sustainability

Numerical models and calculations

Mannheim HYDRUS-1D Modelling – Mar 2017 Event Calibration

Calibration of the HYDRUS-1D [87] model for the Mannheim site consisted of varying saturated hydraulic conductivity values for the six interpreted soil layers shown in Figure S1.1 to match observed water levels at two of the three observation wells (Node 1 / CPP5 and Node 3 / CPP3). The hydrological event selected for this calibration was the Mar 2017 event, a small event where ponding (~ 2 cm depth) occurred in the base of the topographic depression for 0.26 days and the creek water level only responded to a small degree (creek water levels increased by up to 10 cm). This event was chosen to avoid the potential superposition of recharge influences on the local water table when infiltration beneath both ponded water in the base of the topographic depression and the creek occurred. The water level, temperature, and weather data used in the HYDRUS-1D models of the Mannheim site are available from [65]. Snowmelt estimates were developed based on rainfall data from the Mannheim site and snowpack thickness data from the Roseville weather station [94].

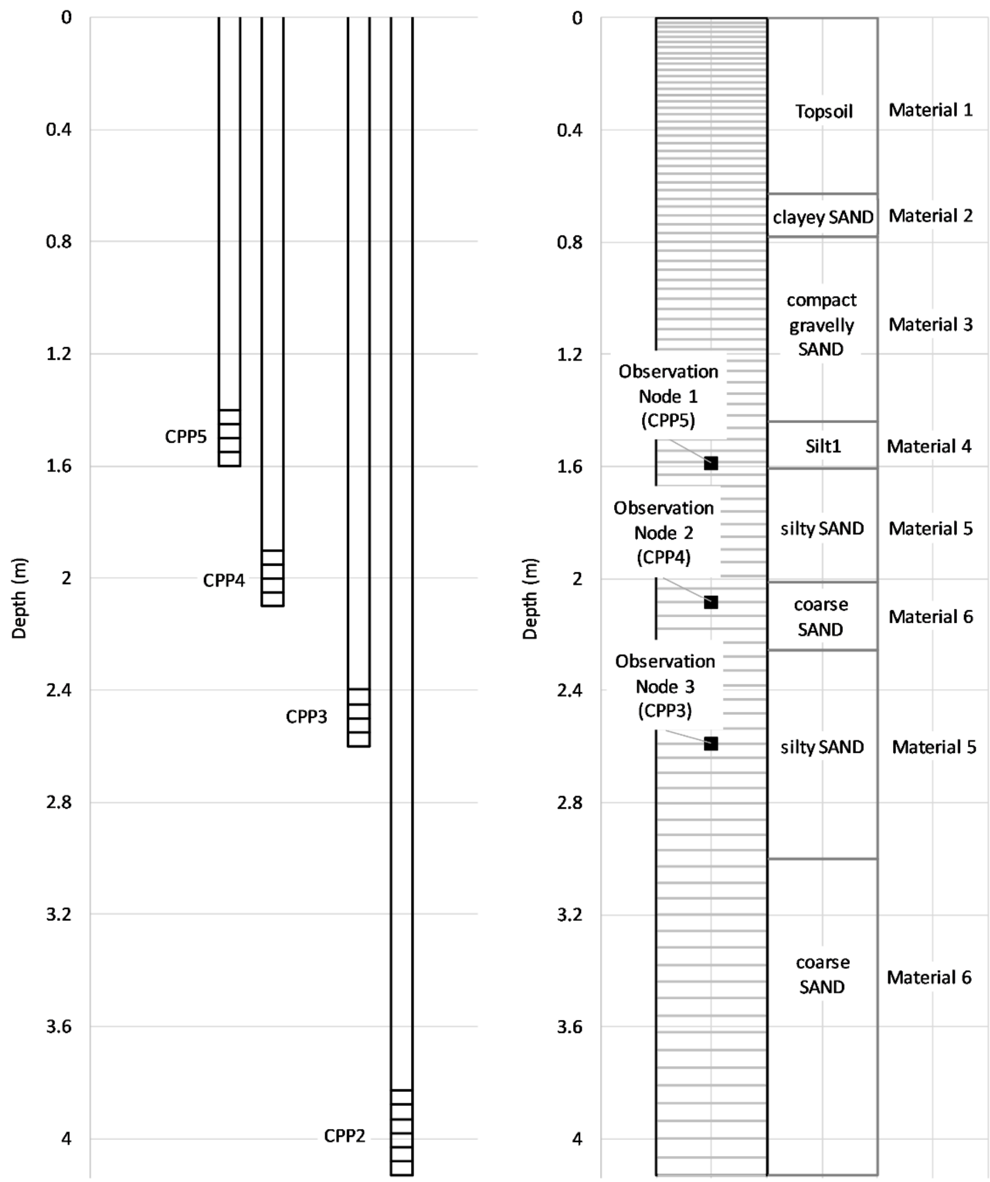

Figure S1.1. Observation well screen depths and model layers representing the soils beneath the topographic depression at the Mannheim site.

The domain for this model consisted of 102 nodes vertically spaced by about 1.6 cm at the top (density = 0.25) and by about 7 cm at the bottom (density = 1), representing a soil column of 4.13 m in height. The height of the column was selected to be the depth of the deepest observation well screen installed beneath the base of the topographic depression. Observation nodes were assigned at the (screen bottom) locations of the observation wells within the profile (CPP3 – 2.6 m depth, CPP4 – 2.1 m depth, and CPP5 – 1.6 m depth), where the pressure transducer measurement points were located. Water levels observed at the deepest observation well (CPP2 – 4.13 m depth) were used to set the transient, specified head boundary condition at the bottom of the model domain. A combination of specified head and specified flux boundary conditions was applied at the top of the column. Observed (pressure transducer) ponding levels at the ground surface were used to specify pressure head values when the presence of surface water was indicated by the pressure transducer data. A specified flux of 0 m/day was assigned after ponding ceased. Precipitation was not included directly in this simulation; instead, its effects were included indirectly by specifying ponding depth at the ground surface. Variable specified temperatures were used as boundary conditions at the top and bottom of the domain for heat transport. The temperatures at the top of the column were assigned based on data from the pressure transducer device at the ground surface, while the temperatures at the bottom were assigned based on the data from the pressure transducer device in observation well CPP2. Figure S1.2 shows the water level elevation (metres above sea level, or "m asl") and temperature variations applied at the boundaries during the Mar 2017 Event. Water levels measured with the pressure transducers were adjusted based on their average differences with periodic manual readings.

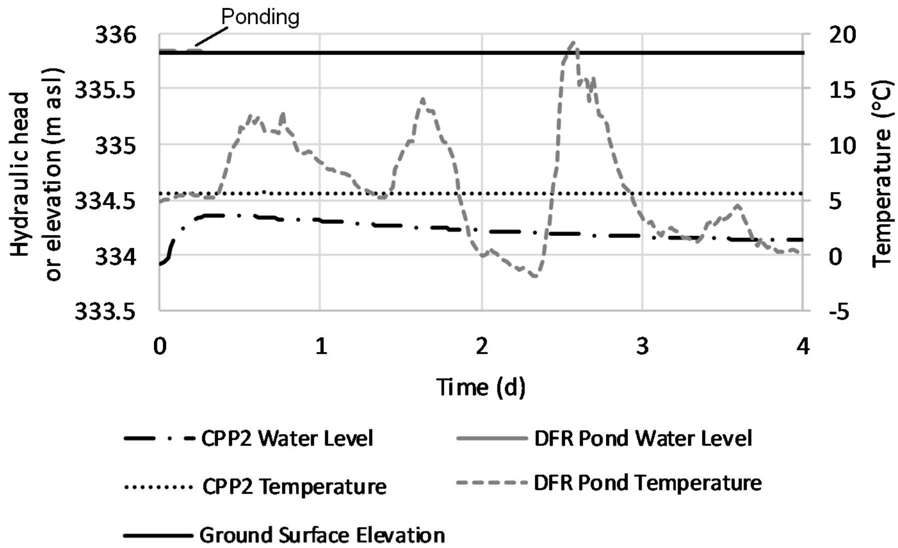

Figure S1.2. Hydraulic heads and temperatures at the top and bottom boundaries during the Mar 2017 Event [65].

Initial pressure head conditions (Figure S1.3a) were developed based on the observed pressure heads at the observation points that were below the water table prior to the event. Nodes with a depth equivalent to an observation location were assigned the pre-event pressure head observed prior to the start of ponding. Other nodes were assigned values that varied linearly between the observation points, and a unit gradient was used to specify initial pressure heads above the shallowest water level observation (CPP4). Initial temperatures (Figure S1.3b) were specified as the values from pressure transducers or soil temperature sensors at equivalent depths and were specified to vary linearly in between observation depths. The heat transport parameters used were the default values in HYDRUS-1D for either loam (material layers 1, 2, 4, and 5) or sand (material layers 3 and 6) for the Chung and Horton [80] method. The solid fraction value for each layer was calculated based on estimated porosity.

Calibration was conducted within HYDRUS-1D for the hydraulic conductivity values of the soil layers. The initial, minimum, and maximum values specified for the calibration process are shown in Table S1.1. The unsaturated moisture content and hydraulic conductivity functions of pressure head were modelled using the van Genuchten-Mualem approach within a single porosity medium with no hysteresis. The van Genuchten parameters for the moisture retention curves of the soil material layers were specified based on literature values (UNSODA database [88]; Table S1.1) in association with observations of soil consistency and moisture content [29].

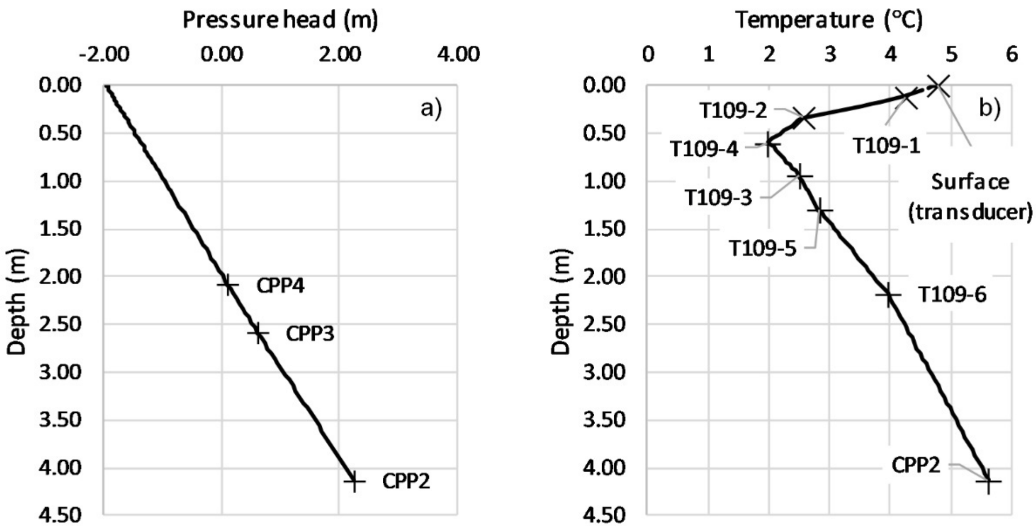

Figure S1.3. Initital conditions [65] for the Mar 2017 Event calibration: (**a**) pressure head, and (**b**) temperature.

Table S1.1. Soil properties.

Soil layer	θr* (-)	θs† (-)	α‡ (1/m)	n§ (-)	Ks¶ (m/day) (minimum, maximum, initial)
Material 1, Topsoil	0.1	0.4	1.2	1.39	4.8 (0.1, 10, 2.0)
Material 2, Silt1	0.1	0.4	1.2	1.39	4.0 (0.001, 4, 0.5)
Material 3, Gravelly Sand	0.05	0.3	1.5	3.8	72 (0.1, 86.4, 10)
Material 4, Silt2	0.1	0.4	1.2	1.39	0.018 (0.01, 3, 0.3)
Material 5, Silty Sand	0.08	0.37	2.5	2.3	0.11 (0.1, 25, 0.3)
Material 6, Coarse Sand	0.08	0.33	3.5	3.2	64 (0.1, 86.4, 2)

* Residual moisture content
† Saturated moisture content, assumed equivalent to porosity
‡ van Genuchten air entry pressure
§ van Genuchten fitting parameter
¶ Saturated hydraulic conductivity

The times in HYDRUS-1D were specified as their Julian Day equivalents, accounting for fractions of days. Parameters for calculating evaporation (such as solar radiation) were not specifically added to this calibration simulation because the short duration of the simulation and the colder temperatures were assumed to be associated with negligible evaporation. This assumption was checked by running the model in an additional scenario with evaporation parameters measured at weather station WS4 on site (solar radiation, maximum and minimum air temperature, relative humidity, and wind speed [65]) to verify that evaporation was only a small fraction of cumulative infiltration. The solar radiation parameters were available at a 15 min time scale and were applied at this scale. Nine missing wind speed values were filled using the average of the two values immediately before and after the missing value(s). The latitude and altitude of the field site, and the heights of the wind speed (300 cm) and temperature sensors (200 cm), were specified; other parameters were set to the defaults within HYDRUS-1D. The Penman-Monteith method was selected for estimating evaporation, and cumulative evaporation was found to be less than 5 mm.

The results after calibration are shown in Figure S1.4. Figure S1.4a shows the match between observed and simulated water levels at observation wells CPP3, CPP4, and CPP5. The simulated groundwater levels generally represent a reasonable match with CPP5 observations, visually. The rising limb of the groundwater hydrograph at CPP5 was matched with a similar rate of water level increase, but the recession was more pronounced and then more gradual than observed after 0.5 days. The simulated water levels for CPP4 are a poor match for the observations. The CPP4 observations were very similar to the CPP3 observations, suggesting a possible hydraulic connection despite the fact that these two observation wells were installed in different boreholes. For this reason, the CPP4 water levels were not used for calibration. The simulated hydrograph at CPP3 has a peak that overestimates the observed peak by 0.23 m, but the rate of recession is well represented. The presence of multiple coarser and finer soil layers at this site likely hindered the ability to fit the CPP3 data more accurately. Figure S1.4b compares observed and simulated temperatures at the three observation wells represented by observation points within the domain. The simulated temperatures were within 1°C of the observations. The short duration of this simulation and the low degree of temperature variation prevented further analysis (e.g., calibration) based on these temperature data.

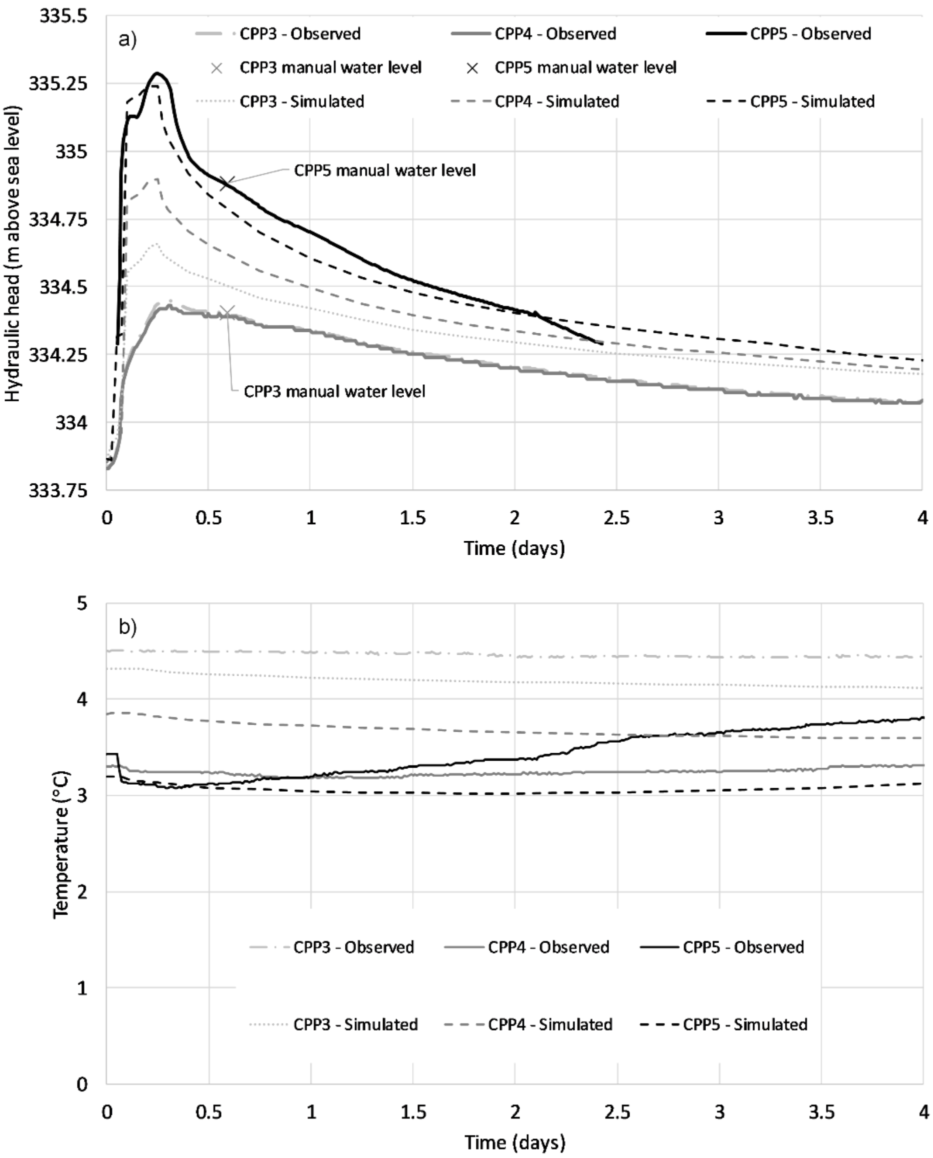

Figure S1.4. Mar 2017 Event [65] calibration results for (**a**) hydraulic head and (**b**) temperature.

The maximum potential recharge was approximated by the cumulative infiltration during each HYDRUS-1D model simulation. The recharge estimate based on the cumulative infiltration during the Mar 2017 simulation was 191 mm (Figure S1.5).

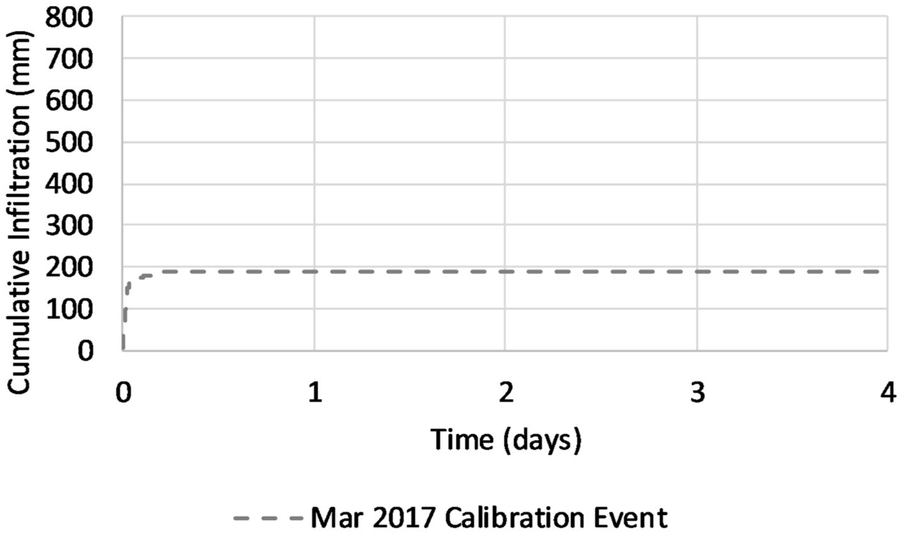

Figure S1.5. Cumulative infiltration for the Mar 2017 Event simulation, after calibration.

Mannheim HYDRUS-1D Modelling – Nov 2014 Event Simulation

The calibrated hydraulic conductivity values and other soil properties from the Mar 2017 Event simulation were used to model one large event. The Nov 2014 Event was the largest event on record (from Nov 2014 to Apr 2018) in terms of rainfall magnitude and duration of ponding at the Mannheim site. Field data [65] such as water levels and temperatures recorded at the observation wells CPP2, CPP3, CPP4, and CPP5, and by a pressure transducer located at the ground surface near the base of the topographic depression were again used to specify variable specified head and variable specified temperature at the top and bottom of the model domain (Figure S1.6), and to set the initial conditions (Figure S1.7). Initial conditions were specified as described for the Mar 2017 Event, with linear interpolation between values specified at column depths equivalent to instrument depths. Data related to evaporation calculations, such as incoming solar radiation, air temperature, relative humidity, and wind speed (Figure S1.8) were specified at a 15 min time scale using the site observations from [65]. For example, the incoming solar radiation was converted from units of W-hr/m^2/15 min time step to MJ/m^2/day by multiplying by 0.0036 MJ/W-hr and then by the number of time steps per day (96). The Penman-Monteith method was used to estimate potential evaporation within HYDRUS-1D.

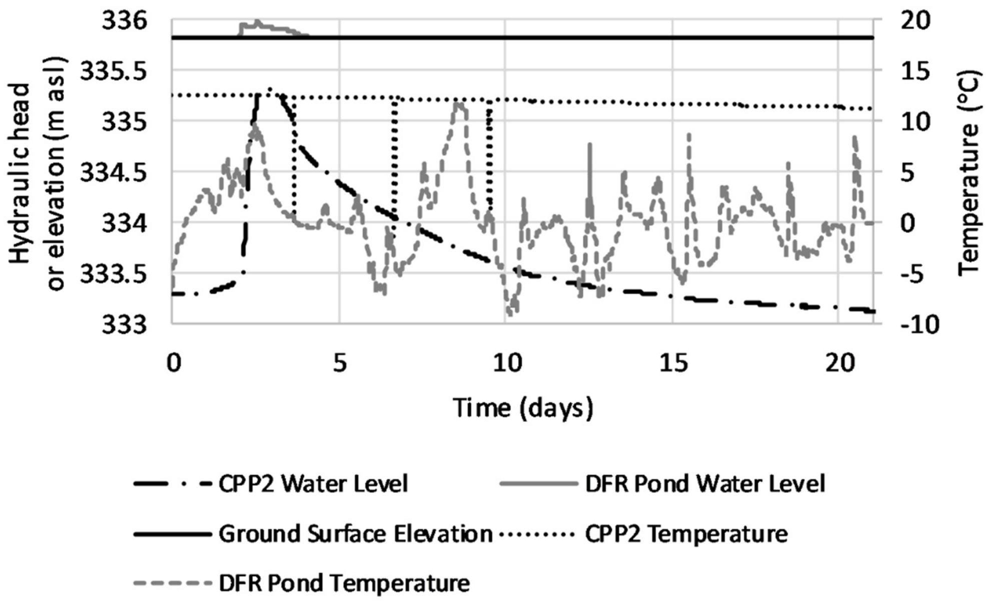

Figure S1.6. Hydraulic heads and temperature at the column boundaries during the Nov 2014 Event [65].

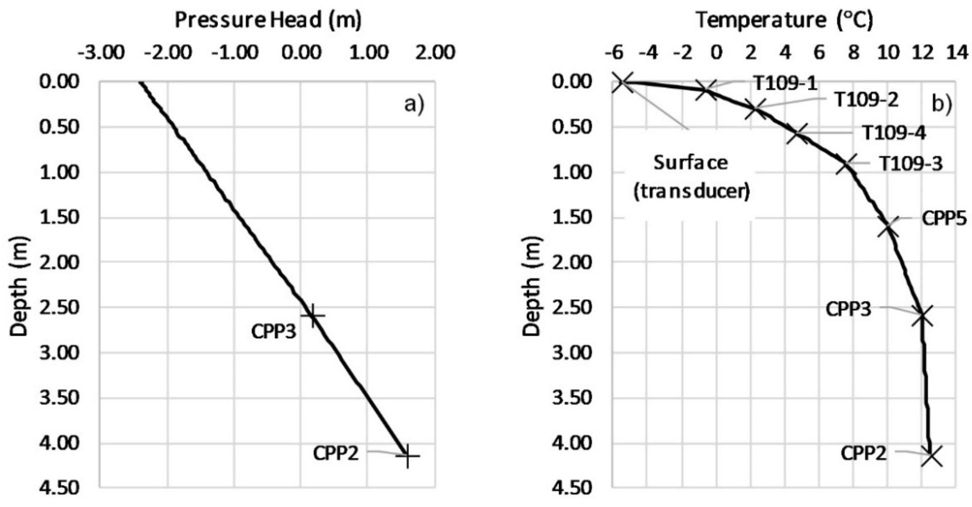

Figure S1.7. Initial conditions [65] for (**a**) pressure head and (**b**) temperature for the Nov 2014 Event.

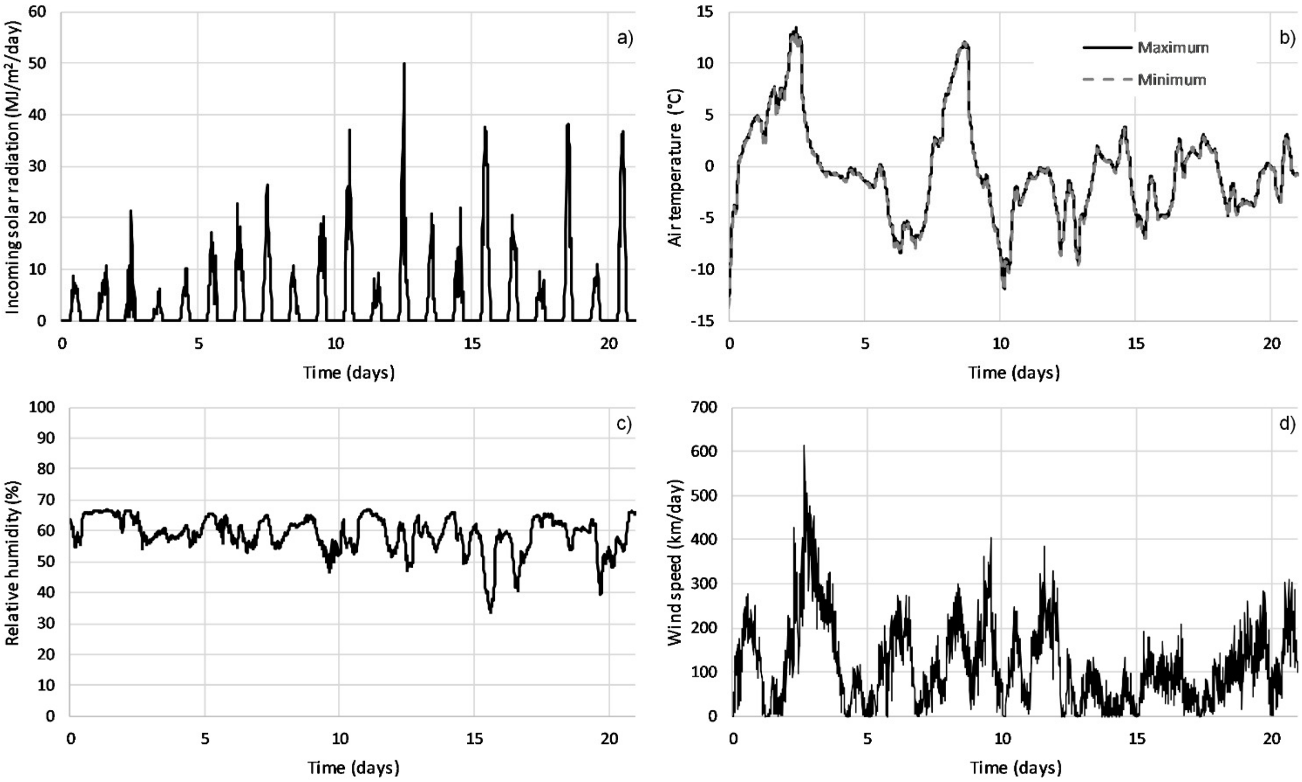

Figure S1.8. Data [65] for evaporation calculations: (**a**) incoming solar radiation, (**b**) air temperature, (**c**) relative humidity, and (**d**) wind speed.

Precipitation was included as a specified flux for time periods with no ponding at the ground surface. Ponding was largely the result of overland flow into the base of the topographic depression at the Mannheim site. Effective precipitation, equal to rainfall plus estimated snowmelt, was used in the Nov 2014 Event simulation. Rainfall was measured on site with a tipping bucket rain gauge at weather station WS4 [29]. Daily snowmelt amounts were estimated as described in the next section. These daily totals were applied over several hours at a rate of 0.5 mm/15 min or 0.25 mm/15 min on days with estimated snowmelt > 0 mm, starting at 9 am. Rainfall and snowmelt were added on a time step by time step basis. The total effective precipitation during the Nov 2014 Event was 91.2 mm (Figure S1.9), where snowmelt was estimated on four days with an overall total of 18 mm. A smaller amount of total effective precipitation (38.8 mm; Figure S1.9) was applied during the simulation because precipitation flux was not specified during the duration of ponding (shown on Figure S1.6). The amounts shown in Figure S1.9 were applied within the model after conversion to fluxes in m/day; any precipitation related to the period of specified head (1.969 days to 4.021 days in the Nov 2014 simulation) was ignored.

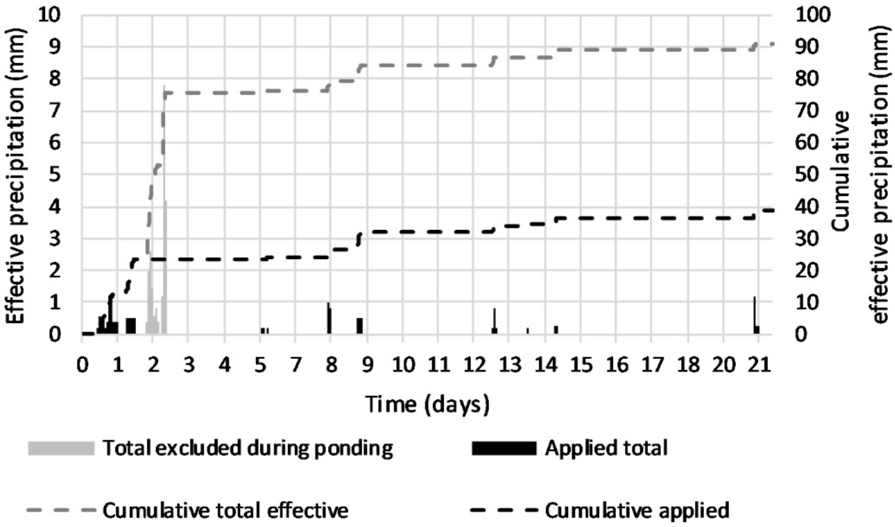

Figure S1.9. Total and applied precipitation during the Nov 2014 Event [65].

Figure S1.10 shows the comparisons of observed and simulated values for hydraulic head and temperature as a means of verification of the calibrated hydraulic conductivity values. Overall, the peak water levels are well represented by the model. The downward spikes on Figure S1.10 were the result of water sample collection at the observation wells. The rate of water level rise and the peak water level at CPP5 were simulated quite well (peak within 0.12 m), though the simulated recession occurred more rapidly (Figure S1.10a). The observed water levels at CPP3 and CPP4 were very similar, and the peak was well matched by CPP4 in the simulation. The recession at CPP3 and CPP4 was again poorly matched by the simulation. Water level recession in the field could have been influenced by lateral flow, which cannot be represented in this 1D model. Temperatures during the Nov 2014 Event were well matched at CPP3 and CPP4 (within about 0.5°C), though temperatures were up to 1.6°C lower than observed at CPP5 by the end of the simulation (Figure S1.10b). Cumulative infiltration was 392 mm during the Nov 2014 Event simulation, with 8 mm of evaporation.

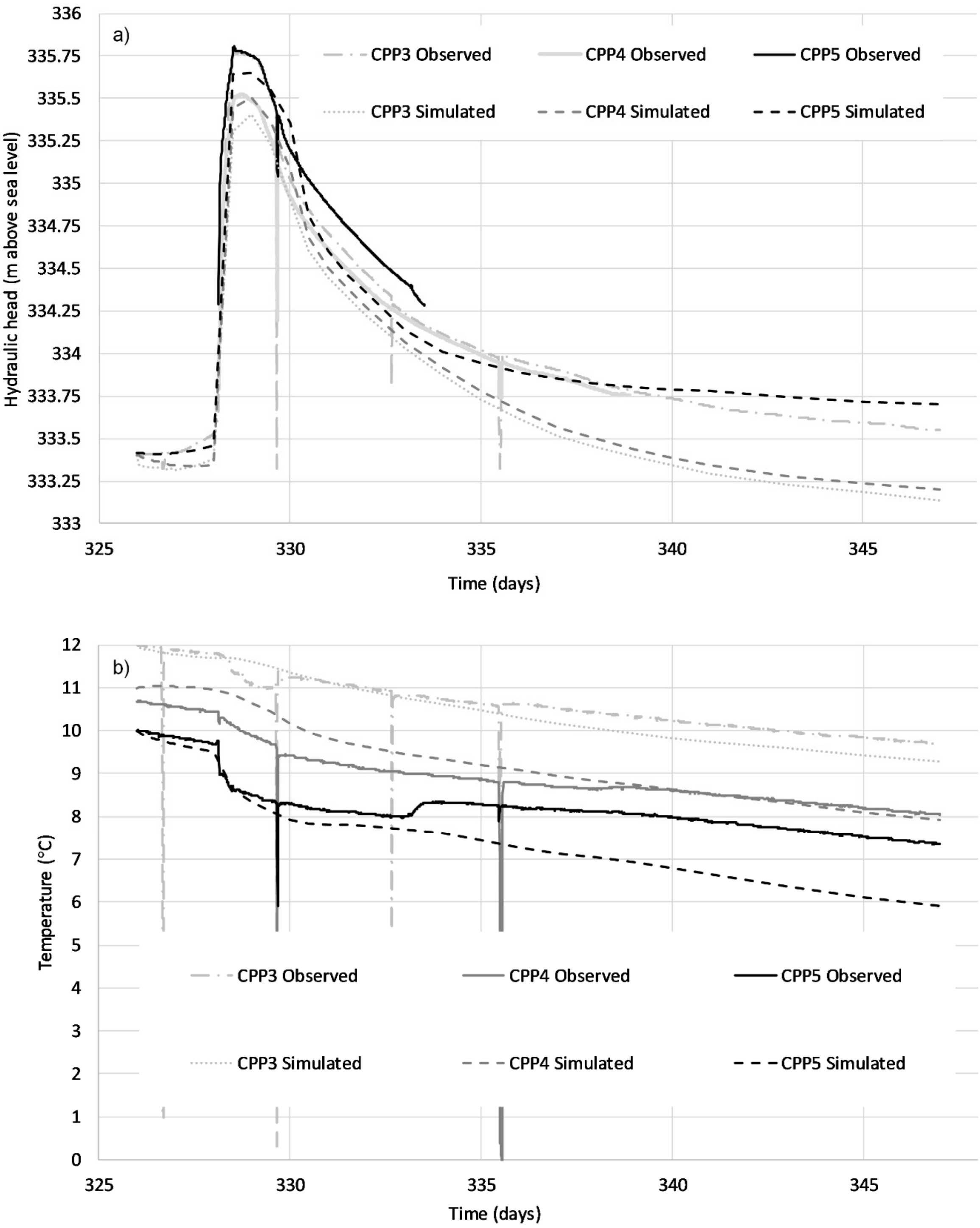

Figure S1.10. Comparison of observed [65] and simulated (**a**) hydraulic head and (**b**) temperature during the Nov 2014 Event.

Summary of Thornton and Mannheim HYDRUS-1D models

Table S1.2. Summary of HYDRUS-1D models for the Thornton (T) and Mannheim (M) sites.

Scenario	T *	T (Stn 3) †	T (Stn 4) †	T (Stn 5) †	M ‡	M ‡
Date	Mar 2010	Mar 2015	Mar 2015	Mar 2015	Mar 2017	Nov 2014
Number of soil layers	11	6	5	5	5	5
Height of 1D column (m)	3.49	1.60	1.65	1.65	4.13	4.13
Event simulation duration (day)	14	20	20	20	4	21
Effective overland flow/ponding duration § (day)	1.38	1.29	3.79	1.75	0.26	2.05
Range of hydraulic conductivity values for soil layers (m/s)	5.6E-7 – 2.0E-3	2.3E-8 – 1.2E-4	1.3E-6 – 6.7E-5	1.2E-6 – 6.7E-5	2.9E-7 – 3.2E-4	2.9E-7 – 3.2E-4
Cumulative Infiltration (mm)	153	46	709	422	191	392

* [62].
† [63]; "Stn" = "Station"
‡ Described above
§ Estimated overland flow or ponding duration contributing directly to infiltration, i.e., when soils were not frozen and surface water levels were recorded at the specific location represented by the model.

Limitations of recharge estimation methods

Limitations of the recharge estimates at the two sites could include errors associated with field data collection, a mismatch of method assumptions and field conditions, or inappropriate selection of model parameters.

Improper equipment installation could allow preferential flow along the outside of observation well casings or through disturbed soil backfilled above soil moisture or temperature sensors. In particular, leakage along improperly sealed boreholes could lead to inaccurate interpretations and modelling of event responses in shallow observation wells. The use of multiple types of data (e.g., groundwater and surface water levels, groundwater and surface water temperatures, soil moisture, and soil temperature) and multiple observation locations over multiple years and at different study sites decreases the probability that the general idea that localized recharge can occur near public supply wells in unconsolidated sediments is false, or at least, false at the field sites examined.

A poor match of method assumptions and actual field conditions is a limitation of the HYDRUS-1D modelling, and of the WTF and Darcy's Law calculations employed at the Mannheim site. Representing a 3D reality with a 1D model is a simplification that poses an obvious limitation. The uncertainty of this was not quantified in the case studies. The WTF method also simplifies reality, ignoring antecedent moisture conditions in the vadose zone prior to an event and the 3D nature of groundwater flow away from water table mounding beneath localized infiltration. The Darcy's Law calculation involved the assumption of saturated flow, though actual field conditions could have been heterogeneously saturated.

The selection of model parameters is another source of uncertainty. The many parameters employed during the HYDRUS-1D modelling each have uncertainty. The sensitivity of model results to each parameter would differ. The use of field-derived parameters and calibration to observation serves as a helpful but inconclusive form of connection to field conditions. The specific yield parameter for the WTF method was calculated by Menkveld [64] as the difference between typical maximum and minimum soil moisture readings based on a neutron probe. This value would have associated uncertainty and the value selected was near the low end of the literature range [64]. The hydraulic conductivity used for the Darcy's Law estimate of recharge flux during the analytical estimate by Menkveld [64] could potentially have uncertainty up to an order of magnitude, though field infiltration tests were performed to assist the estimation.

Mannheim HGS Modelling

Figure S1.11 shows the model grids for the HGS modelling by [29]. The domain used for calibration of the near-surface soils (soils beneath the base of the topographic depression < 6 m deep) is shown in Figure S1.11a. Its dimensions were 100 m by 100 m in plan view, and the depth varied between 23 and 26 m based on the interpolated depth of the underlying aquitard. Forty-nine layers between 50 nodal surfaces were used, and there were 692 nodes outlining 1302 elements per slice. The domain used for calibration of the main aquifer hydraulic conductivity is shown in Figure S1.11b. This domain was a wedge with an arc angle of 18.64°, an outer radius of 2400 m, and a height of 24.14 m; there were 38 nodes per slice and 70 layers. The domain used to simulate solute transport is shown in Figure S1.11c. This domain was also a wedge with the same arc angle as in Figure S1.11b, but its length was 183.6 m, and it had 320 nodes per slice and 71 layers. One of the layers from the longer wedge domain was split into two for this domain. This shorter wedge had smaller elements (lateral nodal spacing ≤ 0.3 m between the base of the topographic depression and the well at the apex of the wedge, and vertical nodal spacing ranging from 0.17 m to 1 m) to minimize numerical dispersion. See [29] for further details.

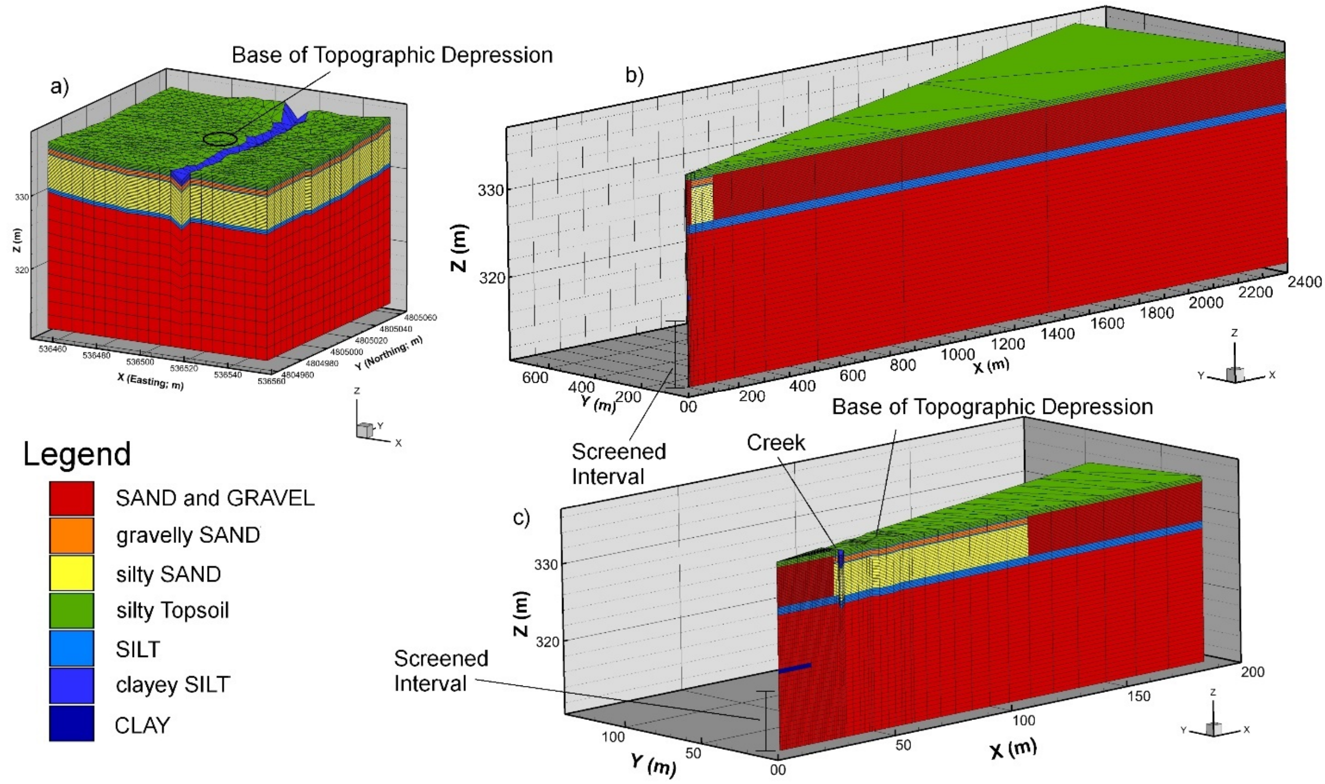

Figure S1.11. HGS model domains representing the Mannheim site [29]: (**a**) domain used for calibration of the near-surface soils, (**b**) domain used for calibration of the main aquifer hydraulic conductivity, and (**c**) domain used to simulate solute transport.

The HGS modelling conducted in the present study builds on the method of [29] in terms of using a degree-day method to estimate the timing of snowmelt applied during the solute transport runs. Total daily precipitation was calculated as the sum of observed rainfall [65] at the WS4 weather station at the Mannheim site, and a snowmelt estimate derived from 1) observed snowpack thickness [94] at the Roseville Environment Canada weather station (8 km from the site) and 2) a simple degree-day method (e.g., [76]):

$$M = aT, \tag{S1.1}$$

where M is the potential daily snowmelt (cm), a is the degree-day factor or ratio (cm°C^{-1}day^{-1}), and T is the number of degree-days (°C day). The actual amount of daily snowmelt depends on the available snow water equivalent present in the snowpack on a given day, in addition to M. The value of T was calculated as the product of the mean daily temperature and one day.

Uniform snowfall and snowmelt in the area was assumed based on limited available snowpack thickness data. The arithmetic average of seven local weather stations' measurements was within 2 cm of the snowpack observations at Roseville during the winter season of 2014-2015 [29]. The degree-day method was applied from Nov 2013 to Apr 2018 and employed daily mean temperature data [94] from the Roseville station. Missing temperature values were obtained from the average of minimum and maximum daily temperatures [95] at the University of Waterloo weather station (15 km from Roseville; 8 km from the Mannheim site). Missing daily snowpack thickness values in the Roseville record were estimated as the average of the observations immediately before and after the missing day or series of days. The method employed a constant degree-day ratio of 0.725 cm°C^{-1}day^{-1} that was obtained by minimizing the sum of squared errors between the cumulative snowmelt calculated using the snowpack thicknesses observed at Roseville [94] and the cumulative snowmelt estimated by the degree-day method. This ratio is slightly higher than the recommended ratios for non-forested areas (up to 0.7 cm°C^{-1}day^{-1} in June [76]) but is similar to the arithmetic mean value (0.743 cm°C^{-1}day^{-1}) obtained by [96] for a site in Manitoba (Mar-Apr). The value for each watershed must be determined empirically [96,97]. The weather station at the Mannheim site and the Roseville weather station are each located in suburban areas, which may influence their temperature and precipitation records. Possible snow accumulation on top of the rain gauge at the Mannheim site, leading to snowmelt recorded as rain, was assumed to be 0 mm during this analysis.