**Model description**

The classical model for water transport through soil is the Richards equation (Richards, 1931). In this paper a modified version of the Richards equation was used to incorporate the influence of root exudates on soil water surface tension, soil-water contact angle and soil hydraulic conductivity:

Here is the soil water pressure head with initial condition , is the soil water content is the soil hydraulic conductivity, and is the final time. The soil water content and hydraulic conductivity functions are expressed using the formulations of (van Genuchten, 1980) and (Mualem, 1976):

, (4)

The function [-] is the effective saturation, the parameter is the inverse air-entry pressure head, and are shape parameters with , and the saturated soil water content and residual soil water content are given by respectively. Within the hydraulic conductivity function the parameter is the saturated hydraulic conductivity, and are required to incorporate the hysteretic effect of wetting and drying regimes on the saturated hydraulic conductivity and the function is the relative hydraulic conductivity. The constant is included in the formulation of so that it meets conditions imposed by the methods used to generate simulations. The notation and is used to indicate the reference saturated and residual water content values that are constant and do not depend on whether the soil is wetting or drying.

As already mentioned, the model accounts for the hysteretic relationship between water content and pressure head regarding whether the soil is wetting or drying. This phenomenon is incorporated through the inverse air entry pressure head and saturated hydraulic conductivity as follows:

where and . To maintain the continuity of at a time when a switch occurs between soil wetting and drying, the residual and saturated water contents are formulated as follows (Kool & Parker, 1987):

Likewise, the parameters and are formulated to maintain the continuity of at wetting/drying switches (Vogel & Zhang, 1996);

and

The influence of the concentration of exudates suspended in soil water and exudates dried to the soil surface is incorporated in the inverse air entry pressure head as follows (Karagunduz et al., 2001):

where is the surface tension of the soil water, is the contact angle between soil water menisci and the surface of soil particles and , are the default inverse air entry pressures during drying and wetting if no exudates are present in either form.

The effect of exudates is also incorporated into the saturated hydraulic conductivity in the following way

Where are the default saturated hydraulic conductivities during wetting and drying if no exudates are present and determines the extent to which an exudated-induced reduction in surface tension increases hydraulic conductivity.

The expressions for surface tension and contact angle as functions of the concentrations of suspended and dried exudates are fitted to the data of Read et al., (2003) and Zickenrott et al., (2016) respectively:

A graph of a blue line

Description automatically generated

A graph of a graph

Description automatically generated with medium confidence

The dynamics of the exudates in solution and the dried exudates are given by the following differential equations

where is the coefficient of diffusion of exudates through soil water, is the advective flux of soil water and is the bulk density of Nafion. The terms and are the rates at which dried exudate joins the soil water solution and exudate in solution dries to the pore surface respectively.

Finally, the movement of dye within the chambers is modelled using an additional differential equation

Here is the concentration of dye in solution and is the diffusion coefficient of the dye in solution.

A finite element scheme, with an implicit Euler discritisation in time, was used to approximate solutions to the coupled system of equations (1), (16), (18) and (20), and, hence, simulate the dynamics of water content, exudate concentrations and dye concentrations within the chambers for each of the scenarios tested experimentally.

Most parameter values in equations (1), (2), (16)-(19) and (20) were taken from previously published literature, and for those relating to soil hydraulics it was assumed that coarse sand would be the best approximation to the values of Nafion. However, the reference inverse air-entry pressure heads and saturated hydraulic conductivities , were altered considerably from the values cited in the literature in order to reflect the hydrophobicity of dry Nafion that was observed in the control infiltration experiments. The full list of parameters can be found in Table 1. After this, the values of and remained to be determined.

Table : Parameter values

|  |  |  |
| --- | --- | --- |
| Parameter | Value | Source |
|  |  |  |
|  |  | (Benson et al., 2014) |
|  |  | (Benson et al., 2014) |
|  |  | (Benson et al., 2014) |
|  |  | (Benson et al., 2014) |
|  |  | (Carsel & Parrish, 1988) |
|  |  | (Carsel & Parrish, 1988) |
|  |  | (Scott et al., 1995) (Average taken) |
|  |  | (Oberbroeckling et al., 2002) |
|  |  | (Syms, 2017) |

**Model calibration**

**Approximating the value of**

To calibrate the value of , data was used from the 5-day infiltration experiment () where initial exudate concentrations were

and observations of the dye concentration between depths and at times were compared against a control experiment in which no exudates were present. The coupled models for water transport (1), (2), exudate dynamics (16)-(19), and dye transport (20), (21) were set up according to these initial conditions and, for this calibration procedure, the rates of exudate drying and saturation were set to . Using Bayesian optimisation (Brochu et al., 2010), simulations were sequentially run from the coupled system at different values of and the value for which simulations most accurately matched experimental results was .

**Approximating the values of and**

The find the values of and data was used from the experiment with initial conditions , and the experiment with initial conditions:

The coupled models for water transport (1),(2), exudate dynamics (16)-(19), and dye transport (20), (21) were set up according to these initial conditions with and Bayesian optimisation was used to approximate the values of and that best allowed the predicted dye concentrations in the lower third of the domain to simultaneously match the experimental results for both initial conditions and . The parameter values arrived at by the Bayesian optimisation scheme were and

.

**Results**

Using the model system (1), (2), (16)-(19), (20), (21) calibrated with values simulations were then run of the experiments that had been carried out. The agreement between the dye concentrations in the bottom third of the chamber that were recorded from experiments and the those that were simulated by the model was recorded and can be seen in Table 2. Figures 1 and 2 give visual representations of the agreement for the experiment where exudates were initially in solution in the upper third of the chamber and the experiment where they were initially dried in the central third of the chamber respectively.

Table : Agreement of calibrated model with experimental data.

|  |  |  |  |
| --- | --- | --- | --- |
| Initial condition | Dye concentrations in lower third of chamber () | | |
|  |  |  |
| No exudates – experiment |  |  |  |
| No exudates – simulation |  |  |  |
| Exudates in solution in upper third of chamber – experiment |  |  |  |
| Exudates in solution in upper third of chamber – simulation |  |  |  |
| Exudates dried in barrier – experiment |  |  |  |
| Exudates dried in barrier – simulation |  |  |  |

A graph with a red line

Description automatically generated

Figure : Model/experiment agreement when exudates initially in solution in upper third of chamber.

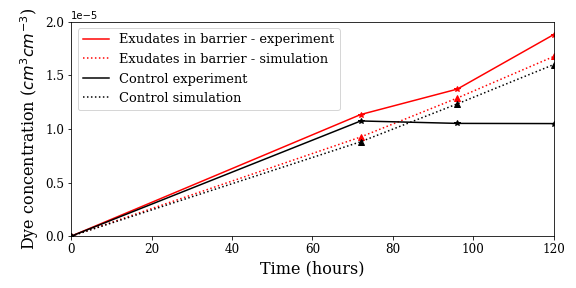


Figure : Model/experiment agreement when exudates initially dried in central third of chamber.