Response to the referees – sand-2026-11

We thank the three referees for their careful reading and constructive comments. They led us to re-examine the setups of all codes and to identify the causes of the deviations between the breakthrough curves. The main revisions are:

- The setups were harmonized: in both models, all codes now use a common grid, the same transport boundary condition at the recharge boundary and the same van Genuchten parametrization; in the 1D soil model, they also use the same time steps. The common grid proved essential in the 2D landfill model, whose downstream results are very sensitive to the grid; in the soil model, a refinement test confirmed that the grid is fine enough.
- The causes of the deviations of DuMux were identified and corrected: an absorbing transport boundary condition and an additional saturation factor in the dispersion flux (soil model), and an averaged initial saturation and a dispersion tensor that used only the face-normal velocity (landfill model).
- All results were recomputed. DuMux and d^{3}f++ now agree in both models; SPRING agrees in the soil model and yields lower maxima downstream in the landfill model, caused by a lower water content in its unsaturated zone. The saturated soil cases were verified against an analytical solution.
- The introduction was extended by a literature review, the equations were revised for consistency, a table compares the numerical methods of the codes, and the discussion and conclusions were rewritten on the basis of the new results.

The comments are summarized in italics. Line and equation numbers in the comments refer to the submitted manuscript, all other references to the revised manuscript.

RC1

1. *The explanation of the differences between the breakthrough curves is not fully consistent.*

   We identified the causes and recomputed all results. Soil model: in the submitted version, DuMux yielded lower maxima, in particular for high dispersivities, because of an absorbing transport boundary condition at the recharge boundary (no-flow in d^{3}f++ and SPRING) and an additional saturation factor in its dispersion flux. Both were corrected; in addition, all codes now use $m = 1 - 1/n$, the same grid and the same time steps (Sect. 3.1). The curves of all codes now agree (Figs. 3–8, Sect. 4.1). Landfill model: in the submitted version, DuMux used a saturation averaged from d^{3}f++ as initial condition, since its steady flow simulation did not converge. Now all codes compute the steady flow field on a common grid (DuMux with the cell-centred TPFA method), and the flow fields of DuMux and d^{3}f++ agree. The comparison also revealed that the DuMux simulations used only the face-normal velocity in the dispersion tensor, which suppresses transverse dispersion in 2D; this was corrected. DuMux and d^{3}f++ now agree at all observation points; SPRING yields up to about 20 % lower maxima at P3/P4 (Figs. 9–11, Sect. 4.2).

2. *The overall structure should be checked; proofreading by a native speaker is recommended.*

   The manuscript was proofread for grammar, spelling and style, also with language editing tools.

3. *Comments within the manuscript.*

a) *"Decay" is mentioned in the abstract and conclusions but not modelled.*

Decay was removed from the abstract and conclusions; Sect. 2.4 states that it is not considered (^{129}I, half-life 1.57×10^7 a).

b) *The statement is not suitable given the differences in Fig. 5.*

The statement was removed; with the revised results, the curves of all codes agree in Fig. 5.

c) *Why were these three codes selected?*

Sect. 2 now explains that the codes represent complementary modelling philosophies and numerical implementations.

d) *FV or FE is not specified.*

The discretization of each code is now stated (Sect. 2.1–2.3, Table 1).

e) *The code descriptions lack a common focus (GRS-436).*

The new Table 1 compares the codes in a common scheme: spatial and temporal discretization, stabilization of advection, flow equation, dispersion tensor and licence. GRS-436 is cited.

f) *Quantitative information on the discretization in space and time is missing.*

Soil model: common grid of 2304 cells (3.9 mm) and the same fixed time steps per case (Sect. 3.1, Table A1). Landfill model: common grid of 58 368 quadrilaterals with the cell sizes, and the time steps of all codes (Sect. 3.2).

g) *The concept of the relative permeability should be explained.*

Darcy's law now contains the relative permeability, and the van Genuchten–Mualem relation is given (Sect. 2.4).

h) *The approach after Frind (1987) used by SPRING should be mentioned.*

In 2D, SPRING forms the dispersion tensor after Scheidegger, as the other codes; the approach after Frind is used only in 3D and therefore not relevant here.

i) *The vertical discretization should be described.*

See the answer on the discretization above (Sect. 3.1, 3.2).

j) *What is the aim of the parameter variations?*

Sect. 3.1 now explains that the cases test the implementation of each transport process individually and in combination, over a range of travel times and peak concentrations.

k) *Is there a difference in the transverse dispersion? The reason for the growing differences in Fig. 5 should be found.*

The differences in the soil model were caused by the transport boundary condition and the additional saturation factor in the DuMux dispersion flux (see the first comment), not by transverse dispersion. After the correction, the curves agree.

l) *The time and concentration axes change from Fig. 3 to Fig. 4.*

All breakthrough curves are now plotted over time in years, and figures with the same parameters in the saturated and unsaturated column share their axes. Figs. 3 and 4 keep different time axes, since sorption increases the travel times from about 7 to 54 a.

m) *The differences due to dispersion are smaller for the unsaturated case 12 than for the saturated case 2.*

With the revised results, dispersion lowers the maximum more strongly in the unsaturated case (SC11 to SC12: 0.62 to 0.10 mg kg^{-1}) than in the saturated case (SC1 to SC2: 0.99 to 0.30 mg kg^{-1}); the sentence was removed.

n) *Lines 243–246 describe effects of multiphase finite-volume modelling; SPRING uses the relative permeability, so advection should be slower in the unsaturated case.*

All codes solve the Richards equation with the same relative permeability. Under the prescribed infiltration, the Darcy flux is the same in the saturated and unsaturated column, so the lower water content increases the pore velocity, and the peaks arrive earlier in all codes. The paragraph was rewritten accordingly and also explains the lower maxima by the compression of the tracer pulse in the saturated zone (Sect. 4.1).

o) *The peak arrival times of SC11–14 are about 1.6 a shorter than those of SC1–4.*

With the revised results, the difference is 1.9 a in all codes; it follows from the higher pore velocity (Sect. 4.1).

p) *The initial saturation of $d^3f{+}{+}$ is used for DuMux, yet differing initial saturations are named as cause of deviations.*

All codes now compute the steady flow field themselves on the same grid, and the statement was removed (Sect. 3.2, 4.2).

q) *The dispersivities are not realistic for an 850 m long model.*

The models are generic; the dispersivities test the implementation of dispersion and are not meant to represent a site. The statement that 1 m may be realistic was replaced (Sect. 4.2).

r) *2D concentration plots are described but not shown.*

The concentration fields of all codes for case 2 at $t = 12$ a were added (Fig. 12, Sect. 4.2).

s) *The transverse vertical dispersivity is too large; transverse vertical and horizontal dispersivities are not distinguished.*

In the vertical 2D cross section, only the longitudinal and the transverse vertical dispersivity act; this and $\alpha_t = \alpha_l/10$ are now stated (Sect. 4.2). The differences at P3 were resolved by the common flow field and the corrected dispersion velocity in DuMux (see the first comment).

t) *Both dispersivities are not realistic for this setup.*

See above.

u) *The dispersivity is usually based on the plume length; the grid then has to be adjusted.*

All codes use the same grid and dispersivities. The grid Péclet numbers in the aquifer (6 and 0.6), the grid sensitivity of the landfill model and a refinement test for the soil model were added (Sect. 3.1, 3.2, 4.2).

v) *Chapter 4 mostly describes the curves; Chapter 5 lacks a discussion of the deviations.*

Sect. 5 now discusses the deviations: the requirements for agreement (transport boundary condition, van Genuchten parametrization, common flow field and grid), numerical dispersion and upwinding in the purely advective cases compared with the analytical solution, and the lower water content in the unsaturated zone of SPRING.

w) *For which cases was upwinding used in DuMux? The approaches should be introduced earlier.*

Sect. 3.1 and Table 1 now give the upwind schemes for both models: none in SPRING, partial in $d^3f{+}{+}$, full in DuMux.

x) *The implementation of the transverse horizontal and vertical dispersivities should be checked again.*

The implementations were checked. The DuMux simulations used only the face-normal velocity in the dispersion tensor; with the full Darcy velocity, as in $d^3f{+}{+}$, the two codes agree (Sect. 4.2).

y) *The deviations of DuMux (SC10, SC18–20, P3 in SC1) should be explained in the conclusions.*

These deviations were caused by the issues described in the first comment and disappeared after their correction. The conclusions now state the agreement of the codes and the remaining differences of SPRING (Sect. 6).

z) *Permeability and porosity are not discussed, although the material properties are said to have a major influence.*

The sentence was restricted to the sorption properties, which were varied; permeability and porosity were the same in all cases (Sect. 6).

RC2

1. *DuMux differs from the Richards-based codes in timing (∼10 %) and amplitude (∼50 %); the differences should be identified and corrected.*

   All codes solve the Richards equation (Sect. 2.4). The causes of the differences were identified and corrected (see RC1, first comment): DuMux now agrees with d^{3}f++ and SPRING in the soil model (Figs. 3–8) and with d^{3}f++ at all observation points of the landfill model (Figs. 9–11).

2. *A literature review on the state of the art is missing.*

   An overview of numerical groundwater flow and solute transport, unsaturated flow, fractured media and radionuclide-transport applications was added to the introduction.

3. *The phrase "the radionuclide ... groundwater model" conflates flow and transport.*

   The wording was revised; the introduction and abstract now distinguish groundwater flow and solute transport as distinct but coupled processes.

4. *"Mostly analytical methods" is too generic.*

   The statement is now restricted to regulatory clearance assessments in Germany, where simplified analytical models are commonly used.

5. *The implementations should be verified against analytical solutions.*

   The saturated soil cases with advection (SC1), dispersion (SC2) and diffusion (SC3) were compared with the analytical solution for a slug in a semi-infinite column (Fig. A2, appendix). For SC2 and SC3, all codes agree with it within $0.02\,\mathrm{mg\,kg^{-1}}$; for SC1, the rectangular pulse is smoothed by numerical dispersion, with peak and timing reproduced (Sect. 4.1).

6. *Transport is based on steady flow, so the flow formulations should not explain the discrepancies; the flow velocities should be analysed.*

   We agree. In the submitted version, DuMux used an averaged initial saturation. Now all codes compute the steady flow field on the same grid. Started from the DuMux steady state, d^{3}f++ changes the pressure by less than 4 mm of head in the unsaturated zone and about 2 cm in the aquifer (Sect. 4.2), so the flow fields agree. The remaining differences between DuMux and d^{3}f++ were traced to the velocity in the DuMux dispersion tensor and corrected (see RC1). SPRING yields the same water table, but a lower water content in the unsaturated zone, since its relative permeability had to be set higher for numerical stability (Sect. 4.2).

7. *Radioactive decay is mentioned but not addressed.*

   Decay is not considered: the tracer represents ^{129}I with a half-life of 1.57×10^7 a. The study is now explicitly restricted to long-lived radionuclides (Sect. 2.4), and decay was removed from the abstract and conclusions.

8. *Spatial distributions are mentioned but not shown.*

The steady-state saturation and pressure profiles of the unsaturated soil column (Fig. A1) and the concentration fields of the landfill model for case 2 (Fig. 12) were added.

RC3

General comments

1. *The novelty of the code comparison should be highlighted.*

   The introduction now states that the contribution is the systematic comparison of three codes for clearance-related groundwater-pathway assessments, not numerical radionuclide-transport modelling itself. Sect. 2 explains the choice of the codes.

2. *Literature on numerical radionuclide transport is missing.*

   See RC2.

3. *The peak concentrations differ by a factor of 2–3; the discrepancies should be resolved or convincingly explained.*

   The causes were identified and corrected (see RC1, first comment). The codes now agree in the soil model; in the landfill model, DuMux and d^{3}f++ agree, and SPRING yields up to about 20 % lower maxima at P3/P4 because of its lower water content in the unsaturated zone (Figs. 3–11).

4. *Numerical setup: spatial discretization methods.*

   d^{3}f++ uses vertex-centred finite volumes, DuMux vertex-centred (soil model) and cell-centred (landfill model) finite volumes, and SPRING finite elements (Sect. 2, Table 1).

5. *Time discretization and time-step selection.*

   All codes use implicit time stepping. In the soil model, all codes use the same fixed time step per case (Table A1); for the landfill model, the time steps of all codes are given in Sect. 3.2.

6. *Numerical grids.*

   Soil model: a common grid of 2304 cells; refining it fourfold changes the maxima of the cases with dispersion by less than 0.5 % (Sect. 3.1). Landfill model: a common grid of 58 368 quadrilaterals (Sect. 3.2); on an unstructured triangular grid, DuMux yields about 50 % (case 1) and 25 % (case 2) lower maxima at P3, which shows that a common grid is essential.

7. *The global mass balance should be analysed.*

   Soil model: the lower DuMux maxima in the submitted version resulted from tracer leaving through the absorbing recharge boundary; now all codes release the same tracer mass (within 3 %). Landfill model: at P1/P2, DuMux and d^{3}f++ release the same mass (within 3 %); SPRING releases about 17 % (case 1) and 13 % (case 2) less, since its lower water content in the unsaturated zone reduces the dissolved initial mass. With strong sorption (case 3), the sorbed mass dominates, and the released masses agree (Sect. 4.2, 5).

8. *The transport equations are not fully consistent; additional verification is recommended.*

   Sect. 2.4 and 2.5 were revised: all transport equations are now written in the concentration $c^\kappa = \varrho_w X^\kappa$, the sorption term and K_d are unit-consistent, and the equivalence of the three formulations is shown explicitly.

Major comments

1. *L. 13–18: the discrepancies are not minor; the abstract should be revised.*

The abstract was rewritten and states the agreement of the codes and the remaining differences of SPRING in the landfill model.

2. *L. 39–41: the statement on little research on coupled flow and radionuclide transport is misleading.*

   The statement was replaced by the literature overview.

3. *All variables should be defined, with units according to common practice.*

   Missing definitions and units were added (e.g. source terms, relative permeability, gravity, water and capillary pressure, dispersivities, diffusion coefficient, adsorbed mass, K_d); the unit of the van Genuchten α was corrected to Pa^{-1}. The storage term of the Richards equation is now written with the water content $\theta = \phi S_w$ (Eq. 1).

4. *The same symbol is used for mass fractions and concentrations.*

   The mass fraction X^κ is used only in the general balance (Eq. 7); all other equations use the concentration $c^\kappa = \varrho_w X^\kappa$, and X_s^κ denotes the adsorbed mass per mass of solid.

5. *Eq. 6 (mass fractions) and Eq. 10 and following are not consistent.*

   K_d is now defined as $K_d = X_s^\kappa / c^\kappa$ in $\mathrm{m^3\,kg^{-1}}$, and the sorbed mass per bulk volume is $(1-\phi)\varrho_s K_d c^\kappa$ (Eq. 10, 11).

6. *The corrected equations should also be verified in the codes.*

   The notation changes do not affect the implementations. In DuMux, the sorption term with $(1-\phi)$ and $\tau = 1$ were set as described in Sect. 2.5. For d^{3}f++ and SPRING, the formulations were confirmed against the code documentation.

7. *L. 148: a tortuosity of 1 is unrealistic; how is it implemented in SPRING?*

   We agree. $\tau = 1$ was chosen to compare the codes without an additional parameter, since d^{3}f++ and SPRING contain no tortuosity factor. It only scales the molecular diffusion, which is small compared to dispersion here. This is now stated in Sect. 2.5.

8. *Geochemistry and decay are not considered.*

   The study is restricted to long-lived radionuclides; see RC2.

9. *The appendix could be expanded with additional runs.*

   The appendix now contains the steady-state profiles of the soil model (Fig. A1) and the comparison with an analytical solution (Fig. A2).

10. *Figs. 4, 5, 7, 8 and 9 suggest different total masses; the global mass balance should be checked.*

    See the mass-balance comment above. Figs. 3–11 were replaced; in the soil model, all codes now release the same mass.

11. *Figure captions and axis labels; definition and normalization of the concentration.*

    The figures show the tracer mass fraction in $\mathrm{mg\,kg^{-1}}$, with an initial value of $1\,\mathrm{mg\,kg^{-1}}$ in the contaminated layer; since the tracer does not change the fluid properties, the results scale linearly with it (Sect. 4.1, caption of Fig. 3).

12. *The discussion and conclusions should be revised after all modifications.*

    Both were rewritten on the basis of the new results (Sect. 5, 6).

Minor comments

1. *Second-order tensors should be bold.*

   Corrected.

2. *Eq. 2: Darcy's law should include gravity.*

   The gravity term and the relative permeability were added (Eq. 2); all codes include gravity.

3. *Eqs. 6, 8, 11: the water content is missing in parts of the transport formulation.*

   The dispersion tensor is formed with the Darcy velocity $\mathbf{v}_f = \theta\mathbf{v}$ and therefore contains the water content; this is now stated after Eq. 9 and shown for SPRING after Eq. 13.

4. *Eq. 7: DuMux uses the inverse tortuosity definition.*

   $\tau \leq 1$ is now introduced as tortuosity factor, the inverse of the tortuosity defined by path lengths.

5. *Eq. 9 is not an equation.*

   Replaced by a sentence.

6. *Eq. 12: the dispersion tensor is not defined; diffusion scaling by tortuosity.*

   The definition of $\mathbf{D}_d$ was added; SPRING contains no tortuosity factor, which corresponds to $\tau = 1$.

7. *Eq. 14: tortuosity scaling for diffusion is missing.*

   The diffusion term of $\mathrm{d}^3\mathrm{f}{+}{+}$ corresponds to $\tau = 1$; this is now stated.

8. *Eq. 15: red highlighting; L. 141–142 need more detail.*

   Both highlighted terms are now explained: the factor $(1 - \phi)$ of the sorption term and the tortuosity factor.

9. *Eqs. 6, 11, 12, 14, 15: the same symbol for mass fractions and concentrations.*

   See major comments.

10. *L. 189: "constant" should be "steady".*

    Corrected.

11. *L. 201–202: hydraulic conductivity, not permeability.*

    Corrected.

12. *L. 212–213: "similar" instead of "identical".*

    Corrected.

13. *L. 214–216: literature review.*

    See RC2.

14. *L. 238: meaning of "tone".*

    Typo, corrected to "zone".

15. *L. 341–342: the agreement is not as good as described.*

    The discussion and conclusions were rewritten and name the remaining differences: the sharper SPRING peaks in the purely advective soil cases and the lower SPRING maxima in the landfill model (Sect. 5, 6).

16. *L. 342–343: the differences may involve different total masses.*

Confirmed: in the soil model, tracer left DuMux through the absorbing boundary (corrected); in the landfill model, SPRING contains less dissolved tracer because of its lower water content. See the mass-balance comment above.