Analysis of Nuclide Transport under Natural Convection and Time Dependent Boundary Condition using TOUGH2

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1 Introduction

After implementation of TOUGH2 at GRS in summer 91, it was first used to analyse the gas transport in a repository for the nuclear waste with negligible heat generation and to verify the results obtained with ECLIPSE /JAV 92/. Since the original version of TOUGH2 does not directly simulate the decay of radionuclide and the time dependent boundary conditions, it is not a appropriate tool to study the nuclide transport in a porous medium /PRU 87, PRU 91/. Hence, in this paper some modifications are proposed to study the nuclide transport under combined influence of natural convection, diffusion, dispersion and time dependent boundary condition. Here, a single phase fluid with two liquid components is considered as in equation of state model for water and brine /PRU 91A/.

2 Modification of TOUGH2 Models

TOUGH2 assumes a constant permeability and does not directly simulate the convergence of a salt rock. Hence, the calculation of porosity ϕ and permeability k is modified:

$\phi = \phi\ (p, T, t) > \phi_{min} = \phi_{min}$ (material domain): input parameter,

$k = k\ (\phi$, material domain): input function, $\phi_p = (1/\phi)\ (\partial\phi/\partial p)$: input parameter,

$\phi_T = (1/\phi)\ (\partial\phi/\partial T)$: input parameter, $\phi_t = (1/\phi)\ (\partial\phi/\partial t)$: input parameter,

p: pressure, T = temperature, t: time,

$(1/\phi)\ (d\phi/dt) = \phi_p\ (\partial p/\partial t) + \phi_T\ (\partial T/\partial t) + \phi_t$.

In the original version of TOUGH2, only the first two terms on the right side of the above equation are included. Employing input parameters and user specified function for k, time dependent porosity and permebility can be determined. Within the original version of TOUGH2, a simulation of time dependent boundary conditions is troublesome. Therefore, user specified functions are introduced to model them:

$p = p\ (t, j_i)$, $T = T\ (t, j_i)$, $X_2 = X_2\ (t, j_i)$,

X_2 : mass fraction of secondary component (brine), j_i : index of a inactive element.

To simulate the decay of a nuclide, which can be represented by the secondary component (brine), following equations are inserted into original version:

$\Delta X_2 = \mathrm{abs}\,(\lambda X_2 \Delta t)$, $X'_2 = X_2 - \Delta X_2$, $X'_1 = X_1 + \Delta X_2$,

X_1 : mass fraction of primary component (water),

λ : decay constant for the secondary component, ' : initial value for the next time step.

In extension to the original version /PRU 87, PRU 91/, a dispersion model for two liquid components (water/brine) is developed by /PRU 93/. Since this dispersion model assumes a full two dimensional configuration, it is inexpedient to analyse a configuration, which consists of drifts and shafts mainly. Therefore, the original version /PRU 87, PRU 91/ is extended to simulate dispersive and diffusive flux G at the interface of two elements:

$\mathbf{G}_{i,diff} = - \rho_F \, \phi f \, \mathrm{grad}\,(X_i)$, $\mathbf{G}_{i,disp} = - \rho_F \, \beta \, \mathrm{abs}\,(u) \, \mathrm{grad}\,(X_i)$,

f = f (direction, material domain) : molecular diffusion coefficient, input parameter,

$\beta = \beta$ (direction, material domain) : dispersion length, input parameter,

u : darcy velocity, ρ : density, index F : fluid; i : component 1 or 2.

The determination of flux G is very similar to flux F in the dispersion model of /PRU 93/. However, this model modification does not assume a full two dimensional configuration as in /PRU 93/ and can easily be applied to a three dimensional configuration containing drifts and shafts and, as shown below, it can save computation time significantly compared to the sophisticated model of /PRU 93/.

To implement all the modifications mentioned above, only two subroutines MULTI and CONVER of the original version are extended. At present, these modifications are implemented in a separate package containing only these two subroutines and are used only with the original version /PRU 91/ and the module EOS-7 for water and brine. In following, both liquid components are treated as water.

3 Results

To verify the modifications explained above, several one dimensional examples are treated in GRS reports /JAV 94, JAV 95/ to estimate the individual impact of discretization, hydrodynamic dispersion, molecular diffusion, time dependent boundary condition and radioactive decay. They also contain various examples on natural convection to verify the original models of TOUGH2. A few of them are summarized below:

Case WL3: Heat conduction under time dependent boundary temperature. On one boundary of a one dimensional configuration, temperature as a linear function of time is imposed; no heat flux is assumed at other boundaries. The analytical solution and the results obtained with the modifications above shows a very good agreement.

Case NH2: Natural convection in a long drift (H << L) with a horizontal temperature gradient. For the steady state with constant material proporties, an analytical solution gives a linear valocity profile over the height H with zero at the center line and maximum magnitude at the drift walls. For H/L = 4/700, the deviation between the maximum Darcy velocity from the analytical solution and TOUGH2-value accounts to be less than 5 %, which is acceptable.

Case NV2: Natural convection in a shaft with a vertical temperature gradient. In this case, a natural convection in the full height occurs, if the Rayleigh number $Ra > Ra_{crit}$, which depends on the ratio heigth/width. TOUGH2 calculations with different Rayleigh numbers showed a proper tendency for the occuring of natural convection.

Case ZH20: Mass transport without dispersion in a one dimensional horizontal drift. In a case of a long drift with a constant tracer mass fraction at the entrance, a constant tracer profile moving with the pore velocity is to be expected. TOUGH2 shows a noticeable deviation due to numerical mixing, which decreases slowly with a finer grid (Fig. 1).

Case ZH21: Mass transport with dispersion. This case is like ZH20 but with a horizontal dispersion length of 10 m. A similar case is considered in /PRU 93/. In Fig. 2, the TOUGH2 results, which are obtained by using the complicated model of /PRU 93/, are compared with the analytical solution. As expected, the case ZH21 is closer to the analytical solution than case ZH20. But, the effect of numerical mixing is so significant that, even if physical dispersion is not included in a numerical model, one might meet the analytical solution with dispersion reasonably well by an appropriate choice of grid. Hence, it is concluded, if a numerical analysis shows an acceptable agrrement with an analytical solution, it does not necessarily mean that the numerical solution reproduces physical effects reasonably well. This case was also repeated with the original version /PRU 91/ and employing the modifications regarding the dispersive flux G in section 2 and not with the complicated dispersion model of /PRU 93/. Both calculations yield practicaly the same results. Hence it is concluded, the modifications are implemented correctly. The computation with model /PRU 93/ was about 4 times slower.

Case ZH22: Nuclide transport without dispersion. This case is same as ZH20 but with a tracer decay constant of 0.001 1/day within drift only and in case ZH23 also at the drift entrance. These cases are selected to verifiy the decay modifications of section 2. The agreement between the analytical solution /JAV 84/ and TOUGH2 results is satisfactory, whereas the deviation is mainly due to numerical mixing (Fig. 3).

All above cases are selected as basic examples to verify TOUGH2. Now, an additional case of nuclide transport under combined influence of natural convection, dispersion and decay in a simple network is considered (Fig. 4). The network with a initial vertical temperature gradient of 0.024 °C/m and with a heat generating waste located at the right end of the drift is discretized with 768 active elements and is analysed with original version of TOUGH2 including modifications of section 2 without employing the complicated dispersion module of /PRU 93/. As the module /PRU 93/ requires a complete two dimensional model including insignificant elements located outside drifts and shafts, it is inexpedient and very time consuming for the present case. Figure 5 shows the tracer distribution at t = 20 years for three different cases. The tracer enters into the drift from the right side and is transported mainly through natural convection. As expected, in case NZ1 tracer mass fraction is far higher than in case NZ2 or NZ3, in which temperature and the tracer mass fraction decay at the drift entrance x = 1396 m with a half life period of 10 years. In present case, the dispersion influences the tracer distribution very insignificantly. In case NZ2 or NZ3, the tracer distribution shows a relative minimum around x = 1270 m, which is due to the time dependent boundary conditions at the drift entrance (see similar example TZ4 in /JAV 95/). Figure 6 shows the distribution of tracer mass fraction of case NZ2 at t = 20 years. Since no other tool is used to check the TOUGH2 results for the cases NZ1 to NZ3, it is difficult to access their accurancy. However, after analyzing various one and two dimensional basic examples, the results of NZ1 to NZ3 seem to be reliable.

4 Conclusions

Several modifications are introudced to simulate time dependent porosity, permeability and boundary conditions and radioactive decay of the secondary liquid component as well as to compute faster the diffusive and dispersive flux mainly for a network consisting of drifts and shafts. After treating various one and two dimensional basic examples to verify TOUGH2 with modifications, it is concluded that a qualified application of TOUGH2 can lead to reasonable results, however the effect of numerical mixing should not be underestimated.

References

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Figure 1

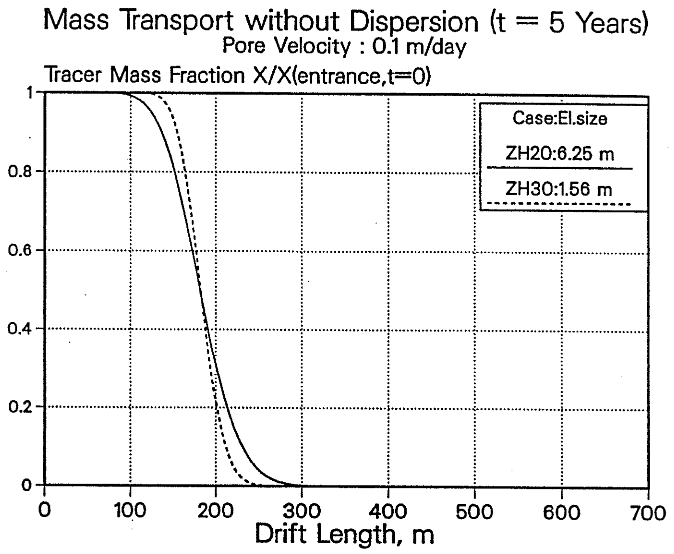

Mass Transport without Dispersion (t = 5 Years)
Pore Velocity : 0.1 m/day

Figure 2

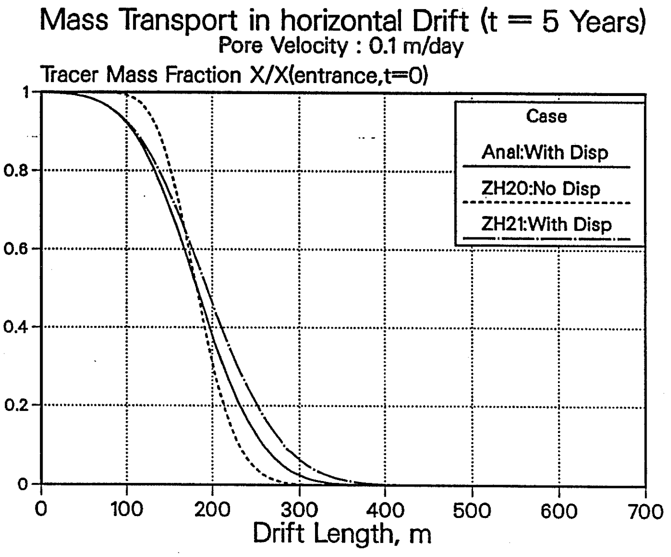
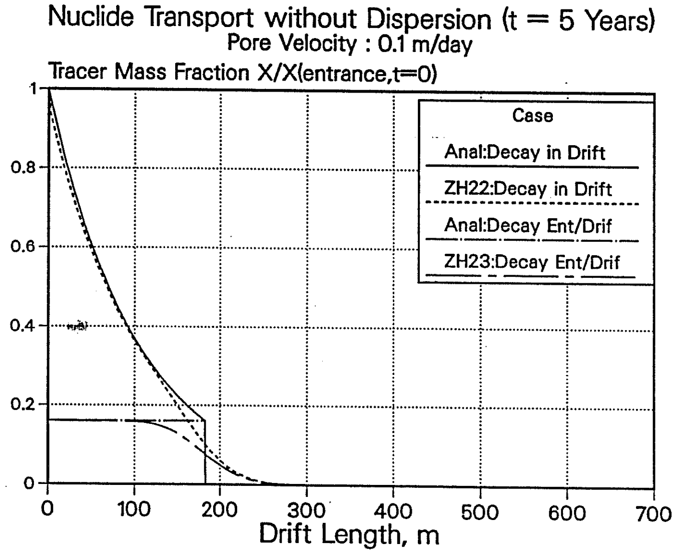

Mass Transport in horizontal Drift (t = 5 Years)
Pore Velocity : 0.1 m/day

Figure 3


Nuclide Transport without Dispersion (t = 5 Years)
Pore Velocity : 0.1 m/day

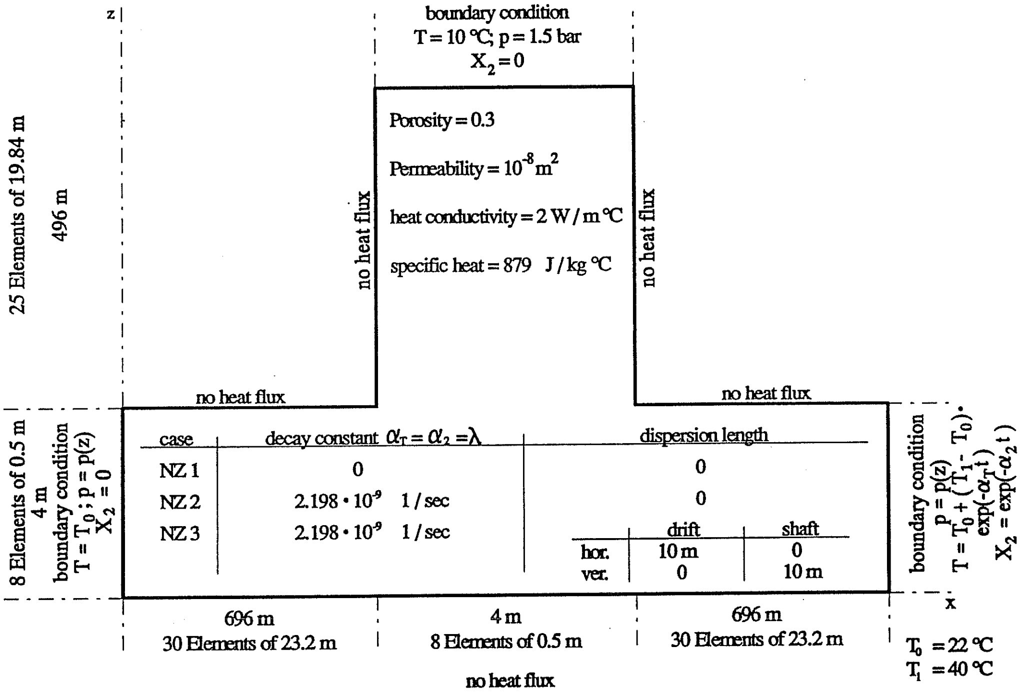


Figure 4 : Model of nuclide transport in a simple network

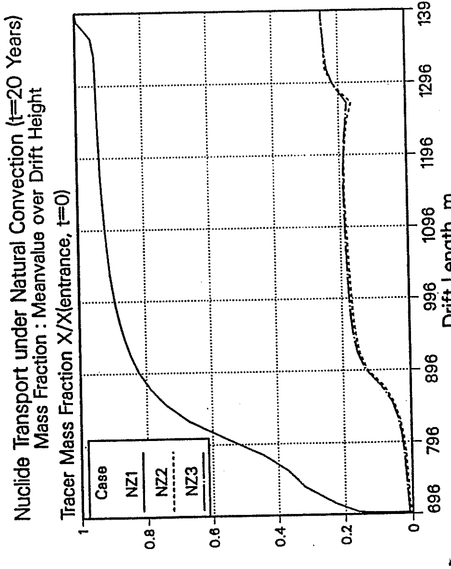


Figure 5 : Nuclide Transport in Network of Fig. 4

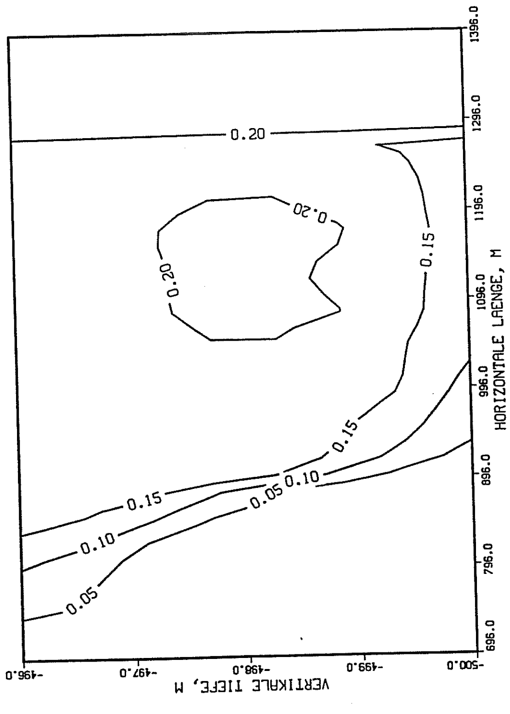


Figure 6 : Tracer Mass Fraction, Case NZ2, t = 20 Years