# REVIEW OF COMPUTER MODELS USED FOR POST CLOSURE SAFETY ASSESSMENT OF NUCLEAR WASTE REPOSITORIES IN THE FRG

P. Bogorinski, B. Baltes, K.-H. Martens
Gesellschaft fuer Reaktorsicherheit (GRS) mbH
Cologne, Federal Republic of Germany

ABSTRACT

In the FRG disposal of nuclear wastes will take place in deep geologic formations. For longterm safety assessment of such a repository, groundwater transport provides a release scenario for the radionuclides to the biosphere. GRS reviewed a methodology that was implemented by the research group of PSE to simulate migration of radionuclides in the geosphere. The examination included the applicability of theoretical models, numerical experiments, comparison to results of diverse computer codes as well as experience from international intercomparison studies. The review concluded that the hydrological model may be applied to full extent unless density effects have to be considered whereas there are some restrictions in the use of the nuclide transport model.

## INTRODUCTION

In the Federal Republic of Germany final disposal of nuclear waste will take place in deep geologic formations (1). Two sites are under detailed investigation. One is the salt dome at Gorleben where a repository for all grades of nuclear wastes is planned. The other is the disused iron ore mine of Konrad where non-heat-generating medium and low-level wastes should be disposed of.

One goal of the investigations is to prove that the waste will be isolated from the biosphere for long time periods. Neither by natural events nor by human activity should radionuclides be released to such an amount that exceeds permissible limits. In the case of a repository being constructed in fractured rock, groundwater will get into contact with the waste and will provide a migration path for the radionuclides from the repository via the geosphere to the biosphere. This is true for the Oxford formation which is the host rock for the Konrad repository. In the case of a repository in a formation like the Gorleben salt dome contact of water with the waste can be excluded under normal conditions. However, the question whether water ingress into the repository must be considered as enveloping accident or not can only be answered by the underground exploration of the salt dome, which started with sinking a shaft some months ago.

In the meantime a methodology to simulate such release scenarios was prepared for the case that water ingress into the repository has to be considered. This work was done by the 'Projekt Sicherheitsstudien Entsorgung (PSE)' during the last years (2). For application of this methodology in a future licensing procedure a critical review is neccessary. Under contract of the Federal Minister for the Environment, Nature Conservation and Reactor Safety, the GRS carried out this review.

## METHODOLOGY

The purpose of PSE was to develop and implement a methodology that can be used to carry out safety analyses for the time periods after closure of a nuclear waste repository. Figure 1 gives an overview of the different models that have to be applied.

The capability of this methodology was demonstrated for a hypothetical repository site for which available data of the Gorleben site were used. It was not intended to carry out a safety study for an actual repository site.

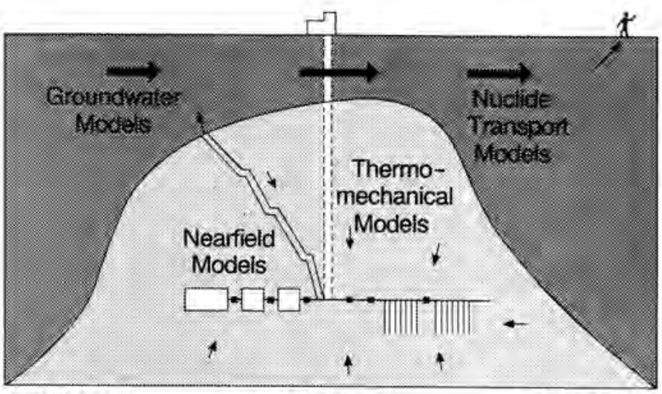


Fig. 1. Overview of the Methodology used for Longterm Safety Assessment.

The different computer models that are in use at PSE and GRS and their interconnection are shown in Fig. 2.

For the near-field analysis, i.e. radionuclide transport within the repository itself, PSE developed a new computer code EMOS. This model together with the MARNIE code that is under development at the GRS for the same purpose is discussed in a separate paper (3).

For the far-field analysis, i.e. transport of the radionuclides from the repository via the geosphere to the biosphere, several aspects have to be considered:

- three-dimensional groundwater flow in porous media or fractured rock due to hydraulic potential, groundwater recharge and discharge

- for salt sites advective and dispersive transport of brine with feedback on the groundwater flow field via density changes
- advective and dispersive transport of radionuclides, which are leaking from the repository, due to groundwater flow
- retardation mechanisms for the radionuclides due to sorption, matrix diffusion and geochemical reactions.

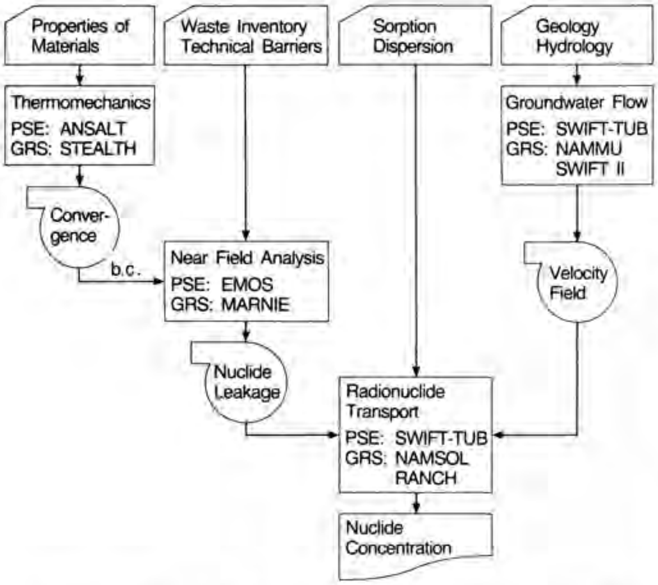


Fig. 2. Computer Models and their Interconnection

To describe these phenomena PSE applied the computer code SWIFT which was originally developed for simulation of waste water injection into deep lying saline aquifers. It was later modified for application in the safety analysis of nuclear waste repositories in salt formations (4). This code was than again modified for application to the German waste repository projects (5).

SWIFT models the groundwater flow in a porous media on the basis of Darcy's law. The advective and dispersive transport of heat and brine are coupled to the groundwater flow via a variable density. The radionuclide transport is considered to be uncoupled due to the low concentrations of the nuclides that do not influence the fluid density. The differential equation system that describe the different phenomena are solved by a finite difference scheme in space as well as in time.

## REVIEW

When we reviewed the PSE methodology we first scrutinized the applicability of the theoretical models used as well as the validity of simplifying assumptions. After that we carried out numerical experiments. A further important part was the comparison of the results with those obtained by a diverse computer code. Finally we included the experience from international benchmark studies into our review. In the following paragraphs examples for these points are given.

### Model Assumptions

In most computer models Darcy's law is applied to determine groundwater flow. There is no question that this is valid for a flow field that is not influenced by density variations. However some sites which are selected for a nuclear waste repository are salt sites like that at Gorleben. In the vicinity of these sites groundwater may highly be mineralized with brine concentrations far above seawater. In these cases there is a strong influence of the density on the groundwater flow. Here phenomena may exist that cannot be described by the classical Darcy equation. Within the HYDROCOIN study it was widely discussed whether the Darcy equation must be extended to cover density dispersion phenomena, as suggested by the Dutch party (Ref. 6). If the need for these additional terms can be verified by appropriate experiments the classical Darcy equation may not be conservative with respect to the transport of radionuclides in highly mineralized groundwaters.

Hydrodynamic dispersion plays an important role as dilution mechanism for the transport of radionuclides in groundwater. This phenomenon is caused by the pore structure of the aquifer. Heterogenities within the porous media influence the dispersion significantly. Molecular diffusion contributes also to the dilution but is only important for very low velocities. Since heterogenities are of statistical nature and therefore not known in detail, an exact solution of the Navier-Stokes equation that describes the flow within the pores is not possible. For this reason simplifying theoretical models were developed.

One assumption often used is that hydrodynamic dispersion follows Fick's law with different dispersivities along the flow axis and perpendicular to it. Since in a finite difference grid flow is normally not parallel to the grid lines dispersivities are split into components and described by a tensor. Comparison of this model with dispersion found in laboratory experiments agreed well.

However evaluation of field experiments showed that dispersivities increased with migration distance. Only for very long distances dispersivities reached asymptotic values that are orders of magnitude larger than those from laboratory experiments. That means that for large-scale problems like migration of radionuclides from a repository through the geosphere the Fickian type dispersion is not correct.

For a better approximation of the dependency of dispersivity from migration distance new models were developed which for example are reported by Gelhar (7) or Naff (8). These are stochastic models which result in a dispersion that varies with travel time and thereby also with distance. However these models are for the moment only applicable to simple geometries and not to configurations that are representative waste disposal problems.

In SWIFT the usual Fickian model is implemented. If low dispersivities are used which may be derived from laboratory or small-scale field experiments this assumption may be considered conservative because it results in lower dilution. However, due to numerical stability criteria of the finite difference method limitations have to be observed for low dispersivities.

### Numerical Experiments

In order to find out which restrictions are imposed by the numerical rather than by the theoretical model, we carried out several numerical experiments with the SWIFT code. Base were simple model regions that can be overlooked easily. As example the result of our investigation on the numerical dispersion that is introduced by the finite difference grid is presented here. We chose a two-dimensional model region through which the water flow is in one case parallel and than in another diagonal to the grid. Longitudinal dispersion was set to a value that is compatible to the numerical criteria imposed by the discretization. Transverse dispersion was set to zero. Dispersion was indicated by a nonsorbing stable tracer. As Fig. 3 shows there was a strong transverse dispersion in the case where the flow was diagonal to the grid whereas the tracer did not spread in the case of parallel flow.

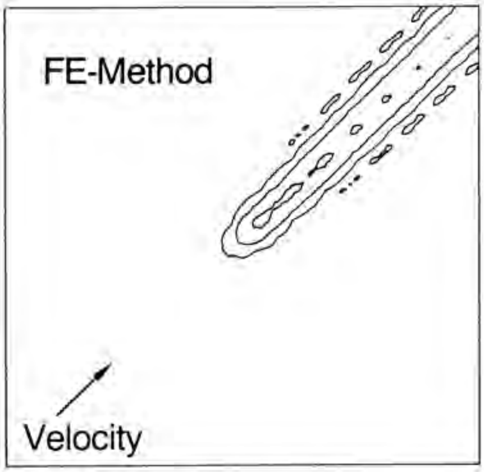


Fig. 3. Concentration contours for a diagonal flow field in a finite difference grid.

To check the magnitude of this transverse numerical dispersion we compared it to selected values of transverse dispersion in the parallel flow field. Figure 4 shows concentration lines perpendicular to the flow axis at a certain distance from the tracer injection point. It can be seen that numerical transverse dispersion introduced by a nonparallel flow can be in the order of the longitudinal dispersion.

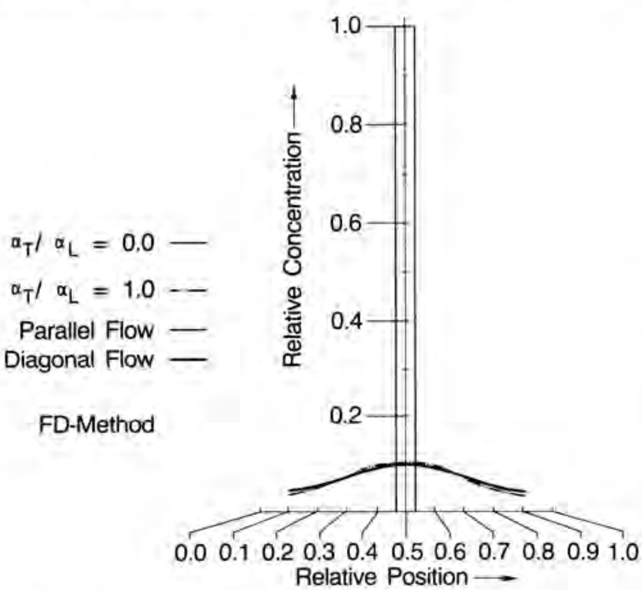


Fig. 4. Comparison of numerical Dispersion in a parallel and diagonal flow field for a finite difference grid.

This numerical dispersion is caused by the fact that the advective transport of the tracer is not calculated in the direction of the flow but is split into components that are perpendicular to the grid lines. By this the tracer is transported into the adjacent blocks off the diagonal direction and from these into the next ones and so on. Therefore this effect should rather be called advective dispersion than numerical dispersion.

Use of Diverse Computer Models

It is common in all fields of safety assessment that results of computer simulations are checked against the results of calculations carried out with diverse computer codes. To give an example we did the same calculation concerning numerical dispersion, as mentioned in the previous paragraph, with a finite element model instead of a finite difference one. The NAMMU program system (9,10) was selected for this purpose.
As Fig. 5 shows spreading of the tracer into the domain off the flow axis due to numerical dispersion is very limited even for diagonal flow.

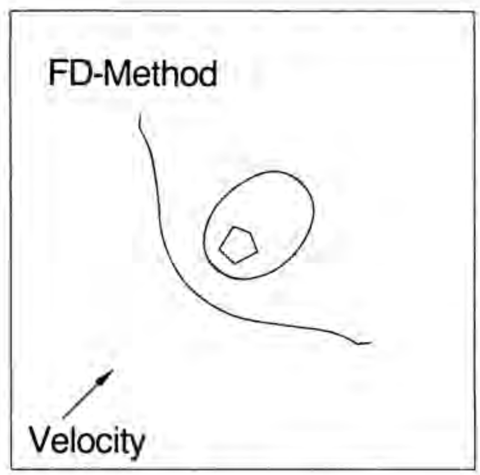


Fig. 5. Concentration contours for a diagonal flow field in a finite element grid.

The same can be seen in Fig. 6 where the concentration lines perpendicular to the flow axis at a defined distance from the injection point is plotted for both the parallel flow and the diagonal flow.

It can be seen that the decrease in the maximum concentration is by about 15 % whereas in the finite difference grid it decreases by 90 %. Thus numerical dispersion is much lower but has to be observed too.

Experience from International Intercomparison Studies

Soon after computer models for the simulation of radionuclide transport from a nuclear waste repository to the biosphere had been developed the need for verification and validation had been realized. This initiated international code intercomparison studies for radionuclide transport INTRACOIN (11) and for groundwater flow HYDROCOIN (6). Both studies are managed by the Swedish Nuclear Power Inspectorate. They include benchmark calculations, comparison to experiments as well as sensitivity studies. The value of these studies corresponds to the interest in special phenomena. For example interest in multidimensional transport had been not very extensive during the INTRACOIN study.

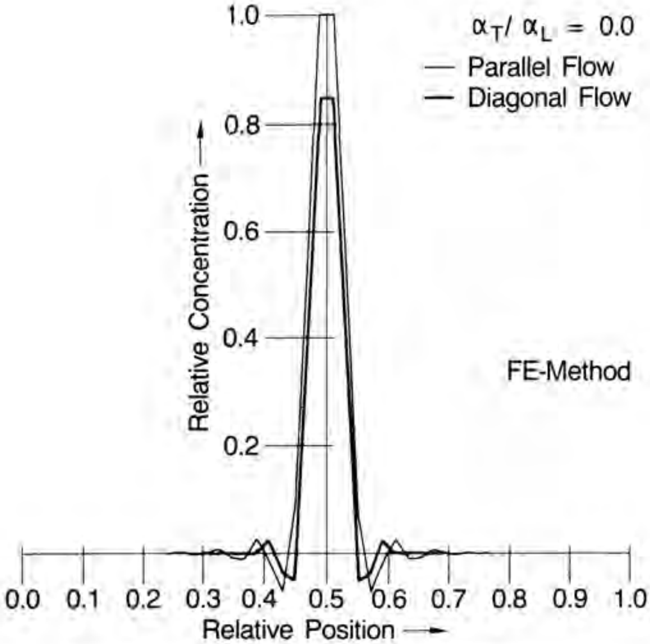


Fig. 6. Comparison of Numerical Dispersion in a Parallel and a Diagonal Flow Field for a Finite Element Grid

However, this effect has to be considered in the safety analysis for German waste repository sites, unless one-dimensional transport can be proved to be conservative.

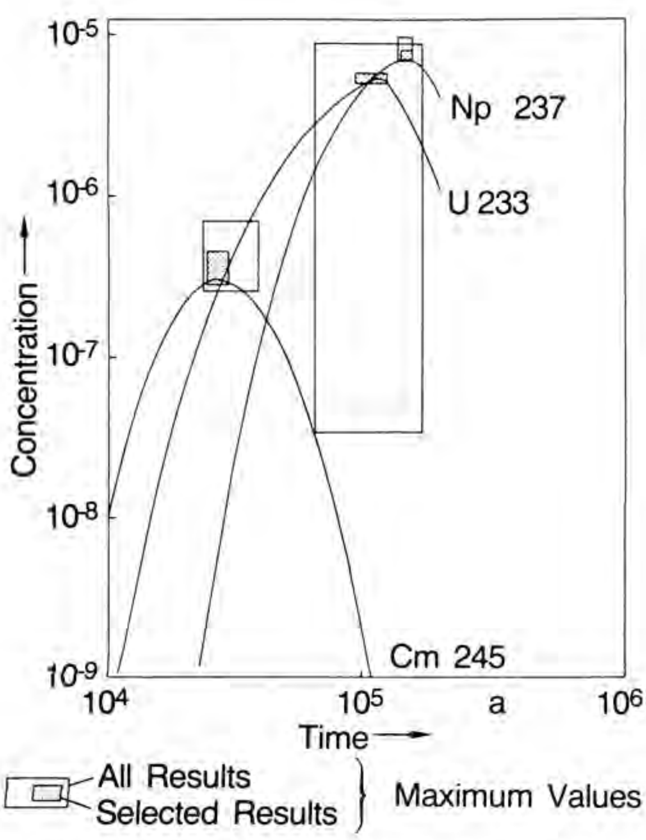


Fig. 7. INTRACOIN Intercomparison Level 1 Case 1 Short-Lived Mother Nuclide, Bad Retention

In this paper we compare the results of the SWIFT-simulations of INTRACOIN-case 1 carried out by the Technical University of Berlin on behalf of PSE with the results of all other teams. Case 1 consists of a one-dimensional transport of a radionuclide chain in a porous medium. Two chains were considered, one with a short-lived mothernuclide and one with a long-lived. Data can be found in Ref. 11. Figures 7 and 8 show the nuclide concentrations at a distance of 500 m from the source as calculated by the TUB-team (12).

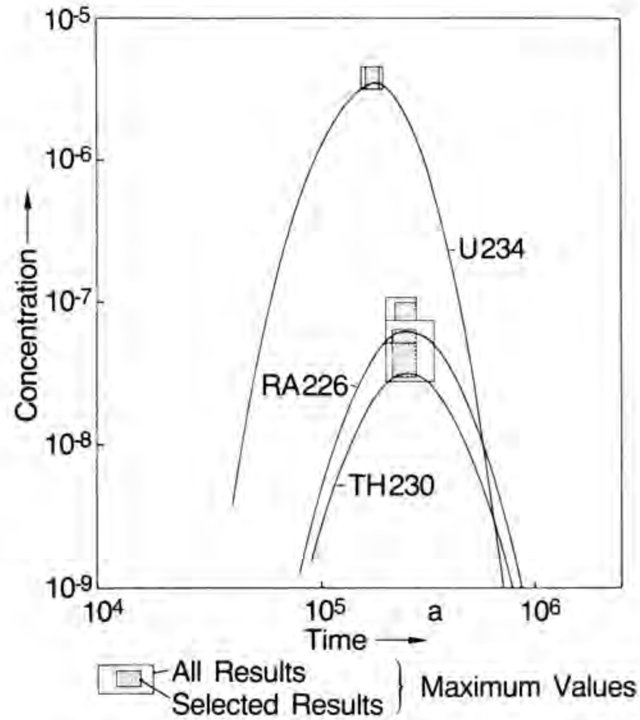


Fig. 8. INTRACOIN Intercomparison Level 1 Case 1 Long-Lived Mother Nuclide, Good Retention

The rectangular areas indicate the range of the calculated maximal concentrations and of the times at which these concentrations are reached. These areas are normally small, however, in one case the spread reached more than two orders of magnitude. The reason for this deviation may be due to the fact that there were differences in the interpretation of the boundary conditions. Thus only 11 simulations out of 28 used the same boundary conditions as applied by SWIFT. If we select these results the spread is much smaller as the shaded areas in the figures show.

The HYDROCOIN study is not yet finished but results from level 1 can be evaluated. Table I gives the results for four cases with travel distance and travel time as performance measure. For details of the case definitions see Ref. 6. The values listed in the table are error factors defined as the ratio of the maximal deviating value to the analytical value or to the average value calculated as geometric mean, respectively.

TABLE I

Evaluation of HYDROCOIN Level 1 Simulation Results
Examples for Selected Trajectories

| Case | Error Factor | | Number of |
|---|---|---|---|
| | Distance | Time | Simulations |
| 2 (Fractured Rock) | 1.02 | 1.23 | 11 |
| 4 (Heat Transport) | 2.45 | 5.80 | 5 |
| 5 (Brine Transport) | 1.11 | 1.27 | 6 |
| 6 (Porous Medium) | 2.88 | 3.47 | 7 |

As the table reveals the error bands in the HYDROCOIN study are much larger than in the INTRACOIN study. This may be due to the fact that the cases selected for intercomparison of groundwater models are much more complex.

From the evaluation of these studies the conclusion can be drawn that radionuclide transport codes can be assumed to be verified for one-dimensional calculation whereas multi-dimensional calculation need more careful assessment. The same is true for groundwater calculations.

## CONCLUSIONS

From our review of the methodology that was implemented by PSE to perform simulations of the radionuclide transport in the geosphere for longterm safety assessment of German nuclear waste repository sites we came to the conclusion that it did not satisfy all requirements to full extent. The SWIFT code may be applied to groundwater problems for actual repository sites under consideration in the FRG without restrictions as far as no density effects have to be modeled. Brine transport calculations would require further investigations, but it seems to be plausible that freshwater models are conservative. Numerical dispersion restricts the applicability of the program to one-dimensional radionuclide transport problems. However, this may also supposed to be conservative.

Our review did not include data. This is a field for a future review as soon as site investigations are finished and data are available or a licensing procedure has started.

## REFERENCES


1. M. BLOSER, "Safety of Radioacitve Waste Disposal - Regulatory Principles and Aspects in the Federal Republic of Germany", this conference.

2. Projekt Sicherheitsstudien Entsorgung, "PSE Abschlußbericht", Berlin (1985).

3. B. BALTES, U. HOLZHAUER, M. BLOSER, "Safety Analyses to the Post Operational Phase of Final Repositories of Radioactive Waste", this conference.

4. M. REEVES, R.M. CRANWELL, "User's Manual for the Sandia Flow and Transport Model (SWIFT) Release 4.81", NUREG/CR-2324. SAND81-2516, Sandia National Laboratory (1981).

5. Projekt Sicherheitsstudien Entsorgung, "PSE-Fachband 18", Berlin (1985).

6. K. ANDERSON, et. al., "HYDROCOIN Level 1 Final Report: Verification of Groundwater Flow Models", Report to be published.

7. L.W. GELHAR, C.L. AXNESS, "Three-dimensional Stochastic Analysis of Macrodispersion in Aquifers", Water Resour. Res., 19, p. 161 (1983).

8. R.L. NAFF, "Dispersitivität eines Grundwasserleiters", PSE-Nr. 84/1B, Projekt Sicherheitstudien Entsorgung, Berlin (1984).

9. R. ATKINSON, A.W. HERBERT, C.P. JACKSON, P.C. ROBINSON, "NAMMU User Guide", AERE-R11364, Harwell, UK (1985).

10. R. ATKINSON, A.W. HERBERT, C.P. JACKSON, P.C. ROBINSON, "NAMSOL User Guide", AERE-R11365, Harwell, UK (1985).

11. "INTRACOIN Final Report Level 1, Code Verification", SKI 84:3, Stockholm (1984).

12. M. GOLKER, E. BOTOW, L. HEREDIA, "INTRACOIN, Level 1 - Benchmark Calculations with Code SWIFT", PSE-Nr. 82/B8, Projekt Sicherheitsstudien Entsorgung, Berlin (1982).