum guide value of 12 for light soils (95th percentile over a one-year period) (DEHP 2014).

The scenarios 2 (simulation Run3b) and 3 (simulation Run3c) differ only in the way effects of major ion chemistry on soil hydraulic properties are treated: only in scenario 3 is reduction in hydraulic conductivity due to major ion composition and corresponding pore space blockage accounted for. Any major ion composition in scenario 2 will not affect hydraulic conductivity.

The effect of solution chemistry on the hydraulic conductivity in the major ion chemistry module is calculated as follows:

$$K(h, pH, SAR, C_0) = r(pH, SAR, C_0)K(h)$$  \hspace{1cm} \text{Equation 6}

where SAR is the sodium adsorption ratio, $C_0$ is the total salt concentration of the ambient solution (meqL$^{-1}$), and $r$ is a scaling factor which represents the effect of the solution composition on the final hydraulic conductivity $[-]$, and which is related to pH, SAR and salinity (Šimůnek et al. 2009). Conceptually the effects relate to clay swelling as a result of changes in ion composition here expressed via the parameters SAR and $C_0$.

We note that other effects of solution chemistry on hydraulic properties such as mineral precipitation resulting in a decrease of pore space and hence decrease in hydraulic conductivity may be equally important to determine a soil’s water balance under irrigation in arid and semi-arid regions. Examples of a more general approach to couple major ion chemistry with soil hydraulic and solute transport parameters are available from Jacques et al. (2013). These authors implemented a Kozeny-Carman type equation to relate the permeability to the porosity in the coupled HYDRUS-PHREEQC simulator which accommodates effects of mineral dissolution and/or precipitation; other relationships were implemented that relate tortuosity (and subsequently diffusion coefficient) to porosity changes.

Both scenarios 2 and 3 use three solution compositions for three consecutive periods:

- Solution 1 is rainwater (used as initial solution, Table 2.3),
- Solution 2 is untreated produced water (used for irrigation, Table 2.7),
- Solution 3 is again rainwater (not currently used, but may be used if precipitation is considered).

2.3.4 VEGETATION PARAMETERS

To simulate the effect of i) water stress separately and ii) both water stress and salinity, two cases are considered. First, the effect of water stress separately was analysed using Feddes’ model (Feddes et al. 1978) (see Figure 2.4 for a conceptual representation and Table 2.8 for relevant parameters). Plant water stress response functions specific for pasture and alfalfa are displayed in Figure 2.5

Whether HYDRUS selects P2H or P2L as the limiting pressure head depends on the value of the potential transpiration rate, $T_p$. If $T_p > r2H$ (0.5 cm/day), then P2H (-200 cm) is selected. If $T_p < r2L$ (0.1 cm/day), then P2L (-800 cm) is selected. If $T_p$ is in between $r2H$ and $r2L$, linear interpolation between P2H and P2L is applied. In this study $T_p = 0.8$ cm/day, hence P2H is selected.

When salinity stress is considered in HYDRUS, a selection must be made whether the effect of salinity stress is additive or multiplicative to water stress. Here the multiplicative Threshold Model function according to Maas (1990) was selected. The Threshold Model has two parameters, the threshold parameter and the slope parameter (Table 2.9). The first parameter represents the value of the minimum osmotic head (the salinity threshold) above which root water uptake occurs without a reduction. The second parameter is the
slope of the curve determining the fractional root water uptake decline per unit increase in salinity below the threshold. Root water uptake reduction parameters for alfalfa were used to investigate combined water and salinity stress as no salinity stress parameters are available for pasture (all other root water uptake parameters are those for pasture).

Table 2.8 Root water uptake reduction parameters without solute stress (based on Wesseling et al. 1991).

<table>
<thead>
<tr>
<th>Feddes' parameters</th>
<th>Pasture</th>
<th>alfalfa</th>
<th>Parameter definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>P0 (cm)</td>
<td>-10</td>
<td>-10</td>
<td>Value of the pressure head below which roots start to extract water from the soil</td>
</tr>
<tr>
<td>P0pt (cm)</td>
<td>-25</td>
<td>-25</td>
<td>Value of the pressure head below which roots extract water at the maximum possible rate</td>
</tr>
<tr>
<td>P2H (cm)</td>
<td>-200</td>
<td>-1500</td>
<td>Value of the limiting pressure head, below which roots cannot longer extract water at the maximum rate (assuming a potential transpiration rate of r2H)</td>
</tr>
<tr>
<td>P2L (cm)</td>
<td>-800</td>
<td>-1500</td>
<td>As above, but for a potential transpiration rate of r2L</td>
</tr>
<tr>
<td>P3 (cm)</td>
<td>-8000</td>
<td>-8000</td>
<td>Value of the pressure head, below which root water uptake ceases (usually taken at the wilting point)</td>
</tr>
<tr>
<td>r2H (cm/day)</td>
<td>0.5</td>
<td>0.5</td>
<td>Potential transpiration rate [LT^{-1}] (currently set at 0.5 cm/day)</td>
</tr>
<tr>
<td>r2L (cm/day)</td>
<td>0.1</td>
<td>0.1</td>
<td>Potential transpiration rate [LT^{-1}] (currently set at 0.1 cm/day)</td>
</tr>
</tbody>
</table>

Figure 2.4 Schematic of the plant water stress response function, α(h), as used by a) Feddes et al. (1978) and b) van Genuchten (1987). The Feddes et al. function was used in this study: for definition of parameters, see Table 2.8 (h1 = P0, h2 = P0pt, h3 = P2L/P2H, h4 = P3).
Figure 2.5 Plant water stress response function, $\alpha(h)$, for pasture and alfalfa as applied in this study.

Table 2.9 Root water uptake reduction parameters with solute stress for alfalfa.

<table>
<thead>
<tr>
<th>Threshold Model</th>
<th>cm</th>
<th>dS/m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threshold(^5)</td>
<td>-1473.52 (cm)</td>
<td>2</td>
</tr>
<tr>
<td>Slope(^6)</td>
<td>9.57854e-005 (1/cm)</td>
<td>7.3</td>
</tr>
<tr>
<td>Osmotic coefficient</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

2.3.5 SUMMARY OF SIMULATION CASES

A total of five different scenarios are considered in the numerical analysis to evaluate (Table 2.10):

- A base case scenario against which other scenarios can be compared: the base case involves soil water balance calculations without i) effects of major ion chemistry on hydraulic properties, ii) effects of salinity stress on root water uptake, iii) effects of competing adsorption between major ions on ion migration in soil;
- Effect of major ion chemistry on hydraulic conductivity (scenarios 2 and 3);
- Effect of three different irrigation water qualities (scenarios 2/3, 4, and 5).

\(^5\) Threshold = -3.8106*(Th\_ECe*2)+0.507 (m), where Th\_ECe = 2 dS/m for alfalfa; the electrical conductivity of the saturation extract is converted into electrical conductivity of the soil water through the multiplication factor 2

\(^6\) Slope= (SI\_ECe/2)/(381.06) (1/m), where SI\_ECe = 7.3 dS/m for alfalfa
Table 2.10 Description of scenarios used.

<table>
<thead>
<tr>
<th>Scenario #</th>
<th>Scenario description (main processes)</th>
<th>Irrigation water quality</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Base case: general solute transport module with single component. Comparison between pasture and alfalfa root water uptake without solute stress</td>
<td>Tracer only (6 cm/day irrigation rate)</td>
</tr>
<tr>
<td>2</td>
<td>Major ion chemistry solute transport without reduction in hydraulic conductivity; root water uptake with multiplicative solute stress</td>
<td>Untreated produced water (6 cm/day irrigation rate)</td>
</tr>
<tr>
<td>3</td>
<td>Major ion chemistry solute transport with reduction in hydraulic conductivity; root water uptake with multiplicative solute stress</td>
<td>Untreated produced water (4 cm/day irrigation rate to avoid water ponding due to reduced hydraulic conductivity)</td>
</tr>
<tr>
<td>4</td>
<td>Major ion chemistry solute transport with reduction in hydraulic conductivity; root water uptake with multiplicative solute stress</td>
<td>Surface water-amended produced water (6 cm/day irrigation rate)</td>
</tr>
<tr>
<td>5</td>
<td>Major ion chemistry solute transport with reduction in hydraulic conductivity; root water uptake with multiplicative solute stress</td>
<td>Treated produced water (6 cm/day irrigation rate)</td>
</tr>
</tbody>
</table>
3 Detailed description of the simulation cases

3.1 Scenario 1: Base case

The base case scenario represents a simplified conceptualisation of water flow and solute transport under irrigation boundary conditions involving water containing only a non-reactive tracer. This scenario does not consider major ion chemistry, root water uptake affected salinity stress, and soil hydraulic properties influenced by salinity. The calculated soil water balance, including root water uptake and actual plant transpiration, will serve as a reference against which other scenarios that do include additional coupled processes will be compared.

Simulated water content (Figure 3.1) and pressure head (Figure 3.2) time series show typical patterns linked to alternating periods of soil wetting during and following irrigation and drying periods in the intermittent periods between irrigation events. At deeper depths in the soil profile, the variations become smaller as the water redistribution becomes increasingly buffered as it moves through soil. Total simulation time for the base case is 30 sec on Personal Computer with an Intel Core i5-2540M CPU and 2.6 GHz.

Figure 3.1 Simulated water content at three depths in the soil profile. Only first 100 days are shown. Arrows show times at which results at observation nodes are outputted for producing profile plots (at 30, 60, 90 days).
Figure 3.2 Simulated pressure head at three depths in the soil profile. Only first 100 days are shown.

The solute accumulation in the soil profile at different depths is shown in Figure 3.3. Note that a unit tracer concentration of 1 mg/L was assumed in the infiltration water. At the shallower depths of 10 and 20 cm the cyclic variation in solute concentration reflects the variation in water content seen in Figure 3.1. Print time steps indicate the time when detailed profile results are outputted to produce graphs like Figure 3.4.

Figure 3.3 Simulation of tracer movement through soil. Tracer is applied through the irrigation water.

Solute concentration profiles are shown in Figure 3.4 at the end of the time period with transpiration and evaporation (lasting four days), before irrigation starts. During this period, as a result of evaporation, water content at the soil surface decreases (Figure 3.1), creating at the same time the pressure head gradient,
which produces upward water flow towards the soil surface. Water flowing towards the soil surface carries with it solute ions, which accumulate at the soil surface during evaporation. Note that during evaporation, water leaves the soil profile while leaving solute ions behind. As a result of decreasing water contents and upward water flow towards the surface (bringing additional solute ions), concentration of solute ions increases significantly during this time period.

As a whole, the solute profiles reflect the equilibrium between infiltration with irrigation water, water and solute redistribution due to transpiration and evaporation, and downward leaching (Figure 3.4). The prominent effects of transpiration and evaporation on the solute profile become further apparent when these processes are suppressed (Figure 3.4). When transpiration is suppressed during the simulations a much smaller solute concentration across the entire soil profile becomes apparent. If subsequently also soil evaporation is suppressed, the effect is much smaller although some further decrease in solute concentration is observed after 365 days. This effect is mainly caused by differences in soil water content between the different models: highest water content is observed when both transpiration and evaporation are suppressed, whereas lowest water contents exist when those processes are included (Figure 3.4). As expected, the effect of suppressing transpiration is much greater than suppressing evaporation (daily potential transpiration rate is 0.8 cm/day while daily potential evaporation rate is 0.2 cm/day). At the top of the soil profile, the water content without ET is 1.7 times larger than when ET is included. This ratio almost corresponds to the ratio of 2.2 obtained by dividing solute concentration with ET and without ET. This demonstrates that higher solute concentration are indeed due to lower water contents following water loss mainly due to transpiration and to a lesser degree due to soil evaporation.

Figure 3.4 Simulated solute concentration following infiltration of solute-containing irrigation water. Comparison of models including ET (solid lines), excluding T (transpiration, dashed lines) or excluding ET (evapotranspiration, symbols) (left). Comparison of simulated soil water content for models including ET, excluding T or excluding ET (right).

Cumulative fluxes are compared for pasture and alfalfa (only water stress functions applied for both crops). As can be observed from Figure 3.5, there is no noticeable difference between the two crops. For both crops, the actual (281 cm) and potential (292 cm) cumulative transpiration flux are very similar, indicating there was little water stress during the simulations (Figure 3.5). The cumulative potential and actual surface flux (infiltration and evaporation) are both negative (downward) and identical, meaning potential and actual evaporation are equal. The cumulative actual bottom flux is slightly negative, meaning a small drainage flux is exiting the soil profile. This is expected as the irrigation rate = 1.2 × potential ET (6 cm irrigation over 5 days/5 cm potential ET over 5 days).
3.2 Scenario 2: Major ion chemistry

This scenario and all subsequent scenarios consider major ion chemistry to simulate behaviour of multiple solutes added to the soil profile through use of produced water (untreated in scenario 2). Consideration of major ion chemistry provides insight in the distribution of individual ions (both in the aqueous phase and adsorbed on the solid phase), the electrical conductivity and the sodium adsorption ratio in soil. The simulations also provide concentrations of minerals such as calcite, dolomite or gypsum. Scenario 2 further links the soil chemistry (i.e. salinity) to salinity stress of plants (in addition to water stress invoked in scenario 1), allowing calculation of reduction in water uptake by vegetation. The reduction in water uptake in turn has an effect on the water and solute distribution in the soil profile (see discussion in Section 3.1), and thus on the drainage flux across the bottom of the profile. Unlike scenario 3, 4, and 5, effects of salinity on hydraulic properties are not considered in scenario 2.

The tracer profile developed over one year simulation is quite different across the three scenarios 1, 2 and 3 (Figure 3.6). If only water stress is accounted for in absence of major ion chemistry (scenario 1), the tracer concentration gradually builds up over the entire soil profile, with a maximum concentration at a soil surface due to a “concentration” effect (Figure 3.14). As a result of soil evaporation (E) and plant transpiration (T), water contents in the top layer are minimal, resulting in an increase of concentrations. Also note that the output is obtained just before irrigation starts (at the end of a period with irrigation at day 1 followed by 4 days of ET), when water contents in the top layer are low (resulting in an increase in concentration). When major ion chemistry is accounted for (scenario 2 and 3), salinity stress is induced resulting in a significant reduction in the root water uptake (Figure 3.14). This in turn changes the water distribution as exemplified by the changes in the solute profile (Figure 3.6): the lower concentrations in the bottom part of the soil profile are due to the higher drainage flux causing dilution of the tracer. In the case of scenario 3 (reduction in hydraulic conductivity due to the soil solution composition), the hydraulic conductivity decreased and caused the water to pond on the soil surface. This caused the tracer to accumulate at the 40 to 50 cm depth for the first 150 days of the simulation.
Figure 3.6 Solute tracer concentration profiles for scenario 1 (left), 2 (middle) and scenario 3 (right).

Water content at a particular depth in the soil profile seems quite constant during the simulation (Figure 3.7); however, this is only so because we print water content profiles at the same time of the irrigation cycle (i.e., just before irrigation starts). On the other hand, there is a gradual increase of water content with depth as a result of the plant water uptake in the top 50 cm.

The simulated SAR and electrical conductivity evolution illustrate high SAR values of over 100 progressing downward the soil profile. The rate at which SAR moves through soil is determined by the migration of Na and Ca. Because Na migration is retarded, SAR migration will be retarded too (Figure 3.9). The precipitation of Ca in the top of the profile further influences the migration of SAR (Figure 3.10). The electrical conductivity progresses much faster because it is mainly determined by chloride (Figure 3.9), and reaches values beyond 10 dS/m (Figure 3.8). Electrical conductivity migration will be retarded if mineral precipitation happens.

The SAR ANZECC trigger value of 20 (sandy-sandy loam soil, see Table 1.5) is exceeded relatively quickly, i.e. down to 40 cm after 150 days. The EC ANZECC trigger value of 0.65 dS/m (see Table 1.5) is exceeded very quickly, i.e. down to 70 cm after 30 days.

Figure 3.7 Water content profiles for scenario 2 (left) and scenario 3 (right).
From the six minerals considered in the Major Ion Chemistry (calcite, dolomite, gypsum, nesquehonite, hydromagnesite, sepolite), only calcite is formed. The concentration of calcite gradually increases with depth as more irrigation water entered the soil (Figure 3.10). The effect of calcite precipitation is clearly reflected in the concentration of dissolved calcium ions (Figure 3.9): close to the surface, dissolved calcium is nearly absent as a result of precipitation of calcite. Using a calcite mineral density 2.72 g/cm³, total porosity from Table 2.1, and soil bulk density from Table 2.2, the calculated mineral volume of precipitated calcite after 365 days was shown to have increased to approximately 0.015 cm³ cm⁻³ at the soil surface; the mineral phase occupies nearly 3% of total soil porosity. While this is a relatively small fraction of the available pore space, this volume is expected to increase as irrigation continues for many years. The long-term effects of salt formation on soil hydrology and plant response needs further corroboration.

There are clear differences in the way the major cations Ca, Mg, Na and K migrate through soil (Figure 3.9). Calcium is mainly affected by precipitation in the top soil; ahead of the precipitation front calcium is only weakly retarded compared to chloride. Magnesium displays accumulation at the soil surface due to a decrease in soil water owing to ET; the similarity between magnesium and chloride indicates the former is little retarded. Sodium displays the largest retardation as is expected from the Gapon cation exchange constant (see Table 2.6). The migration of potassium is somewhat similar to Mg, although it exhibits nearly constant values in the top 30 cm of the soil profile.
Figure 3.9 Simulated concentrations of dissolved major ions Ca, Mg, Na, K, and Cl. ANZECC trigger value for sodium (see Table 1.3).

Figure 3.10 Calcite concentration for scenario 2 (left). Calcite mineral volume after 365 days of irrigation (right).
3.11 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for scenario 2.

The sodium ANZECC trigger value of 20 meq/L (460 mg/L, see Table 1.5) is exceeded relatively quickly, i.e. down to 60 cm after 150 days.

Due to the combined effect of water and salinity stress on root water uptake, the actual transpiration is considerably lower than the potential transpiration (Figure 3.11). The lower transpiration results in more water remaining in the soil and more water draining through the bottom of the profile (123 cm versus 84 cm for scenario 1).

3.3 Scenario 3: Major ion chemistry including effect of salinity on soil hydraulic properties

Scenario 3 was run (Run3c) using the Major Ion Chemistry module and concentrations of major ions associated with irrigation of untreated produced water, while now also considering reduction of hydraulic conductivity due to solution composition (based on the McNeal model).

During the simulations and based on an irrigation rate of 6 cm/day once in five days, the hydraulic conductivity was reduced automatically due to the salinity effect to the point that water could not get into the profile without causing ponding. Therefore, we reduced the irrigation rate to 4 cm/day once in five days to avoid ponding conditions. Under those new soil hydrological conditions, major ion chemistry resulted in the following observations. Compared to the two previous scenarios, the SAR moves downward about two times slower, while also the electrical conductivity reaches lower values at the same depths (Figure 3.12).
The actual transpiration becomes severely reduced, i.e. to 188 cm versus 240 cm for scenario 2 (Figure 3.13). The decrease in root water uptake between -20 and -40 cm soil depth is not due to salinity stress caused by a too high EC. This occurs at the very end of the simulation, when the SAR front reaches the second soil layer, causing the hydraulic conductivity reduction which in turn causes water logging in this area. The reduction in water uptake then is due to a too high pressure head (> -25 cm, see parameter POpt in Table 2.8) to allow water uptake at an optimal rate (Figure 3.14).
Figure 3.14 Root water uptake function for scenario 1 (top left), scenario 2 (top right) and scenario 3 (bottom left). Pressure head exceeds the $P_{\text{Opt}} = -25$ cm threshold after 300 days (bottom right).
3.4 Scenario 4: Amended produced water

Scenario 4 (run3d) considers use of amended irrigation water with chemical composition defined in Table 1.5, while all other processes and parameters are identical to those of scenario 3. The simulated SAR profiles shown in Figure 3.15 demonstrate that the SAR ANZECC trigger value (SAR=20) for sand-sandy loam is exceeded after 365 days for a small section of the profile. The SAR ANZECC trigger value (SAR=5) for light clay is exceeded in the top 30 cm after 150 days, whereas after 365 days it is exceeded for the top 50 cm.

The EC ANZECC trigger value of 0.65 dS/m is exceeded across the entire soil profile after 90 days. The relatively high EC is due to the EC of the irrigation water (1.57 dS/m). In terms of contributions of individual ions in the amended irrigation water to the EC, the most important contributors to EC are sulfate (36% contribution to total EC), sodium (26% contribution to total EC) and chloride concentration (23% contribution to total EC) (Table 1.2).

Optimisation of irrigation water quality can be done by reducing concentration of those ions that contribute most to the total EC, in the above example that is sulfate, sodium, and chloride, where the contribution of each ion to the total EC is calculated using the procedure given in Table 1.2.

![Simulated SAR and EC profiles for scenario 4](image)

Figure 3.15 Simulated SAR (left) and electrical conductivity (right) for scenario 4. ANZECC trigger value for SAR and EC (see Table 1.3).

The cumulative potential and actual surface and bottom fluxes are shown in Figure 3.16. The use of lower salinity irrigation water results in reduced salinity stress: the actual transpiration is slightly higher. As a result, the drainage across the bottom of the soil profile is lower too. This scenario results in a more efficient use of the applied irrigation water.
Figure 3.16 Cumulative potential and actual surface (infiltration and evaporation) and transpiration flux and cumulative actual bottom flux for scenario 4, in comparison with scenario 3.
3.5 Scenario 5: Treated produced water

In scenario 5 (run3e) irrigation water has the chemical composition of treated produced water as defined in Table 1.5, while all other processes and parameters are identical to those of scenario 3 and 4. The simulated SAR profiles now remain below the lowest SAR ANZECC trigger value (SAR=5) for light clay (Figure 3.17). This result is as expected, given the low SAR value (i.e. 1.6) of the irrigation water and the absence of any initial salt built-up in the soil profile (initial SAR value is 1.25 throughout entire soil profile) or without other salt inputs into the soil profile (e.g. from saline shallow groundwater or later inflow from water discharging at the break-of-slope (Biggs et al. 2012)).

The EC ANZECC trigger value of 0.65 dS/m is generally not exceeded across the entire soil profile, except at the very top few centimetres. Although the EC of the irrigation water is low (0.29 dS/m), EC in the top of the soil profile increase to a maximum value of 0.73 dS/m due to evapotranspiration leading to dry soil conditions triggering salt concentration effects. In terms of contributions of individual ions in the treated irrigation water to the EC, the most important contributors to EC are chloride (49.6% contribution to total EC), sodium (21.5% contribution to total EC) and magnesium (11.3% contribution to total EC) (Table 2.7).

![Figure 3.17 Simulated SAR (left) and electrical conductivity (right) for scenario 5. ANZECC trigger value for SAR (light clay) and EC (0.65 dS/m) (see Table 1.3).](image)

Depth distributions of aqueous concentrations of major cations Ca, Mg, Na and K in the soil profile are shown in Figure 3.18. Calcium, magnesium and sodium display similar patterns; accumulation at the soil surface due to a decrease in soil water owing to ET and gradual accumulation at deeper depths due to downward leaching. Sodium displays the largest retardation as is expected from the Gapon cation exchange constant (see Table 2.6). The migration of potassium is somewhat different in the top 30 cm of the soil profile, without a distinctive accumulation as observed with the other ions.

The sodium ANZECC trigger value of 20 meq/L (460 mg/L, see Table 1.5) is not exceeded anywhere in the soil profile.

Figure 3.19 shows concentrations of sorbed/exchangeable cations on the cation exchange sites. While the concentration front for exchangeable Na moves relatively quickly down the soil profile, the front reaching the bottom of the soil profile, other concentration fronts (i.e., for Ca and Mg) move much slower. This is mainly due to large amounts of Na being added with irrigation water and relatively small buffering capacity.
with respect to Na (note that the initial concentration for exchangeable Na was only about 2.6 meq/kg). On the other hand, the initial concentrations of exchangeable Ca and Mg were about 175 and 89 meq/kg, i.e., significantly larger than for Na, resulting in a significantly larger buffering capacity for these two cations.

![Diagram](image1)

**Figure 3.18 Simulated concentrations of dissolved major ions Ca, Mg, Na, K, and Cl.**

From the six minerals considered in the Major Ion Chemistry (calcite, dolomite, gypsum, nesquehonite, hydromagnesite, sepolite), only calcite is formed. The concentration of calcite is highest in the top soil layer where it reaches nearly 0.5 meq/kg (results not shown). Calcite formation in the top layers explains the nearly depth-invariance in aqueous calcium concentration, a behaviour quite different from that of magnesium and sodium.

Time series of soil water content and pressure head at 10 cm depth display wetting-drying cycles as a result of the applied irrigation regime and water redistribution due to evapotranspiration and drainage (Figure 3.20). Every irrigation event adds solutes to the soil which partly migrate downwards while another part accumulates in the top of the soil profile (Figure 3.18).
The pressure head data indicates that the minimum pressure (~ -15 cm) is slightly smaller than the pressure head below which root water uptake is optimal (POpt = -25 cm) (Figure 3.20). On the other hand, the maximum pressure head (~ -272 cm) exceeds the limiting pressure head below which root water uptake is no longer optimal (P2H = -200 cm). In other words, the water uptake by the grass vegetation considered here occurs at a maximum rate for about 3 out of 4 days, whereas at the 4th day it is suboptimal (see schematic root water uptake function in Figure 2.4). A more optimal irrigation regime would involve starting irrigation at day 4 to avoid the soil from becoming too dry.

Figure 3.19 Surface species concentration versus soil depth during irrigation cycles. Total adsorbed concentration for Ca, Mg, Na, and K is constant (279 meq/kg).
Figure 3.20 Calculated soil water content and pressure head at 10 cm depth (scenario 5; pasture). Every five days a 24-hour irrigation event takes place. POpt = pressure head below which root water uptake is optimal, and P2H = limiting pressure head below which root water uptake is no longer optimal (according to Figure 2.4).
3.6 Summary of soil water balance calculations

For each scenario water balance components were calculated based on a 365 day simulation period. Cumulative infiltration, actual transpiration (root water uptake) and evaporation and net drainage (outflow - inflow) values are shown for each of five scenarios evaluated (Table 3.1). The cumulative actual transpiration and evaporation are each expressed as percentage of their respective cumulative potential values (292 and 73 cm, respectively).

For all scenarios except scenario 3 cumulative infiltration equals the imposed value of 438 cm based on a 6 cm/day irrigation rate once every 5 days. Scenario 3 had a reduced irrigation rate of 4 cm/day once every 5 days resulting in a cumulative infiltration of 292 cm. The lower irrigation rate was required to avoid ponding conditions as a result of the reduction in hydraulic conductivity when untreated produced water was applied.

Cumulative actual evaporation reached its maximum value of 73 cm (0.2 cm/day) in all but one scenario (i.e. scenario 3 yielded 69 cm or 95% of the potential value owing to the reduced infiltration generating drier soil moisture conditions and hence reduced evaporation).

The cumulative actual transpiration is a useful metric to evaluate combined effects of soil chemical and soil physical processes on the soil water balance and on plant water stress. In all scenario is the cumulative actual transpiration less than the potential; for scenario 1, 4, and 5 transpiration reaches 281 cm or 96% of the potential value. This very small water stress is most likely due to the sub-optimal irrigation regime which generates soil pressure heads slightly outside the optimal range (see Figure 3.20). Larger differences in actual transpiration exist for scenario 2 (82% of potential value) and 3 (64% of potential value). Scenario 2 applied the combined water and solute stress model – in combination with the major ion chemistry module - to control root water uptake: this resulted in additional stress on plant water uptake, mainly caused by salinity stress. The smaller actual transpiration for scenario 3 (188 cm) is due in part to i) the increased water stress as a result of a drier soil (4 cm/day rather than 6 cm/day irrigation rate, every 5 days), ii) sup-optimal pressure head conditions owing to a decrease in hydraulic conductivity generating near-saturated conditions within the root zone (Figure 3.14), and iii) to salinity stress.

Table 3.1 Water balance components for a 365 day simulation period. Negative infiltration values means inflow; negative net drainage values means outflow.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Cumulative infiltration (cm)</th>
<th>Cumulative actual transpiration (cm)</th>
<th>Cumulative actual evaporation (cm)</th>
<th>Cumulative net drainage (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1: pasture – UPW</td>
<td>-438*</td>
<td>281 [96%]</td>
<td>73 [100%]</td>
<td>-84</td>
</tr>
<tr>
<td>1: alfalfa – UPW</td>
<td>-438*</td>
<td>281 [96%]</td>
<td>73 [100%]</td>
<td>-83</td>
</tr>
<tr>
<td>2: pasture - UPW - MIC - WSS</td>
<td>-438*</td>
<td>240 [82%]</td>
<td>73 [100%]</td>
<td>-123</td>
</tr>
<tr>
<td>3: pasture - UPW - MIC - WSS - KRM</td>
<td>-292*</td>
<td>188 [64%]</td>
<td>69 [95%]</td>
<td>-29</td>
</tr>
<tr>
<td>4: pasture - SAPW - MIC - WSS - KRM</td>
<td>-438*</td>
<td>281 [96%]</td>
<td>73 [100%]</td>
<td>-84</td>
</tr>
<tr>
<td>5: pasture - TPW - MIC - WSS – KRM</td>
<td>-438*</td>
<td>280 [96%]</td>
<td>73 [100%]</td>
<td>-84</td>
</tr>
</tbody>
</table>

UPW : untreated produced water; MIC: major ion chemistry; WSS: water and solute stress model; KRM: hydraulic conductivity reduction model; SAPW: surface water amended produced water; TPW: treated produced water; * 0.06 cm/day once every 5 days; † 0.04 cm/day once every 5 days;

Cumulative net drainage (difference between cumulative outflow and inflow from shallow groundwater) is identical for scenarios 1, 4, and 5. The higher drainage for scenario 2 (-123 cm) is due to the lower transpiration leaving more water in the soil profile that is available for drainage. The lower drainage for
scenario 3 (-29 cm) is the result of the smaller irrigation rate. Note that the decrease in irrigation by ~33% results in a decreased in drainage of ~ 65%. Calculated net drainage from Table 3.1 is considerably higher than calculated values (e.g. 10–20 cm/year) for furrow irrigation on cracking clay soils as reported by (Biggs et al. 2012). Our drainage values are not surprising, given the high irrigation rate applied constantly for a full year.

A comparison of scenario 1 and 2 is interesting from another perspective: it illustrates the effect of including or excluding certain coupled soil processes on water balance components. Scenario 1 has a standard advection-dispersion solute transport model without major ion chemistry. Scenario 2 on the other accounts not only for major ion chemistry, but also calculates salinity effects on root water uptake. This was a link is made between soil geochemistry, soil hydrology and plant water uptake. Accounting for such coupled processes resulted in i) a decrease of the actual transpiration to 82% of its potential value, and ii) an increase in net drainage by 46%. This is a clear demonstration that soil water balance modelling involving major ion chemistry should account for the above interacting processes. Note that the importance of such interacting processes decreases as the applied irrigation water has a less extreme composition (such as the amended and treated produced water).

Mass fluxes of major cations and anions were calculated for upper and lower model boundary (Table 3.2). For all scenarios the mass flux for calcium out of the soil is larger than the mass of calcium added via irrigation. This results from calcium being replaced on the adsorption complex by mono-charged sodium cations whose added concentration is two orders of magnitude larger than that of calcium. As the sodium concentration in the irrigation water decreases when untreated produced water is replaced by surface water amended produced water (scenario 4) or treated produced water (scenario 5), the calcium flux through the bottom of the soil profile also decreases due to decreased competition for adsorption sites between calcium and sodium.

For magnesium the mass flux through the bottom of the soil profile is larger than that added via irrigation only when untreated produced water is used (scenario 2 and 3). For all other scenarios magnesium accumulates in the soil (input flux is larger than output flux via drainage).

The use of treated produced water generates the overall smallest mass flux (for all ions except HCO3) from soil to groundwater.

Table 3.2 Chemical mass fluxes (gram/m²) through upper and lower model boundary for a 365 day simulation period. For upper model boundary negative fluxes are input to the soil; for lower model boundary negative values refer to fluxes leaving the soil. For each element and each scenario, first row is flux through upper boundary; second row is flux through lower boundary.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Ca</th>
<th>Mg</th>
<th>Na</th>
<th>K</th>
<th>HCO3</th>
<th>SO4</th>
<th>Cl</th>
</tr>
</thead>
<tbody>
<tr>
<td>2: pasture - UPW - MIC – WSS</td>
<td>-4.56E+01</td>
<td>-3.93E+01</td>
<td>-6.18E+03</td>
<td>-2.41E+01</td>
<td>-5.64E+03</td>
<td>-9.99E+01</td>
<td>-2.61E+03</td>
</tr>
<tr>
<td></td>
<td>-6.76E+02</td>
<td>-7.91E+01</td>
<td>-6.90E+02</td>
<td>-7.35E+01</td>
<td>-1.44E+01</td>
<td>-7.92E+01</td>
<td>-2.07E+03</td>
</tr>
<tr>
<td>3: pasture - UPW - MIC – WSS – KRM</td>
<td>-3.02E+01</td>
<td>-2.59E+01</td>
<td>-4.07E+03</td>
<td>-1.59E+01</td>
<td>-3.72E+03</td>
<td>-6.58E+01</td>
<td>-1.72E+03</td>
</tr>
<tr>
<td></td>
<td>-4.42E+02</td>
<td>-4.99E+01</td>
<td>-1.69E+02</td>
<td>-3.19E+01</td>
<td>-2.92E+00</td>
<td>-3.80E+01</td>
<td>-9.93E+02</td>
</tr>
<tr>
<td>4: pasture - SAPW – MIC – WSS – KRM</td>
<td>-4.52E+01</td>
<td>-2.86E+01</td>
<td>-8.09E+02</td>
<td>-1.53E+02</td>
<td>-6.04E+02</td>
<td>-1.48E+03</td>
<td>-7.20E+02</td>
</tr>
<tr>
<td></td>
<td>-2.06E+02</td>
<td>-2.07E+01</td>
<td>-5.52E+01</td>
<td>-2.55E+01</td>
<td>-1.01E+01</td>
<td>-9.13E+02</td>
<td>-4.43E+02</td>
</tr>
<tr>
<td>5: pasture - TPW – MIC – WSS – KRM</td>
<td>-4.54E+01</td>
<td>-3.33E+01</td>
<td>-1.26E+02</td>
<td>-1.90E+00</td>
<td>-8.24E+00</td>
<td>-4.39E+00</td>
<td>-2.95E+02</td>
</tr>
<tr>
<td></td>
<td>-5.70E+01</td>
<td>-6.27E+00</td>
<td>-2.80E+01</td>
<td>-1.63E+01</td>
<td>-1.17E+01</td>
<td>-2.74E+00</td>
<td>-1.75E+02</td>
</tr>
</tbody>
</table>

UPW: untreated produced water; MIC: major ion chemistry; WSS: water and solute stress model; KRM: hydraulic conductivity reduction model; SAPW: surface water amended produced water; TPW: treated produced water; "# 0.06 cm/day once every 5 days; "# 0.04 cm/day once every 5 days;
4 Conclusions

Coal seam gas production in Australia will generate vast amounts of produced water with an estimated 150-180 GL/y peak production rate in Queensland alone. This water may be used, when treated or amended with e.g. surface water, for irrigation and stock, town water supply and construction and processing. For instance, assessment of alternative use for treated coal seam gas water for the Central Condamine Alluvium (Queensland) indicates the region has capacity to deliver 854 GL, or around 35% of the historic depletion, by 2050 to irrigators and the Chinchilla Weir water supply scheme. If the water quality is acceptable, also untreated coal seam gas water can be used for agricultural purposes.

An in-depth analysis has been undertaken to inform optimisation of water quality scenarios that will yield minimal long-term effects of dissolved ions on soil and plant health. We evaluated three irrigation scenarios, whereby each scenario applied a different water quality based on whether the produced CSG water was amended with surface water, treated or untreated, and two additional scenarios with differing conceptualisation of water quality evolution in the soil. In four out of five scenarios the HYDRUS-1D code and its major ion chemistry module Unsatchem were implemented to simulate the simultaneous movement of multiple major ions (Na, K, Ca, Mg, Cl, SO4, alkalinity) present in irrigation water in a vegetated soil profile (pasture or alfalfa). The fifth scenario served as a baseline and did not consider addition and transport of multiple major ions.

Simulations with different irrigation water qualities provided detailed results regarding chemical indicators of soil and plant health, i.e. SAR, EC and sodium concentrations. By comparing such indicators in the soil profile with ANZECC water quality guideline values, an assessment was made of the suitability of the applied produced water for long-term irrigation. We also evaluated the build-up of salt in the soil profile and its effect on plant salinity stress, a condition which reduces the capacity for plants to uptake water causing yield reduction. Finally, the simulations also allowed to test if soil hydraulic properties, in particular the hydraulic conductivity, are negatively impacted by salt concentrations owing to clay dispersion.

Results based on five scenarios differing in applied irrigation water quality and invoked coupled processes indicated that use of untreated irrigation water would cause SAR and EC values to significantly exceed the ANZECC guide values. One of the three irrigation scenarios considered use of untreated produced water (EC = 5705 µS/cm and SAR = 77). Because irrigation with produced water is strictly regulated, the purpose of this scenario is to provide useful insights in the type of coupled chemical-hydrological processes that might occur, and what the potential impacts would be on soil and plant health should such water end up in the soil. For example, by using saline irrigation water, we demonstrated that accumulation of monovalent ions causes clay swelling, resulting in a decrease in hydraulic conductivity of a particular soil layer. This in turn caused water stagnation above this layer (pressure head exceeds threshold for optimum water uptake by plant roots), leading to additional plant water stress and reduced transpiration (188 cm versus 240 cm without water stress, or more than 20% less). Due to the lower transpiration, more water resides in the soil profile after irrigation causing drainage to increase by 46% (-123 cm compared to 84 cm).

In case surface water amended produced water was used (at a ratio of 1:3 with EC = 1573 µS/cm and SAR = 11), the calculated soil SAR values were much lower and generally acceptable for sandy to sandy-loam soil (i.e. less than 20). Permissible SAR values for light clay (i.e. less than 5) were still exceeded for most of the soil profile. Results also demonstrated the formation of calcite in the top of the soil profile owing to solute concentration effects under dry soil moisture conditions. This scenario did not result in additional stress on plant water uptake as a result of the acceptable salinity levels.

A final scenario used treated produced water with a relatively low concentration of major ions (EC = 291 µS/cm, SAR = 1.6). The permissible SAR values for light clay were not exceeded, and all other ions remained at tolerable levels. Under these conditions, actual transpiration was not reduced by additional salinity stress, meaning that near optimal soil hydrological and chemical conditions existed for plant growth.
Our analysis further illustrate that accounting for coupled geochemical, hydrological and plant water uptake processes resulted in i) a decrease of the actual transpiration to 82% of its potential value, and ii) an increase in net drainage by 46% when compared to a water balance calculation where such interacting processes were disregarded. This is a clear demonstration that soil water balance modelling involving major ion chemistry should account for the above interacting processes.

The major ion chemistry module Unsatchem implemented in HYDRUS-1D is a very power tool to assess in a very detailed way potential effects of different irrigation water qualities on soil and plant health. This offers a cost-effective way to optimise the quality of irrigation water derived from coal seam gas water and thus ensure soils are managed in a sustainable manner. To further underpin such assessments, field trials providing detailed soil chemical and physical data need to be consider to test the validity of the simulations and to improve process parameterisation. One of the processes that needs improvement and testing is the change in hydraulic properties as a result of mineral precipitation/dissolution causing partial or full pore blockage. Based on a simulation period of a single year, calcite precipitation was found to occupy up to 3% of the soil’s pore space in the top of the soil profile. The long-term evolution of salinity and its effect on soil hydraulic properties, however needs further corroboration.
References


DNRM (Department of Natural Resources and Mines) (2013) Assessment of alternative use options for coal seam gas water proposed for Central Condamine Alluvium recharge schemes. Healthy HeadWaters Coal Seam Gas Water Feasibility Study.


McNeal BL (1974) Soil salts and their effects on water movement, In: Drainage for Agriculture, Edited by J. van Schilfgaarde, Agronomy No 17, Am. Soc. Agr.. Madison, WI.


Toride N, Leij FJ, and van Genuchten MTh (1995) The CXTFIT code for estimating transport parameters from laboratory or field tracer experiments. Version 2.0, Riverside, CA, U. S. Salinity Laboratory, USDA, ARS.


YOUR CSIRO

Australia is founding its future on science and innovation. Its national science agency, CSIRO, is a powerhouse of ideas, technologies and skills for building prosperity, growth, health and sustainability. It serves governments, industries, business and communities across the nation.

FOR FURTHER INFORMATION

Land and Water Business Unit/Water Resource Management Program
Dirk Mallants

<table>
<thead>
<tr>
<th>t</th>
<th>+61 8 8303 8595</th>
</tr>
</thead>
<tbody>
<tr>
<td>e</td>
<td><a href="mailto:dirk.mallants@csiro.au">dirk.mallants@csiro.au</a></td>
</tr>
<tr>
<td>w</td>
<td><a href="http://www.csiro.au">www.csiro.au</a></td>
</tr>
</tbody>
</table>

CONTACT US

<table>
<thead>
<tr>
<th>t</th>
<th>1300 363 400</th>
</tr>
</thead>
<tbody>
<tr>
<td>e</td>
<td><a href="mailto:enquiries@csiro.au">enquiries@csiro.au</a></td>
</tr>
<tr>
<td>w</td>
<td><a href="http://www.csiro.au">www.csiro.au</a></td>
</tr>
</tbody>
</table>