Water Balance Model for a Generic Near-Surface Disposal Facility - 10029

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ABSTRACT

Water movement into, within and out of a near-surface disposal facility determines discharges to groundwater and as such can have a major impact on the current and future safety of a facility. However, understanding spatial and temporal variations in near-field flows often poses a challenge to design optimisation, risk and safety assessments, as numerical modelling of spatial heterogeneities and temporal changes are highly resource and data intensive. In order to aid analysis of near-field flows a modelling tool was developed based on a simplified representation of a generic near-surface disposal facility. The model, implemented in GoldSim, is designed to be used in assessments of hydraulic performance of various design options and their influence on releases from the disposal facility over time. The model provides a highly flexible, and user friendly tool to analyse performance of the engineered barrier system (EBS) in support of a safety assessment, an optimisation study or design development. However, results so far demonstrate 'proof of concept', only and further model development is planned.

User input requirements include the definition of the design to be simulated, facility and component dimensions, rainfall, evapotranspiration, and runoff to calculate cap infiltration, and the hydraulic conductivities of the engineered components for the calculation of vertical flow. A user interface aids easy selection and input of these parameters. The model calculates elements of the water balance (inflow, outflow and change in storage) for each component. Component performance changes over time as a function of barrier degradation as defined by the user. Given that the future performance of the EBS and future climate conditions are inherently uncertain, a probabilistic approach has been adopted. The main model outputs include time variant volumetric flows (inflow through cap, overflow in the case of a 'bathtub' scenario and vertical outflow through the base), and time dependent groundwater water level within the facility.

In order to demonstrate the capabilities of the model, an example application is presented. Input values have been chosen so that they are broadly representative of a facility of this type. Probabilistic simulations were conducted for a simulation period of 5,000 years. Results form the demonstration model indicates a scenario of gradually increasing infiltration and a slower degradation of the base liner leading to saturation of the waste in the facility. Given the assumed input parameter values, the best estimate for this model simulation is that overtopping may occur but it is marginally more likely not to. The generated overflow rate can be significant (that is, up to the same order of magnitude as infiltration). Sensitivity analysis identified annual rainfall and degraded hydraulic conductivity of the base liner as the key parameters for overtopping.

INRODUCTION

Water movement into, within and out of a near-surface disposal facility determines discharges to groundwater and as such can have a major impact on the current and future safety of a facility. The development and optimisation of facility design requires some understanding of the impact of the engineered barriers on such water movement, and as such on the safety of the facility. Given the heterogeneous nature of the facility, consisting of the waste form and the engineered barriers, the resulting water movement (here termed near-field flow) is also highly heterogeneous in nature. The degree of this heterogeneity is dependent on the properties of the waste form and the engineering design of the facility. In addition to this, near-field flows can also vary greatly over time in response to climate change and evolution (normally degradation) of the engineered barriers.

Understanding spatial and temporal variations in near-field flows often poses a challenge to risk and safety assessments, as modelling a high level of spatial heterogeneities and temporal changes is highly resource and data intensive. As a consequence, near-field flows are generally treated in a simplified manner (e.g: assuming no change over time or assuming a homogenous near-field).

A simplified water balance model could provide practical assistance to safety assessment and design optimisation by providing a tool that can be used to assess the water balance of a near-surface facility in response to assumed design scenarios, changes in the design and geometry of specific design components, rainfall, evapotranspiration and runoff, hydraulic performance of the main engineered components, and possible system evolution scenarios, including those for the climate and for barrier degradation. Main elements of the water balance that need to be considered for this purpose include infiltration through a cap, vertical outflow through the base of a facility, facility overflow due to overtopping (if the model predicts that this is likely to occur), and water storage and saturation depth in facility components.

It is recognised that a simplified model will have significant limitations as compared with detailed numerical models. It is suggested however that there is a wide a gap in terms of resource requirement, data needs and turnaround time between qualitative approaches and the numerical models used for assessment of EBS performance and resulting near-field flows. A tool, based on a simplified conceptual model could bridge such a gap, and used

- to inform qualitative assessment of EBS performance, for example as part of a group elicitation in a workshop setting by calculating flows resulting from elicited EBS performance parameters,
- to gain insight of possible flow scenarios resulting from assumed EBS design and performance scenarios in support of a post-closure safety assessment,
- in scoping calculations to inform facility design and optimisation,
- to identify most important design features of the EBS with respect to long-term performance,
- to identify key uncertainties associated with the performance of the EBS, and
- to identify key FEPs that need to be better characterised.

SCOPE, PURPOSE AND LIMITATIONS

A water balance model for a generic near-surface disposal facility has been developed and implemented in GoldSim [2]. The model is designed to be used in assessments of the hydraulic performance of various design options. The purpose of the model is to aid an assessment the performance of an engineered barrier system (or EBS) and its influence on releases from the disposal facility over time. Such assessments may be part of an operational and/or post closure safety assessment, an optimisation study or design development.

The model is configured so that it facilitates the representation of typical disposal concepts and their variants, and allows easy definition of input parameters through a user interface. It calculates elements of the water balance (inflow, outflow and change in storage) for each component based on infiltration, facility design and hydraulic performance of the components. Component performance changes over time as a function of system evolution (barrier degradation). Given that the future performance of the EBS and future climate conditions are inherently uncertain, a probabilistic approach has been adopted.

The conceptual model implemented in GoldSim is highly simplified and involves infiltration through a cap as a function of rainfall, evapotranspiration and runoff, and vertical flow through the other barriers based on Darcy's Law. There are two main reasons for the simplifications adopted. Firstly, the main purpose is to provide a flexible tool that is able represent various design options according to user requirement. A modelling approach involving the development of complex models would be inconsistent with this aim. Secondly, the model described in this paper represents work in progress, intended only to be a demonstration of the approach and proof of concept.

One of the main simplifying assumptions adopted in the current version of the model is that it includes vertical flows only. This is considered appropriate for the demonstration of the approach, as vertical flows tend to dominate in near-surface facilities. However, in situations where horizontal flow into or out of a facility is a significant component of the water balance (e.g. due to the presence of localised or regional water bodies above the level of the base of the facility, or significant lateral water movements within facility due to the use of drains) the presented model is not applicable. It may be said therefore that the model is applicable to facilities for which the water table is below the facility and where horizontal flow within the facility is also of little interest.

The following assumptions and model limitations are noted in addition to the assumption of vertical flows only:

- Unsaturated water movement is not considered as its calculation is beyond the scope of this model. This assumption is equivalent with the assumption that saturated and unsaturated vertical hydraulic conductivities are equal. In effect, unsaturated flow is taken to be equal to saturated flow. This simplification is likely to overestimate vertical flow.
- There is no groundwater adjacent to the facility that is also above the level of the base of the facility. This is required as the simple approach adopted is not applicable to consider conditions when a large body of groundwater interacts with the facility. As a consequence of this assumption, it follows that flow into the facility occurs only through the cap as infiltration, and horizontal flow through the sides of facility or 'upflow' through base are not considered.

- There are two possible pathways for outflow: vertical flow through the base of facility, and ‘overflow’ that is flow out of the facility due the overtopping. Overflow occurs from the component directly underneath the cap.
- Degradation of engineered components and waste form over time occurs between initial (as built) and final (degraded) states. Interim states are not considered as a simple function over time is considered to adequately represent barrier degradation for the purpose of this model.

CONCEPTUAL MODELS AND METHOD OF CALCULATION

The conceptual model was developed on the basis of features, events and processes (FEPs) identified as of key importance for the water balance of a of a generalised disposal facility. Key FEPs include:

- disposal concept (determines relationship between components),
- engineering components (which are considered, how are they represented),
- flow into the EBS (infiltration),
- flow routing between components (dependent on disposal concept being represented),
- vertical flow between components,
- flow out of the EBS (vertical outflow through the base and facility overflow),
- water storage within components potentially leading to component ‘overflow’,
- water level (depth) within components, and
- barrier performance (degradation) as a function of time.

Disposal Concepts

Based on descriptions and definitions given in [1], the following major disposal concepts are represented.

- *Covered trench.* This is the oldest and simplest of the disposal concepts that consist of placing waste into excavated trenches and covering the filled trenches with soil. Typical of this concept is the original trench disposal system at the Low Level Waste Repository (LLWR) near Drigg in the UK.
- *Closed vault.* This consists of a concrete vault into which is placed packaged and/or treated waste. The voidage may be backfilled and the structure closed with concrete slabs, which may be sealed by, for example, asphalt. The whole structure is then protected by an earthen cap. Examples of this disposal concept may be found at the Centre de l’Aube in France, El Cabril in Spain and Rokkasho-Mura in Japan.
- *Domed vault.* This concept is best typified by the IRUS disposal facility in Canada, in which infiltration is controlled by placing waste in a dry permeable layer and covering the waste with an impermeable concrete roof that is subsequently protected by an earthen cap.
- *Open vault.* In this concept, a low permeability cap is placed over the filled vault without emplacement of a concrete slab. Waste is however pre-treated to minimize voidage. This concept is used at the LLWR site in the UK.

Conceptual Model of a Generalised Disposal Facility

The conceptual model of a generalised disposal facility considered in the water balance model is shown in Fig. 1. The components represented in the model break down to two categories: those that are considered in any simulation independently of user choice (‘hardwired’) and those that are optional. The user can select which (if any) of the optional components are considered in any simulation. Optional and ‘hardwired’ components are highlighted with colour coding in Fig. 1. The engineering components included in the conceptual model (indicated with numbers 1 – 8 in Fig. 1) are as follows

1. Cap (always represented),
2. Concrete vault top slab (optional),
3. Waste form (always represented but can be trench or vault type),
4. Concrete vault bottom slab or impermeable layer (optional),
5. Backfill consisting of permeable (e.g. granular materials) or less permeable (e.g. grout) material (optional),
6. Concrete vault side walls (optional),
7. Base liner (optional),
8. Engineered wall. (optional).

The conceptual model breaks down the EBS into two parts: a cap that allows a fraction of the rainwater into the rest of the facility as infiltration, and below-ground components consisting of interconnected 'boxes' or cells that are characterised by their geometry (area, depth), hydraulic conductivity and porosity[1]. The most basic design that can be represented consists of a cap (1) and the waste form (3). Other components can be added as required, including concrete vault top and base slab, a permeable layer beneath the waste, backfill and base liner. It is noted that although vertical walls (6 and 8) are included in the conceptual model, these are not considered in the calculation of vertical flow.

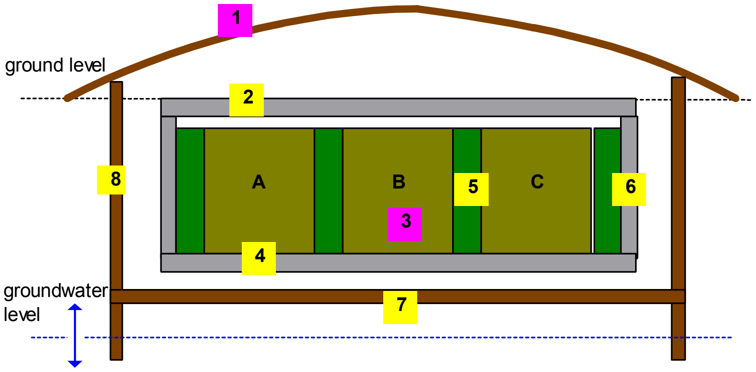

Fig. 1. Conceptual Model of Generalised Disposal Facility Showing the Engineering Components.

Routing of vertical flows depends on the disposal concept and the engineered components being selected. Flow routings for the four disposal concepts are shown Table I, using the component numbers already given. Optional components are indicated in brackets. For disposal concepts including backfill, vertical flow through backfill is considered separately from flow through the waste form (Flow1 and Flow2 in Table I). This allows representation of fast flow through backfill material consisting of granular material, if such is chosen.

Table I. Flow Routing for Each Disposal Concept.

Disposal concept	Vertical flow	Flow routing (numbers designate components) (a)
Covered Trench		1 → 3 → (7) → Out
Closed vault	Flow 1	1 → 2 → 3 → 4 → (7) → Out
	Flow 2	1 → (5) → 4 → (7) → Out
Domed vault		1 → 2 → 3 → 4 → Out
Open vault	Flow 1	1 → 3 → 4 → (7) → Out
	Flow 2	1 → (5) → 4 → (7) → Out

(a) Numbers designate components; numbers in brackets designate optional components.

Table II shows the method of representation of each component and the associated parameter requirements. The key aspects described in Table II include the calculation of inflow, outflow and the consideration of water storage changes for each component. To fully understand the representation of these processes, it is necessary to understand the relationship between the various components in terms of flow linkages. This is illustrated in Fig. 2 that shows a conceptual model of the flows considered in the water balance model, including flows into and out of the facility and flows between the components of the EBS.

Note that 'overflow' between EBS components is a computational device to account for the finite water holding capacity of the various components. For instances when inflow per unit time is higher than the remaining volumetric capacity after outflow has been accounted for, excess water is re-assigned to the overlying component. If that component is also full, the excess amount of water is in turn re-assigned to the next component up if one is present, or if not, it is taken to represent overflow from the facility as a whole. This method of calculation is not intended to represent physical flows between components, but a condition whereby there can be overflow due to excess infiltration.

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[1] With the exception of the liner.

Table II. Method of Representation of EBS Components and Parameter Requirements.

EBS component	Method of representation				Parameters required (a)
	Inflow to component	Outflow from component	Water storage	Consideration of overflow	
Cap	calculated from rainfall	based on cap efficiency	not considered	inflow always exceeds outflow	cap efficiency
Concrete vault top slab	as per outflow from overlying component	based on Darcy equation	change in water storage allowed	exceeding water storage capacity leads to facility overflow	plan area, depth, $K_{ver}(t)$, n(t)
Waste form	as above	as above	as above	exceeding water storage capacity leads to overflow to overlying component or to facility overflow.	plan area, depth, $K_{ver}(t)$, n(t)
Concrete vault bottom slab	as above	as above	as above	exceeding water storage capacity results in overflow to overlying component.	plan area, depth, $K_{ver}(t)$, n(t)
Permeable layer beneath concrete vault	as above	as above	as above	as above	plan area, depth, $K_{ver}(t)$, n(t)
Backfill	as above	as above	as above	as above	plan area, depth, $K_{ver}(t)$, n(t)
Base liner	as above	as above	not considered	Inflow always exceeds outflow	plan area, depth, $K_{ver}(t)$

(a) $K_{ver}(t)$ – Time dependent vertical hydraulic conductivity, n(t) – Time dependent drainable porosity

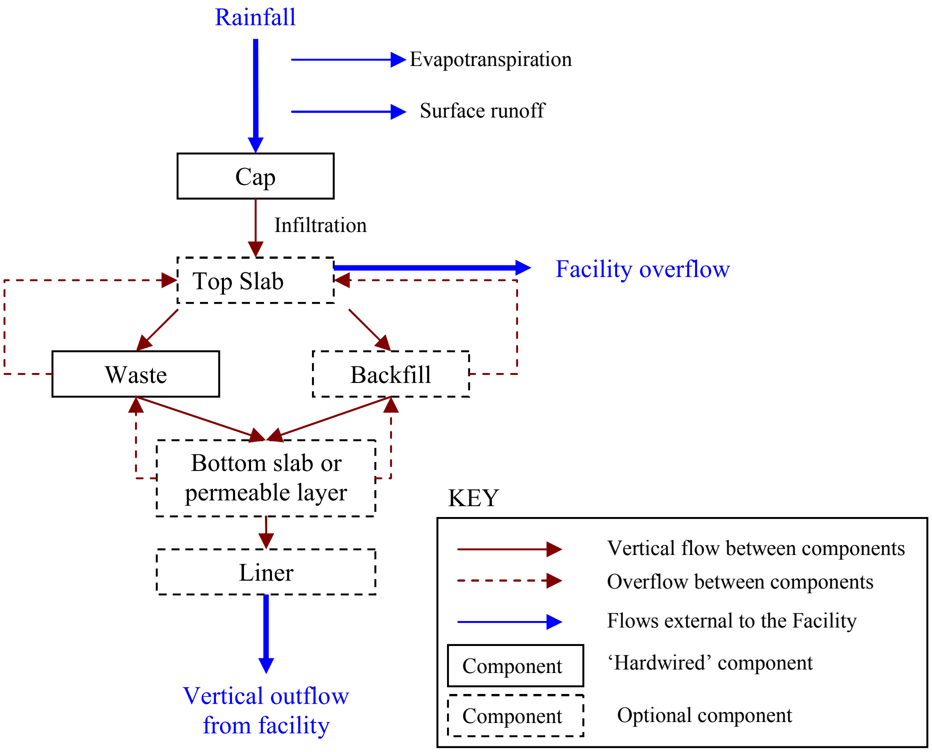

Fig. 2. Conceptual Model of Flows Considered in the Water Balance Model

Representation of most below-ground components is optional. Barrier degradation causes changes to component hydraulic conductivity and porosity. Water moves vertically from the cap through below ground components, a sequence of which is determined by the disposal concept being modelled and components being considered. Flow through a component is determined by incoming flow (generating a head of water), the thickness and area of the component, its hydraulic conductivity and the vertical hydraulic gradient, according to Darcy's Law.

With the exception of the liner, below-ground components are allowed to hold water subject to the available (unsaturated) pore volume. The water level in each component changes with time subject to a balance of inflows and outflows. A component becoming saturated causes 'overflow' to an overlying component, that is, in essence water may be 'backing up' in the system as a function of components saturating from the bottom up and thereby causing 'bath tubbing'. 'Bath tubbing' causes overtopping of the facility and is characterised by overflow from the component directly beneath the cap (facility overflow). This essentially represents a condition when infiltration is greater than the capacity of the below-ground components to hold or conduct water vertically out of the system.

Infiltration

Infiltration through the cap is calculated on the basis of Eq.1 (see also Fig. 2)

$$Inf = R - (ET + SR + SubSR) \qquad \text{(Eq. 1.)}$$

where Inf (m y^{-1}) is infiltration through cap, R (m y^{-1}) is rainfall, SR (m y^{-1}) is surface runoff and $SubSR$ (m y^{-1}) is subsurface runoff. Rainfall and evapotranspiration are user-defined input parameters. Surface runoff is calculated as

$$SR = Rc\ (R – ET) \qquad \text{(Eq. 2.)}$$

where Rc (unitless) is the runoff coefficient. A runoff coefficient of 1 represents all rainfall becoming surface runoff and a runoff coefficient of 0 represents no runoff. Subsurface runoff is defined as a function of the water flow reaching the liner layer in the cap (that is the flow remaining after evapotranspiration and surface runoff have been accounted for) and cap efficiency (η_{cap}, unitless)

$$SubSR = (R - ET - SR)\ \eta_{cap} \qquad \text{(Eq. 3.).}$$

Cap efficiency of 1 represents a fully water tight cap liner layer (no infiltration) and a cap efficiency of 0 represents a fully inefficient cap ($Inf = R – ET - SR$). Therefore, the expression used to calculate infiltration is

$$Inf = (R – ET)\ (1 – Rc)\ (1 - \eta_{cap}) \qquad \text{(Eq. 4.).}$$

Note that of the parameters used to calculate infiltration, only cap efficiency is time dependent. It is therefore cap efficiency that determines changes in infiltration over time.

Calculation of Vertical Flow

As illustrated in Fig. 2, vertical flows considered in the model include inflow and outflow for the concrete top slab (if represented), waste form, bottom slab (if represented) and flow out from the disposal facility through the base liner (if represented). Such flows are essentially determined by the overall inflow into the system (that is, infiltration through the cap) and the vertical hydraulic conductivity of the components. The calculation of 'overflow' between components requires the calculation of water storage in each component and is detailed below.

For any given component, outflow depends on the relative value of the vertical hydraulic conductivity of the engineered component being considered (Comp2) and the vertical hydraulic conductivity of the engineered component above Comp2 (Comp1). Two cases are possible:

1. Comp2 is more permeable or has the same permeability as Comp1 ($KVer\_Comp2 > KVer\_Comp1$), and

2. Comp2 is less permeable than Comp1 ($KVer\_Comp2 < KVer\_Comp1$).

For case (1), flow through Comp2 (Q_Comp2) equals flow through Comp1 (Q_Comp1) at all times. However, the calculation of flows for case (2) is more complicated. In this case, depending on the amount of flow through Comp1, a head of water could develop on top of Comp2 leading to the development of a vertical gradient across the unsaturated depth of Comp2 ($VGrad\_Comp2$). The calculation of this gradient is detailed below. Maximum flow may than be calculated on the basis of Darcy's Law. As already noted, actual flow through Comp2 is dependent on inflow from Comp1. Therefore, flow through Comp2 is calculated as a minimum of the following two quantities: (i) inflow from Comp1 and (ii) maximum flow through Comp2:

$$Q\_Comp2 = min\ ((Q\_Comp1),(KVer\_Comp2 * Area\_Comp2 * VGrad\_Comp2)) \tag{Eq. 5.}$$

Calculation of Vertical Gradient

The intention is to calculate the vertical gradient across an engineered layer, or component (Comp2). The assumption for this calculation is that a head of water has developed (or is going to develop) over the course of the model run due to the accumulation of water on the top of the component (that is, in Comp1). Such accumulation of water may occur due to the inflow of water to the boundary between Comp1 and Comp2 being higher than flow through Comp2. For the purpose of the calculation, it is assumed that Comp2 is fully saturated. According to [3] and based on the above assumptions, the hydraulic head gradient (Δh) for a low permeability percolation layer may be calculated as

$$\Delta h = (h_1+z_1) / z_1 \tag{Eq. 6.}$$

where h_1 (m) is the pressure head on top of Comp2 and z_1 (m) is the thickness of Comp2.

Water Storage

As already described, water storage is calculated for most components (see Table II), based on the balance of inflows and outflows. Water storage is calculated on the basis of

$$(Storage) = (Initial\ storage) + (Addition\ rate) - (Withdrawal\ rate) \tag{Eq. 7.}$$

Elements of the water storage calculation for time step *i*, component N (*CompN*) are given as follows.

$$(Initial\ storage) = V_{Store,CompN,i-1} \tag{Eq. 8.}$$

where $V_{Store,CompN,i-1}$ (m^3) is water storage for component N for time step *i-1*. This calculation requires an initial value for $V_{Store,CompN,i}$. This is to be provided as a user input based on assumptions about the initial saturation state of the disposal facility, porosity and geometry of the component. The rate of water addition is calculated as

$$(Addition\ Rate) = Q_{in,tot,CompNi} = Q_{VerIn,CompN,i} + Q_{OverIn,CompN,i} \tag{Eq. 9.}$$

where $Q_{VerIn,CompN,i}$ is vertical inflow (m^3 y^{-1}) to *CompN* from the overlying component at time step *i*, and $Q_{OverIn,CompN,i}$ is the overflow (m^3 y^{-1}) to *CompN* from underlying component at time step *i*. Withdrawal rate is calculated as

$$(Withdrawal\ rate) = Q_{Out,tot,CompNi} = Q_{Out,CompN,i} + Q_{Over,CompN,i} \tag{Eq. 10.}$$

where $Q_{Out,CompN,i}$ is vertical outflow (m^3 y^{-1}) from *CompN* to underlying component at time step *i*, and $Q_{Over,CompN,i}$ is the overflow (m^3 y^{-1}) from *CompN* to overlying component at time step *i*.

Water Balance

Water balance is calculated for each component based on the generic water balance given as

$$0 = (FlowIn) - (FlowOut) + (change\ in\ storage) \tag{Eq. 11.}$$

The elements *(FlowIn)* and *(FlowOut)* are identical to the elements *(Addition rate)* and *(Withdrawal rate)* described above. The element *(change in storage)* for time step *i*, component N is given as follows

$$(change\ in\ storage) = (V_{storage,CompN,i} - V_{storage,CompN,i-1}) / \Delta t \tag{Eq. 12.}$$

where $V_{storage,CompN,i}$ (m^3) is storage in *CompN* at time step *i*, $V_{storage,CompN,i-1}$ (m^3) is storage component N at time step *i-1* (that is at the previous time step) and Δt is the length of time step *i* (y).

Calculation of Component Overflow

Calculation of component overflow is based on the following generic equation.

(Component overflow) = (Available water storage capacity) – (Balance of inflows and outflows) (Eq. 13.)

Elements of the component overflow calculation for time step *i*, component N are given as follows.

(Available water storage capacity) = $(V_{StoreMax,CompN,i,} - V_{Store,CompN,i-1})$ (Eq. 14.)

where $V_{StoreMax,CompN,i,}$ (m^3) is the water storage capacity of component N at time step *i*. Volumetric capacity of components is calculated from the geometry and total porosity, and is time dependent as a function of assumed porosity changes over time.

$V_{StoreMax,CompN,} = A_{CompN} * D_{CompN} * n_{CompN,i}$ (Eq. 15.)

where A_{CompN} is the plan area of CompN (m^2), D_{CompN} is the depth CompN (m), and $n_{CompN,i}$ is the porosity of component N at time step *i*. The component *(Balance of inflows and outflows)* is provided as part of the water balance calculation, detailed above.

It is noted that the calculation of component overflow necessarily includes a recursive loop, in that it is based on available storage at the start of the time step *i*, when inflows and outflows calculated for this time step are not yet known. GoldSim resolves this loop by using values from the previous time step to calculate overflow. This however also results in apparent water balance errors for periods of model simulation characterised by highly transient flows.

Water Depth in Components

Water depths (m) in components ($D_{Water,Comp}$), are calculated as a function of component geometry, porosity and water storage. For time step *i*, component N this is given as follows

$D_{Water,CompN,i} = (V_{Store,CompN,i} / n_{CompN,i}) / A_{CompN}$ (Eq. 16.)

System Evolution

The assessment of near-surface disposal systems requires consideration of long timescales (thousands of years), depending on the decay properties of the radionuclides disposed in the facility. Over such long timescales, both the facility and its environment will evolve. For the purpose of the water balance model, this means that there is a requirement both to represent the time dependent performance of engineered components and to consider time dependent changes in boundary conditions.

The main boundary condition of the model in its current format is flow from rainfall that penetrates the surface of the cap. Consideration of time dependant changes to this flow involves the assessment of potential future climates and their impact on rainfall, evapotranspiration and runoff. Such analysis is not included in this modelling exercise, and therefore rainfall, evapotranspiration and runoff are treated as constant over time (although subject to significant uncertainties).

Evolution (degradation) of engineered components and their resulting time dependent performance is however included in the model. The key performance parameters for each component are given in Table II. Time dependent values for these parameters are determined by linear interpolation as a function of the initial ('as-built'), final (degraded) component performance, time for degradation and elapsed time from

$P_{CompN}(t) = P_{CompN,ini} + ((P_{CompN,deg} - P_{CompN,ini}) / T_{CompN,degrade}) * ETime)$ (Eq. 17.)

where $P_{CompN}(t)$ is the value of performance parameter for component N at time *t*, $P_{CompN,ini}$ is the initial, or 'as-built' performance (usually occurring at $t = 0$ y), $P_{CompN,deg}$ is the degraded performance (at $t = T_{CompN,degrade}$), $T_{CompN,degrade}$ is time (years) of degradation for component N and *ETime* (years) is the elapsed simulation time. Note that *ETime* = *t* if the component is assumed to be built at the start of the assessment.

Approach to Treatment of Uncertainty

There are significant uncertainties associated with the performance of engineered barriers as represented in the water balance model. This is partly due to a high degree of simplification involved in representing a complex system in a simple model (conceptual uncertainty), and partly due to the fact that future performance cannot be predicted with full confidence (predictive uncertainty). Both types of uncertainty are anticipated to further increase with time, as the system evolves. The system being modelled consists of a mixture of man made and natural materials. Long term performance of man made materials for a timescale that is beyond that for which relevant analogues can be found is inherently uncertain, as is the performance of a complex system that is subject to a number of environmental factors.

Some of these uncertainties are treated in the model through the use of probability distribution functions (pdf[2]) for parameters that describe component performance. These are: rainfall, evapotranspiration, runoff coefficient, cap efficiency and the vertical hydraulic conductivity of below ground components.

IMPLEMENTATION IN GOLDSIM

The GoldSim software tool [2] was selected for its versatility, its capability to represent uncertainty in complex systems and also for its user friendly features. This section describes the main features of the water balance model as implemented in GoldSim version 10.0.

Generic Features, Model Structure and Simulation Settings

The model is designed to be as self-explanatory as possible. This is achieved by widespread use of comments and graphical illustrations within the model. The dashboard feature is used to manage user inputs, access to the main results and to allow easy navigation of the model.

The water balance model consists of a total of 825 elements that are organised into ‘containers’ in a logical order (in this case largely around the representation of key FEPs). ‘Localised containers3’ were used to represent the four main disposal concepts. This approach allows for easy incorporation of additional disposal concepts, should that be required in the future. Data requirements and calculations common to all disposal concepts (that is: infiltration, component performance, materials and facility geometry) are held at the higher level in the model, arranged in their separate containers. Data needs and calculations specific to the four disposal concepts are held in separate localised containers. Global switches (assigned to a value of 0 or 1 by user input) are used to determine whether calculations need to be conducted for a specific localised container (representing a disposal concept). This is implemented by making these containers conditional on the value of the corresponding switch.

By default, the simulation time is set to 5,000 years, with 1-year time steps for the first thousand years, and 10-year time steps for the remainder of the assessment. Testing indicated that this produces reasonably good model performance for most design configurations and ranges of parameter values, while resulting in comparatively quick model runs. Model performance is measured in terms of water balance errors both at the component or the facility level. The model can be run in deterministic or probabilistic mode. GoldSim uses Monte Carlo simulation techniques to calculate the effects of uncertainty in model inputs on model outputs.

Representation of Key FEPs

The four disposal concepts are represented separately (in the localised conditional containers already described) according to the different flow routings they entail. User selection of engineering components is implemented through the use of GoldSim Selector elements. These elements use an if..then logic to specify how a particular parameter is calculated as a function of some state of the system. In this case, vertical flow is calculated depending on whether the switch for the corresponding upstream or downstream component had a value of 0 or 1, according to user input. Selection of the disposal concept and the inclusion of optional components are implemented via user input through the dashboard.

GoldSim Expression elements were used to calculate infiltration on the basis of Equations 4. Similarly, the FEPs associated with engineering components (flow in and out, water storage) were also calculated by a series of GoldSim Expression elements using the appropriate equation, given above. A combination of these Expression elements and the Selector elements allowed calculation of component specific flow and saturation conditions according to flow routing appropriate to the selected design configuration.

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[2] A mathematical representation of the relative likelihood of a variable having certain specific values.

[3] A localised portion of the model such that any element names in the local region are hidden from elements outside of that region. This allows the use of the same element name in the model at various model regions (as long as these are localised). This in turn makes possible copy and paste operations when developing a model.

Vertical gradients are calculated on the basis of Equation 6 using GoldSim Expression elements. Consideration is given to whether the overlying component or components are saturated which would increase the head on the component for which the calculation is conducted by creating an uninterrupted water column spanning three components[4]. This is implemented by using GoldSim Status elements (to monitor saturation state of components) and Selector elements (so that the appropriate calculation could be conducted depending on the state of the overlying components). Once vertical gradients are determined, flow out from each component can be calculated on the basis of Equation 5 using GoldSim Expression elements. Flow out from a component is taken to be flow into the underlying component according to flow routings determined above.

Water storage in each compartment is calculated by the GoldSim Reservoir elements. Reservoir elements accumulate flows and generate an overflow once a pre-determined storage capacity is exceeded. Initial value to Reservoir elements (that is: the amount of water held in the component being represented at the start of the simulation) has been assigned according to Equation 8. Volumetric flow additions are determined by inflows to component (Equation 9), and withdrawals are determined by outflows (Equation 10). An upper bound is set to storage capacity, given by the pore volume of each component (Equation 15).

Overflow rates are calculated in GoldSim through the use of the Euler integration method, which assumes that the Addition Rate and Withdrawal Rate represent constant rates over the next time step. As a consequence, the calculated overflow rate also represents the overflow rate over the next time step. In addition, it is noted that although the method applied in GoldSim to calculate overflow using the Reservoir element always conserves mass, this does not imply that the result is perfectly accurate. In fact, the accuracy of the result is a function of the time step, since GoldSim is approximating continuously varying functions (i.e., rates and bounds) using stair-step functions. Both of the above points have implications for the water balance check conducted within the model. It is stressed however that the calculated water imbalance for a single time step does not necessarily indicate an erroneous calculation, it may be due to the methods applied to calculate overflow. What is important is that the water balance over several time steps should approximate zero.

Any change in water storage is calculated on the basis of Equation 12 using GoldSim Reservoir, Previous Value and Expression elements. The depth of water in components is calculated on the basis of Equation 16 using GoldSim Expression elements. Finally, outflows from the facility are given by outflow from bottom component (= vertical outflow), and overflow from component directly beneath cap (through base= facility overflow). The precise component that provides these flows depends on disposal concept and optional components selected.

Inputs and Outputs

Input requirements are detailed in Table III. Note that for parameters that are allowed to change over time, two input values need to be provided: an initial and final (degraded) value that corresponds to performance for simulation time larger than or equal to 'time required for component degradation'.

The main outputs from the model are:

- probabilistic time history of calculated infiltration (m^3 y^{-1}),
- probabilistic time history of calculated vertical outflow (m^3 y^{-1}) through the base of the facility,
- probabilistic time history of calculated facility overflow (m^3 y^{-1}) due to overtopping, and
- probabilistic time history of water depth (m) in waste.

Other model output that is generated to allow more detailed analysis of the results includes:

- probabilistic time history of calculated component performance parameter (for time dependent parameters),
- probabilistic time history of calculated component specific outflows,
- probabilistic time history of change in facility storage, and
- probabilistic time history of component and facility water balance.

These outputs may be generated for each disposal concept separately from a single simulation run.

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[4] The component for which the calculation is conducted (Comp2) is assumed to be saturated, as already described. Therefore, for cases when the overlying component (Comp1) is also saturated, the head on the top of Comp2 should include the full depth of Comp1, plus the head of water in the component above that, and so on.

Table III Parameter Input Requirements for Water Balance Model.

Group	Input parameters	Units	Time dependency	Treatment of uncertainty
Cap infiltration	Rainfall	mm y^{-1}	constant	stochastic (g)
	Evapotranspiration	mm y^{-1}	constant	stochastic (g)
	Surface runoff fraction	unitless	constant	stochastic (g)
	Cap efficiency (a)	unitless	time dependent	stochastic (g)
	Time required for cap degradation	year	n/a	deterministic
Component performance	Vertical hydraulic conductivity (a, b)	m sec^{-1}	time dependent	stochastic (g)
	Total porosity (a, c)	unitless	time dependent	deterministic
	Time required for component degradation (b)	year	n/a	deterministic
Component geometry	Plan area (d)	m^2	constant	deterministic
	Depth (b)	m	constant	deterministic
Initial conditions	Initial storage (c)	m^3	initial value only	deterministic
EBS design selection	Disposal option selector switch (e)	n/a	n/a	n/a
	Waste type selector (f)	n/a	n/a	n/a

(a) Initial and final degraded values are required to determine time dependency.
(b) Required for all components with the exception of the cap.
(c) Required for all components with the exception of the cap and base liner.
(d) Required for all components.
(e) Check box for each disposal options (multiple selection is allowed).
(f) Check box to choose between trench or vault waste form (multiple selection is not allowed).
(g) Default values have also been defined to allow deterministic model runs.

GoldSim dashboard provides a useful user interface to enter the required input parameters and to access the results. The dashboard has been used at two levels: at the model root (a single top level dashboard), and at the localised container level (four design concept specific dashboards). The former is used to determine generic input (such as design selection, facility dimensions, infiltration parameters and component performance parameters). The latter allows selection of optional components and waste form to be represented and provides access to design-specific model outputs.

User selection of the main component performance parameters (initial and degraded hydraulic conductivities, time of degradation) are selected from a pull down menu from pre-selected values. In the case of vertical hydraulic conductivities, these range between 1E-04 and 1E-10 m sec^{-1} and include seven values with an order of magnitude difference between them. Pre-determined values for 'time of degradation' ranges between 50 years and 3,000 years, and allow a selection between five values. It is noted that pre-selected values are provided for user convenience only, and can readily be altered on requirement by modifying or disabling the dashboard. The remaining input parameters are entered manually by the user. Note that stochastic properties of input parameters cannot be determined through the dashboard in the current model configuration.

MODEL DEMONSTRATION

In order to demonstrate the capabilities of the water balance model, an example application is described briefly. It is stressed that this is for demonstration purposes only, and is not based on a real-life facility. However, the input values were chosen so that they are broadly representative of a facility of this type. For a real-life application, site specific considerations will dictate the selection of the appropriate input data, which therefore may differ significantly from the values used in this example.

Model Setup and Inputs

The open vault design concept with a vault waste form and including backfill and base liner has been selected for model demonstration. The backfill is assumed to consist of granular material. The simulation time is for 5,000 years, assuming that each component is at their ‘as-built’ condition at the start time of the simulation run. Probabilistic simulations have been run for 1,000 realisations using Latin Hypercube Sampling to ensure that the parameter space is spanned uniformly.

Input parameters used in the demonstration run are given in Table IV and Table V. It has been assumed that at the start of the assessment, the facility is essentially dry (1% moisture content). Stochastic properties of parameters used to determine infiltration are fully described in Table V. For component hydraulic conductivities, the log normal distribution has been selected with both the mean and the standard deviation taken to be equal to the reference hydraulic conductivity value (that is: the value given in Table V). This gives a parameter value distribution of about two orders of magnitude between the 5th and 95th percentiles. This is considered a reasonable representation of uncertainty associated with the hydraulic conductivity of engineered barriers for the purpose of illustrative model runs.

Results

Output from the demonstration model run is shown in Fig. 3 (time history) and Table VI (tabulated results for selected time steps). Note that results in Fig. 3 are shown on a log-log scale. Using a log scale for the independent variable (simulation time) allows better illustration of changes that occur at the early times into the simulation in response to changes in rainfall. Using a log scale for the dependent variable is appropriate as the calculated flows vary by several orders of magnitude in response to changes in component hydraulic conductivity. At first sight, uncertainty bands appear to narrow with time in Fig. 3. This is however a false impression generated as a consequence of using a logarithmic scale for the output. Widening of uncertainty bands with time can be correctly assessed from Table VI.

Table IV Component Geometry and Hydraulic Performance Parameters for the Demonstration Run.

Component	Plan area (m^2)	Depth (m)	K ($m\ s^{-1}$)		Distribution	Porosity		Time for degradation (year)
			Initial	Degraded		Initial	Degraded	
Cap (a)	100,000	n/a	n/a	n/a	Normal	n/a	n/a	1,000
Vault top slab	100,000	1	1.E-09	1.E-06	Log-Normal	0.3	0.3	1,000
Waste form (b)	90,000	5	1.E-08	1.E-06	Log-Normal	0.3	0.3	1,000
Backfill (c)	10,000	5	1.E-04	1.E-06	Log-Normal	0.5	0.3	300
Bottom slab	100,000	1	1.E-09	1.E-06	Log-Normal	0.3	0.3	1,000
Base liner	100,000	1	1.E-10	1.E-08	Log-Normal	n/a	n/a	3,000

(a) See Table V for performance parameter (cap efficiency) values and stochastic properties
(b) Vault waste form
(c) Assumed to consist of granular material

Table V Parameters Used To Determine Cap Infiltration In The Demonstration Run.

Parameter	Unit	Stochastic properties				
		Distribution	Mean	St dev	Min	Max
Rainfall	mm $year^{-1}$	Normal	1000	200	500	1500
Evapotranspiration	mm $year^{-1}$	Normal	250	50	0.0	500
Runoff coefficient	unitless	Normal	0.2	0.05	0.0	0.5
Cap efficiency - initial	unitless	Normal	0.99	0.05	0.75	1.00
Cap efficiency - degraded	unitless	Normal	0.50	0.05	0.25	0.75

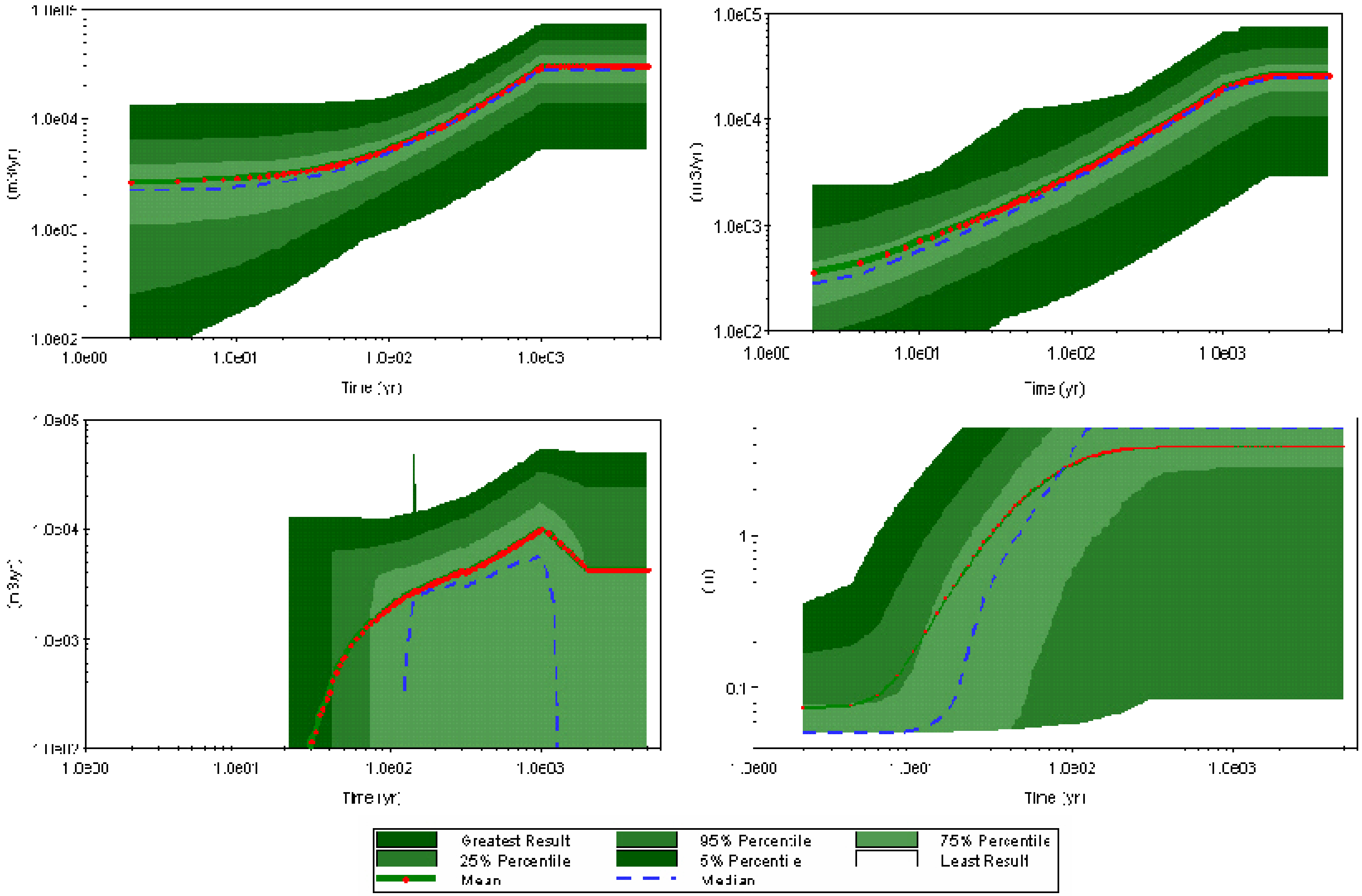

Fig. 3. Results from demonstration model run showing probabilistic time histories for infiltration through the cap (m^3 year^{-1}, top left), vertical flow through the base (m^3 year^{-1}, top right), overflow due to 'bathtubbing' (m^3 year^{-1}, bottom left), and saturation depth in the waste (m, bottom right). Note that results are plotted on a log-log scale.

Table VI Tabulated Results From Demonstration Model Run For Selected Time Steps.

Output	Time (year)	Mean	5%	25%	75%	95%
Infiltration through cap (m^3/year)	0	2,612	203	1,001	3,786	6,448
	100	5,363	2,236	3,557	6,712	9,763
	1,000	30,119	13,546	21,184	38,154	52,377
	5,000	30,119	13,546	21,184	38,154	52,377
Vertical outflow through base of facility (m^3/year)	0	285	51	121	363	794
	100	2,964	944	1,732	3,779	6,140
	1,000	20,057	6,053	12,137	26,133	40,468
	5,000	25,872	10,390	17,846	32,366	47,033
Overflow due to 'bath tubbing' (m^3/year)	0	0	0	0	0	0
	100	1,947	0	0	4,065	7,255
	1,000	10,061	0	0	17,324	33,900
	5,000	4,248	0	0	4,180	23,639
Saturation depth in waste (m)	0	0.05	0.05	0.05	0.05	0.05
	100	2.97	0.06	0.60	5.00	5.00
	1,000	3.84	0.08	2.83	5.00	5.00
	5,000	3.84	0.08	2.83	5.00	5.00
Facility water balance error per time step (percentage of infiltration)	2	0.13	-2.05	-0.78	0.49	3.18
	100	-1.47	-5.88	-2.22	0.00	0.00
	1,000	0.00	0.00	0.00	0.00	0.00
	5,000	0.00	0.00	0.00	0.00	0.00

According to Table VI and Fig. 3, infiltration increases over time from about 2,500 (mean) m^3 $year^{-1}$ at the start of the simulation run to about 30,000 (mean) m^3 $year^{-1}$ at t=1,000 years, when the cap is fully degraded. There is considerable uncertainty associated with these results as a consequence of parameter uncertainties.

The trend established by infiltration is also followed by outflow rates through the base of the facility. This increases from about 290 (mean) m^3 $year^{-1}$ at the start of the simulation run to about 20,000 (mean) m^3 $year^{-1}$ at t=1,000 years and finally to about 25,000 (mean) m^3 $year^{-1}$ at t=5,000 years by which time all components are degraded. Uncertainty associated with outflow also increases with time, but remains slightly below the levels calculated for infiltration in absolute terms. This is mostly due to the fact that outflow is smaller than infiltration. If the comparison made in relative terms (that is: as compared against the corresponding mean value), uncertainties associated with calculated outflow rates are higher compared to those for infiltration. This is expected as outflow is a function of a number of additional input parameters that are also uncertain.

The difference between infiltration and outflow results in increasing storage within the facility until reaching full saturation and finally leading to 'bathtubbing'. From Fig. 3, the waste form reaches saturation levels within a few hundred years into the simulation for considerable numbers of model realisations. However, the mean value[5] of waste saturation remains below the top of the waste for all times. It may be said therefore that the best estimate for this model simulation is that overtopping may occur but it is marginally more likely not to. According to Fig. 3, the critical time for overtopping is between 20 and 100 years simulation time, during which time the likelihood of overtopping increases steeply. At 20 years, fewer than 5% of realisations lead to overtopping while at 100 years more than 25% of realisations result in overtopping.

Overflow rates resulting from overtopping range between zero and about 50,000 m^3 $year^{-1}$, with mean values increasing from zero at the start of the assessment to approximately 16,000 m^3 $year^{-1}$ after 1,000 years. As already described, in more than 25% of model realisations, overtopping does not occur at any time and there is therefore no overflow. Before about 20 years simulation time, even the greatest results[6] do not lead to overtopping (overflow is zero). The general trend according to Fig. 3 is an increasing overflow rate over time. The steep rise in overflow rates

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[5] As calculated from output from all realisations for each time step (indicated 'Mean' in Fig. 3)

[6] Greatest value of independent variable from all realisations for each time step ('Greatest Result' in Fig. 3)

between about 20 and 100 years may be attributed to the trends observed for waste saturation. Between about 100 years and 1,000 years it may be attributed to the trends observed for infiltration. Essentially, between 20 and 100 years, the key process is the increasing depth of water in the waste (itself largely due to a relatively impermeable base) while between 100 and 1,000 years the key process is the increased infiltration (largely due to cap degradation).

A brief sensitivity analysis has also been conducted. Annual rainfall and degraded hydraulic conductivity of the base liner have been identified as the key parameters that determine facility saturation and overtopping. This is consistent with expectations for this type of facility. The model is particularly sensitive to values of annual rainfall between 680 mm year^{-1} and 760 mm year^{-1} (water depth increasing from 1.3 m to 5.0 m with other parameter values at the central value), and degraded hydraulic conductivity of the base liner between 1.2E-08 and 2.0E-8 m sec^{-1} (water depth decreasing from 5.0 m to around 1.0 m with other parameter at the central value). Note that that these sensitivities fall in a range that may be considered as the mid range of the corresponding parameters. This suggests that a confident prediction of system performance for the modelled design is inherently difficult, as the system responds very sensitively to changes within credible ranges of key input parameter.

Model performance in terms of calculated water balance shows a trend of decreasing error per time step. It decreases from about 5% at the initial time steps to less than 1% by about 120 years, less than 0.1% by about 200 years and less than 0.001% by about 300 years for most of the model realisations. This trend reflects the transient nature of the system at the start of the simulation, which is also illustrated in Fig. 3, and is one of the reasons behind the use of logarithmic scale for the independent variable.

SUMMARY

A water balance model for a generic near-surface disposal facility has been developed and implemented in GoldSim. The model can be used in assessments of the hydraulic performance of various design options and provides a highly flexible, and user friendly tool to analyse performance of the engineered barrier system (EBS) in support of a safety assessment, an optimisation study or design development. The ability to represent a variety of design options and barrier degradation scenarios via simple user interface is a unique feature of the model that should be very useful.

In order to demonstrate the capabilities of the water balance model, an example application is presented. Input values have been chosen so that they are broadly representative of a facility of this type. The open vault design concept with a vault waste form and including backfill and base liner has been selected for model demonstration. The simulation time is for 5,000 years. Probabilistic simulations have been run for 1,000 realisations.

Results form the demonstration model indicates a scenario of gradually increasing infiltration due to cap degradation and a slower degradation of the base liner over time leading to saturation of the facility. Given the assumed input parameter values, the best estimate for this model simulation is that overtopping may occur but it is marginally more likely not to. The critical time of system evolution is between about 20 and 100 years, during which time the saturation depth of the waste increases steeply. The generated overflow rate can be significant (that is up to the same order of magnitude as infiltration), but is subject to a high degree of uncertainty. Sensitivity analysis identified annual rainfall and degraded hydraulic conductivity of the base liner as the key parameters for overtopping. However, it also showed very high sensitivity at the mid range of the corresponding parameter values which suggest that a confident prediction of system performance for the modelled design is inherently difficult.

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