

Figure 4 Example of the influence diagram tool (biosphere compartment).

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Figure 5 Example of the tool that supports the grouping process. FEP groups are automatically identified (right) on the basis of various selection criteria (left).

## 2.1.1.6.1.4 Scenario Workshop

The applicability of the tools developed in 2003 was tested during a scenario workshop held at the TNO-NITG premises on 18-19 June 2003 (Appendix B).

Being ahead of the post workshop document, to be completed by the end of July 2003, the main conclusions of the workshop are:

the methodology and tools support a tractable FEP analysis process,

the methodology and tools may contribute to a transparent FEP analysis process if the following aspects are improved:

- 1. definitions and rules with respect to the screening and interaction process should be well documented;
- 2. the list of Features should be re-configured in order to easily deal with the different ranges of abstraction levels of individual FEPs;
- 3. the definition, scope and relation to safety of some FEPs should be described more clearly;
- 4. the tools need small adjustments to increase their user-friendliness. Examples are the complicated mouse-handling within the interaction matrix and the inability to present circular relationships within the influence diagrams;
- 5. possible interaction between scenario elements in different compartments (e.g. overburden FEPs interacting with biosphere FEPs) has not been covered during the workshop, however, is part of the FEP analysis process and should be available in the FEP analysis tools.

## 2.1.1.6.1.5 Future Work

In July and August 2003, the aspects for improvement as identified during the scenario workshop will be worked out. This includes:

Further development of the tools that support the FEP analysis and scenario formation.

Documentation of the user-manual that supports the tools.

Possible integration with the Quintessa IEA FEP database, depending on financial support by the IEA Greenhouse Gas R&D Program.

In addition, the SAMCARDS base case (reference) scenario and variant scenarios should be defined in terms of model representation before end of August 2003. The development of scenarios should follow from the newly developed FEP analysis and scenario formation methodology.

## 2.1.1.6.2 Process modeling

In the description of the status of the physical-chemical modeling, we will concentrate on the results obtained so far for the case of a leaking seal, and the modeling of this case with the reservoir-seal model and the shallow subsurface model.

#### 2.1.1.6.2.1 Reservoir-seal model

#### Introduction

The reservoir-seal model has extensively been described in the Phase 1 status report of SAMCARDS (Wildenborg et al, 2003). In that report, a sensitivity analysis was reported for the case of a leaking (high

permeable) seal. Results of this sensitivity analysis showed that three dimensionless numbers dominated the  $CO_2$  fluxes to the shallow subsurface (at 300 m below ground level). These numbers were:

$$\Pi_{3} = \frac{k_{vo}}{H^{2}} \qquad \Pi_{6} = \frac{\Delta \mathbf{r}gH}{\mathbf{m}_{v} \frac{Q_{i}}{D^{3}}} \qquad \Pi_{7} = \frac{Q_{i}T_{i}}{D^{3}}$$
where
$$?? = ?_{water} \cdot ?_{CO2} = \text{density difference water and CO}_{2} [M L^{-3}]$$

$$g = \text{acceleration of gravity } [L T^{-2}]$$

$$Q_{i} = \text{injection rate } [L^{3} T^{-1}]$$

$$T_{i} = \text{injection period } [T]$$

$$H_{water} = \text{water viscosity } [M L^{-1} T^{-1}]$$

H = depth of reservoir [L] D = thickness of reservoir times porosity [L]  $k_{vo}$  = average vertical permeability of overburden [L<sup>2</sup>]

These dimensionless numbers can be interpreted as the resistance of the overburden, the ratio of buoyancy and viscous forces, and the amount of  $COP_2$  that can be stored.

The time-dependent  $CO_2$  fluxes at a depth of 300 m below ground level were approximately described by six numbers. Fig. 6 shows a typical example of such a breakthrough as a function of time. Also given in this fig. Is the radius around over which  $CO_2$  breakthrough occurs, also as a function of time.

In order to minimize the amount of data that has to be passed on from the reservoir/seal model to either the shallow subsurface model or the marine compartment model, the curves shown in fig. 6 are approximated by six numbers, defining:

- 1. the first time of  $CO_2$  breakthrough  $A_x$  in the fig.);
- 2. the maximum  $CO_2$  flux ( $B_y$  in the fig.);
- 3. the time the maximum  $CO_2$  flux occurs ( $B_x$  in the fig.);
- 4. the maximum radius over which  $CO_2$  fluxes occur ( $D_y$  in the fig.);
- 5. the time at which the maximum radius occurs ( $D_x$  in the fig.);
- 6. the time of the end of breakthrough ( $C_x$  in the fig.).

These numbers have been chosen such, that both the time-dependence of the  $CO_2$  flux and the area over which  $CO_2$  escapes are reasonably well described, and that, as a consequence, the total amount of  $CO_2$  that escapes from the system is well approximated.



Figure 6 CO<sub>2</sub> breakthrough from the reservoir seal model

# 2.1.1.6.2.2 Monte Carlo simulation

In order to quantify the effect of parameter uncertainty on the  $CO_2$  fluxes from the reservoir-seal model to the shallow subsurface model, Monte Carlo simulations were performed. For a number of controlling physical parameters, probability distributions were defined, and a set of parameter combinations were generated based on these distributions.

Parameter	Units	Distribution	Low	Mean	High
Salinity	%	Triangular	8.5	10.5	12.5
Injection rate	Sm³/d	Uniform	900 000	1 000 000	1 100 000
Injection period	Yrs	Uniform	90	100	110
Seal vert permeability	ln(mD)	Lognormal	ln(1)-1	$\ln(1)$	ln(1)+1
Shale vert permeability	ln(mD)	Lognormal	ln(0.01)-1	ln( <b>0.01</b> )	ln(0.01)+1
Res. hor permeability	ln(mD)	Lognormal	ln(100)-1	ln( <b>100</b> )	ln(100)+1
Porosity average	-	Triangular	0.12	017	0.20

Table 2 Parameter distribution for Monte Carlo simulations reservoir -seal model

Table 2 shows the parameters, their mean values and the distributions and the ranges used in the Monte Carlo simulations. The types of distributions chosen, and the possible ranges of the parameters are, to a certain extend, arbitrary, and based on expert opinion of the members of the SAMCARDS team.

For the Monte Carlo simulations, the depth and the thickness of the reservoir have not been varied. The reason for this is, that a changing depth or thickness would necessitate the generation of a new (geometric) model for each parameter combination. Since the behaviour of the model is controlled by a set of dimensionless numbers, changing the depth and thickness of the reservoir is not really necessary.

The water properties, density  $\rho$  and viscosity  $\mu$  are related to the salinity, the temperature and the pressure. Functional relations have been used as given by Batzle and Wang (1992). The temperature distribution is assumed to be according to the geothermal gradient, and, hence, is known. The pressure is initially assumed to be known at reservoir depth, and is during the simulation related to the injection and the flow of water and CO<sub>2</sub>.

The vertical resistance of the overburden, one of the controlling parameters in the system, is mainly determined by the vertical permeability of shale, the type of formation in the overburden with, by far, the smallest permeability. Permeabilities of all other types of formations in the overburden have been kept constant.

The seal vertical permeability for this exercise is much larger than can be expected in real world systems. As has been stated in the previous status report (Wildenborg et al, 2003), this has to do with the type of leakage mode investigated here.

Given the fact that the behaviour of the reservoir-seal system is to a large extend controlled by three dimensionless numbers, we expect that  $1000 (10^3)$  combinations of parameters is sufficient to define the probability density functions of the numbers describing the time dependent CO<sub>2</sub> fluxes from the reservoir-seal model. Consequently, 1000 parameter combinations have been drawn according to the distributions and ranges as given in table 2. In drawing these parameter values, it has been assumed that there is no correlation between the parameters. For each of the parameter combinations, the time dependent CO<sub>2</sub> fluxes to the shallow subsurface have been calculated.

# 2.1.1.6.2.3 Shallow subsurface and atmosphere

## Introduction

Within the SAMCARDS project, the subsurface model calculations for the different leakage modes will be carried out by Lawrence Berkeley National Lab. (LBNL). A number of steps are required to generate the stochasic output in terms of the  $CO_2$  fluxes to the atmosphere and  $CO_2$  concentrations in the shallow aquifer:

- 1. definition of the conceptual model for the shallow subsurface;
- 2. definition of the parameters to be varied and the corresponding distributions;
- 3. definition of the required output;
- 4. simulate base case leaking seal mode (by LBNL) and evaluate results;
- 5. generate input for multiple cases (using the  $CO_2$  fluxes and radii from the reservoir-seal model);
- 6. performing Monte Carlo calculations (by LBNL);
- 7. interpretation of results.

## Conceptual model

The base case model that has been developed in phase 1 of the SAMCARDS project (Wildenborg et al, 2003) has been reevaluated, and the conceptual model as shown in fig. 7 was developed. The model considers a  $CO_2$  flux into the shallow subsurface (the upper 300 m) from the bottom of the model due to a leaking seal. The flux is time dependent and has a certain infiltration radius that is time dependent too. These are generated by the reservoir/seal compartment model. In the subsurface the  $CO_2$  is subject to