iTOUGH2-IFC: An Integrated Flow Code in Support of Nagra's Probabilistic Safety Assessment

User's Guide and Model Description

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Prepared for:

National Cooperative for the Disposal of Radioactive Waste (Nagra)
Wettingen, Switzerland

January 2009

This work was supported by a grant (Order No. 6425) from the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra), Wettingen, Switzerland. The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC02-05CH11231.

Table of Contents

1. Introduction 1
2. Requirements 3
2.1 Functional Requirements 3
2.1.1 Functional Requirements Related to Repository Layout 3
2.1.2 Functional Requirements Related to the Hydrogeologic Environment 6
2.1.3 Functional Requirements Related to Accepted FEPs 6
2.2 Interface Requirements 8
2.3 Performance Requirements 9
3. Software Design 10
3.1 General Approach 10
3.2 Standard TOUGH2 Simulation Capabilities 11
3.3 Implementation of Relevant Processes 13
3.3.1 Representation of Resaturation Process 13
3.3.2 Representation of Gas Generation 13
3.3.3 Representation of Pathway Dilation 13
3.3.4 Representation of Mechanical Processes 14
3.3.5 Representation of Chemical Processes 16
3.4 Initial Conditions and Simulation Period 16
3.5 Addressing Interface Requirements 17
3.6 Replicating Reference Waste Emplacement Tunnel 17
4. IFC Representation of Repository System 19
4.1 Model Domain and Dimensionality 19
4.2 Representation of Key Model Components 19
4.2.1 Representation of Far Field 19
4.2.2 Representation of Waste Emplacement Tunnels 20
4.2.3 Representation of Other Backfilled Underground Structures 22
4.2.4 Equivalent Conceptual Repository Model 22
4.3 Mesh Generation 23
4.3.1 General Approach 23
4.3.2 Submesh Geosphere 26
4.3.3 Submesh Representative Emplacement Tunnels 27
4.3.4 Submesh Intermediate-Level Waste Facility 28
4.3.5 Submesh Operations and Construction Tunnels 29
4.3.6 Submesh Backfilled Underground Structures 29
4.4 Hydrogeologic Properties 30
4.5 Parameters of Geomechanical and Geochemical FEPs 38
4.6 Initial and Boundary Conditions 41
4.7 Parameters Potentially Varied in PSA Calculations 44
5. Input Formats 47
5.1 Replicating System States to Boundary Elements 47
5.2 Geomechanical and Geochemical Processes 48
5.3 IFC-PICNIC Interface 55

6. Testing of Code Modifications 59
- 6.1 Replicating System States to Boundary Elements 59
- 6.2 Flowpath Dilation 62
- 6.3 EDZ Self-Sealing, Tunnel Convergence, and Uplift 67
- 6.4 Geochemical Sealing 70

7. Test Simulation 73

8. Summary and Concluding Remarks 88

9. Comments and Recommendations....................89
- 9.1 Testing of Assumptions 89
  - 9.1.1 Resaturation and Multi-Component Gas Generation.................... 89
  - 9.1.2 Gas Migration within Waste Emplacement Tunnels 89
  - 9.1.3 Appropriateness of Representative Emplacement Tunnel Approach 89
  - 9.1.4 Coupled Hydrologic-Mechanical Effects under Two-phase Conditions.................... 89
- 9.2 Simulation Capabilities not Invoked by Current Base-Case Model 90
  - 9.2.1 Water Consumption 90
  - 9.2.2 Gas Production Limited by Water Availability 90
  - 9.2.3 Consistency in Treatment of Property Changes.................... 90
  - 9.2.4 Representation of Uplift.................... 90
  - 9.2.5 Representation of Fractures 91
  - 9.2.6 Representation of Gas Channeling Effects 91
- 9.3 Miscellaneous Comments 91
  - 9.3.1 Initial Conditions 91
  - 9.3.2 Performance-Affecting Parameters and Options 92

10. Acknowledgment 93

11. References....................94

A1. Code Modifications....................1

A2. Unix Script File for Meshgeneration 2

A3. Supporting Fortran Mesh Manipulation Programs 7

A4. Template iTOUGH2-IFC Input File 10

List of Figures

Figure 1. Preliminary PSA concept (Nagra, 2008c, AN 08-381, Enclosure 1)...............2
Figure 2. Plan view of the repository layout for SF/HLW/ILW in Opalinus Clay (after Nagra, 2006, NIB 06-07, 2006, Appendix 4). 5
Figure 3. Three-dimensional view of the repository layout. 5
Figure 4. Hydrogeological framework model of a repository in the Opalinus Clay of the Zürcher Weinland (Nagra, 2002c, NTB 02-06, Figure 3.5-1) 20
Figure 5. Equivalent conceptual repository model...23
Figure 6. Three-dimensional view of computational mesh of IFC model; submesh of geosphere (gray), local aquifers (cyan), representative waste emplacement tunnels (red), operations and construction tunnels (green), and other backfilled tunnels (blue). 24
Figure 7. (a) XY-, (b) XZ-, and (c) YZ-views of computational mesh of IFC model; submesh of geosphere (gray), waste emplacement tunnels (red), operations and construction tunnel submesh (green), and other backfilled tunnels (blue) 25
Figure 8. Three-dimensional view of representative waste emplacement tunnel model 28
Figure 9. Three-dimensional view of intermediate-level waste facility........................28
Figure 10. Three-dimensional view of connection between representative waste emplacement tunnel and operations tunnel...29
Figure 11. Excerpt of TOUGH2 block showing input format for replicating system state from parent to daughter elements. 48
Figure 12. Excerpt of TOUGH2 block `IFC` showing input format for geomechanical and geochemical FEPs. 54
Figure 13. Excerpt of TOUGH2 block `PICNIC` showing input format for IFC-PICNIC interface. 56
Figure 14. Excerpt of TOUGH2 output file showing information about IFC-PICNIC interface...57
Figure 15. Excerpt of file IFC_q.dat, created by iTOUGH2-IFC, providing flow rates at cross section to PICNIC...58
Figure 16. Set-up of test case to verify implementation of replication feature; (a) reference case; (b) test case...59
Figure 17. TOUGH2-IFC input file for testing the replication feature; reference case ..60
Figure 18. TOUGH2-IFC input file for testing the replication feature; test case 61
Figure 19. Comparison between reference case (symbols) and test case (lines) for verification of replication feature..62
Figure 20. TOUGH2-IFC input file for testing pathway dilation 63
Figure 21. Excerpt from TOUGH2-IFC output file, showing pathway dilation input parameters and results 66
Figure 22. TOUGH2-IFC input file for testing pathway dilation 68
Figure 23. Comparison between prescribed (lines) and calculated (symbols) permeabilities in elements subject to EDZ self-sealing and uplift. 69

Figure 24. Comparison between prescribed (lines) and calculated (symbols) porosities in elements subject to EDZ self-sealing and tunnel convergence. 69
Figure 25. TOUGH2-IFC input file for testing geochemical sealing 71
Figure 26. Flow rate through test cell with and without time-dependent geochemical sealing. 72
Figure 27. CPU time as a function of simulation time for a simulation with and without the inclusion of geomechanical and geochemical FEPs 73
Figure 28. Excerpt of iTOUGH2-IFC output file 87

List of Tables

Table 1. Functional Requirements Related to Repository System 4
Table 2. Functional Requirements Related to the Hydrogeologic Environment 6
Table 3. Functional Requirements Related to the Accepted FEPs 7
Table 4. Interface Requirements 8
Table 5. Performance Requirements 9
Table 6. Simulation Capabilities of Standard TOUGH2 and iTOUGH2 12
Table 7. Vertical stratification of geosphere model 26
Table 8. Material Properties, EDZs 30
Table 9. Material Properties, Backfill and Sealing Materials 31
Table 10. Material Properties, Opalinus Clay 32
Table 11. Material Properties, Steeply Dipping Discontinuity 32
Table 12. Material Properties, Dogger 33
Table 13. Material Properties, Lias and Upper Keuper 33
Table 14. Material Properties, Lower Keuper 34
Table 15. Material Properties, Wedelsandstein Aquifer 34
Table 16. Material Properties, Sandsteinkeuper Aquifer 35
Table 17. Material Names and Description 36
Table 18. Parametric Models for Special FEPs and Related Coefficients 38
Table 19. Boundary Conditions in Aquifers 42
Table 20. Neumann Boundary Conditions (Gas Generation Rates) 43
Table 21. Time-Dependent Gas Generation Rate for LMA1 and LMA2 in Kilograms per Second and Cubic-Meter of Waste 43
Table 22. Parameters Potentially Varied in PSA Calculations 44

1. Introduction

This document describes the development and use of the Integrated Flow Code (IFC), a numerical code and related model to be used for the simulation of time-dependent, two-phase flow in the near field and geosphere of a gas-generating nuclear waste repository system located in an initially fully water-saturated claystone (Opalinus Clay) in Switzerland. The development of the code and model was supported by the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra), Wettingen, Switzerland.

Gas generation (mainly H_2, but also CH_4 and CO_2) may affect repository performance by (1) compromising the engineered barriers through excessive pressure build-up, (2) displacing potentially contaminated pore water, (3) releasing radioactive gases (e.g., those containing ^{14}C and ^{3}H), (4) changing hydrogeologic properties of the engineered barrier system and the host rock, and (5) altering the groundwater flow field and thus radionuclide migration paths. The IFC aims at providing water and gas flow fields as the basis for the subsequent radionuclide transport simulations, which are performed by the radionuclide transport code (RTC). The IFC, RTC and a waste-dissolution and near-field transport model (STMAN) are part of the Integrated Radionuclide Release Code (IRRC), which integrates all safety-relevant features, events, and processes (FEPs). The IRRC is embedded into a Probabilistic Safety Assessment (PSA) computational tool that (1) evaluates alternative conceptual models, scenarios, and disruptive events, and (2) performs Monte-Carlo sampling to account for parametric uncertainties. The preliminary probabilistic safety assessment concept and the role of the IFC are visualized in Figure 1.

The IFC was developed based on Nagra's PSA concept. Specifically, as many phenomena as possible are to be directly simulated using a (simplified) process model, which is at the core of the IRRC model. Uncertainty evaluation (scenario uncertainty, conceptualization uncertainty, parametric uncertainty) is handled by the outer shell of the PSA model; it is not further discussed in this report. Moreover, justifications for the inclusion or exclusion of FEPs as well as for certain simplifying assumptions are available or can be obtained using detailed process models and other supporting information.

The IFC is both a numerical code and a model of a repository system. The numerical code is a modification of the multiphase, multicomponent simulator TOUGH2 (Pruess et al., 1999), as implemented within the iTOUGH2 (Finsterle, 2007abc) framework. The code modifications are mainly concerned with the implementation of relevant FEPs as outlined in Nagra (2007a, AN 07-115), as well as removal of processes and features that are not needed within the IFC; the modifications are summarized in Appendix A1. In addition, the IFC includes a model, i.e., a simplified representation of the repository system. Specifically, a computational grid was generated, which includes the emplacement tunnels for spent fuel, high-level wastes, as well as long-lived intermediate-level wastes. Moreover, the model represents engineered barriers (backfill, seals, plugs, etc.), various tunnels and other underground facilities, and includes a simplified representation of the geological structure, i.e., the host rock (including the excavation disturbed zone (EDZ) around the underground openings), confining units, local aquifers, and a highly-transmissive zone. The IFC model was designed in close collaboration with Nagra.

This report describes all functional requirements of the IFC and how they are implemented in the IFC. The input formats needed to invoke added modeling capabilities are documented. Finally, the IFC model grid is described, and results from a test simulation are presented.

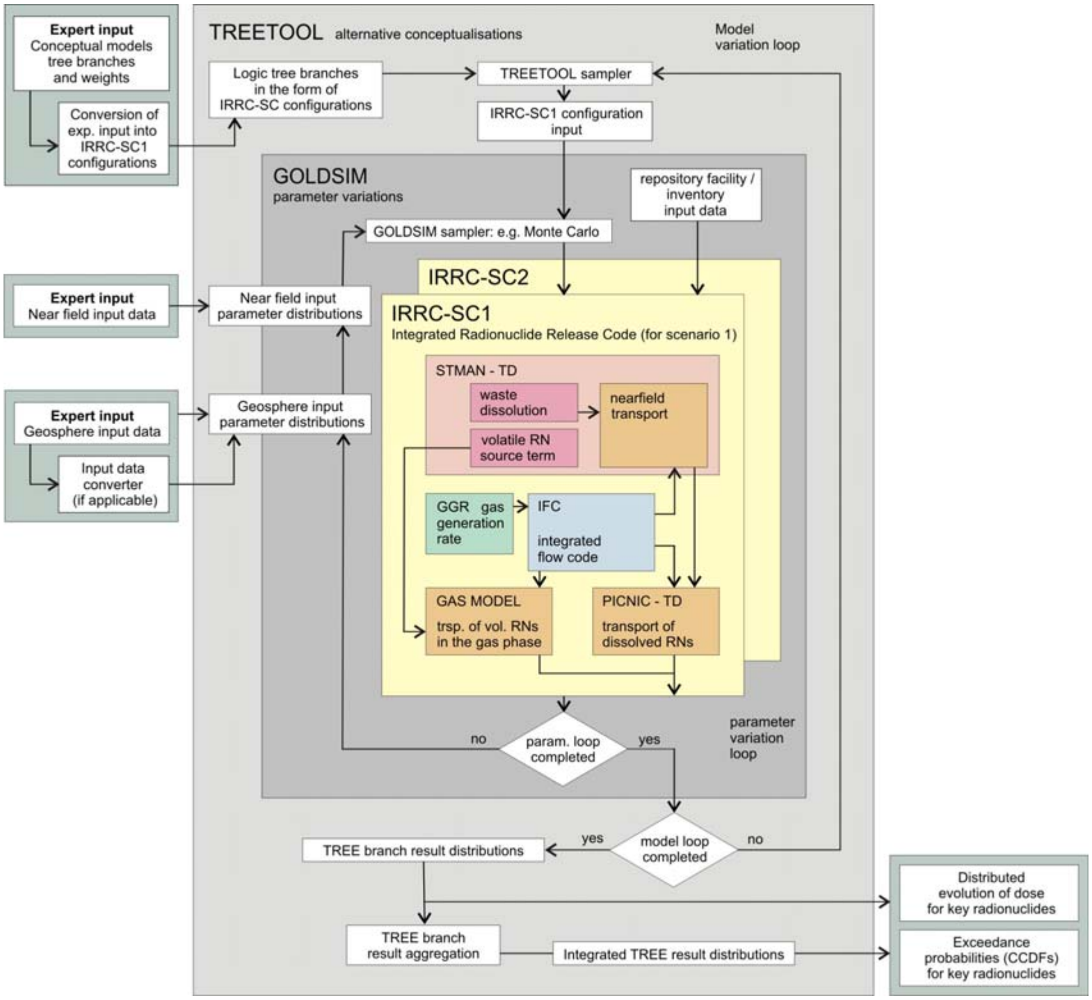

Figure 1. Preliminary PSA concept (Nagra, 2008c, AN 08-381, Enclosure 1)

2. Requirements

The intended use of the IFC within a probabilistic performance assessment framework for the Swiss nuclear waste disposal program defines functional, interface, and performance requirements for the software. In general, the code needs to be able to handle features, events, and processes that are considered safety-relevant; these are specified in a list of accepted FEPs (Nagra, 2007a, AN 07-115). Moreover, the specifics of the Swiss repository system need to be appropriately represented. Integration of the IFC into the PSA concept also requires that the code is computationally efficient and robust, and that it can be integrated with other IRRC components.

The IFC is not intended to be a general-purpose simulation program; it only has to be able to handle a finite number of processes for a specific set of repository layouts, environments, and conditions. The sophistication with which individual processes are represented is limited by their respective treatment in the safety report for a repository in the Opalinus Clay (Nagra, 2002b, NTB 02-05; see also Nagra, 2007b, Order 960.09, p. 2, Bullet 2). The processes may be appropriately abstracted or simplified in accordance with their expected relative impact on overall repository performance. Only post-closure conditions after the thermal pulse will be considered.

The specific functional, interface, and performance requirements for the TOUGH2-based IFC are summarized in the following subsections. The requirements are numbered for later reference. The implementation of each requirement is discussed in Section 3.

2.1 Functional Requirements

The functional requirements define the requested functionality to be implemented in the IFC. They are grouped into requirements related to (1) the representation of the repository system, (2) the hydrogeologic environment, and (3) safety-relevant FEPs as identified in Nagra (2007a, AN 07-115).

The IFC will be used for probabilistic safety assessment calculations for a repository for spent fuel (SF), vitrified high-level waste (HLW), and long-lived intermediate-level waste (ILW) and a related pilot facility. The repository is sited in Opalinus Clay, as described in Nagra (2002b, NTB 02-05, Section 4.4). For the purposes of the IFC, the individual components of the repository system and their geometries will need to be represented in a simplified, albeit defensible manner, taking advantage of symmetries and reduced model dimensionality, where appropriate.

2.1.1 Functional Requirements Related to Repository Layout

A plan view of the repository layout is shown in Figure 2; a three-dimensional rendering is shown in Figure 3. The repository elements to be considered are summarized in Table 1.

Table 1. Functional Requirements Related to Repository System

#	**Requirement**	**Comment/Reference**
R1	Represent flow conditions within and in the vicinity of waste emplacement tunnels of the main SF/HLW/ILW and pilot facilities.	The main facility consists of an array of 800 m long, parallel emplacement tunnels with a diameter of 2.5 m; the spacing between tunnels is 40 m (Nagra, 2002b, NTB 02-05, Section 4.5.1).
R2	Represent flow through and along the backfill material.	Compacted bentonite backfill for SF/HLW tunnels and pilot facility (Nagra, 2002b, NTB 02-05, Fig. 4.5-7); bentonite/sand mixtures in access and operation tunnels (Nagra, NIB 06-07, 2006, Section 9.3.2); mortar in ILW; crushed Opalinus Clay in access tunnel above Opalinus Clay; compacted bentonite and gravel in seals and shaft (Nagra, 2002a, NTB 02-02, Fig. 8.6).
R3	Represent flow through and along the excavation disturbed zone (EDZ)	EDZ has approximately one order of magnitude increased permeability than undisturbed Opalinus Clay (Nagra, 2002b, NTB 02-05, Section 5.5.1).
R4	Represent operation tunnels, access tunnel (ramp), construction tunnel, shaft, central area, and other backfilled underground structures	See Figure 2.
R5	Represent seals and plugs	See Nagra (NIB 06-07, 2006, Appendix 15) and Nagra (2002b, NTB 02-05, Sections 4.5.3.4 and 5.5.1).

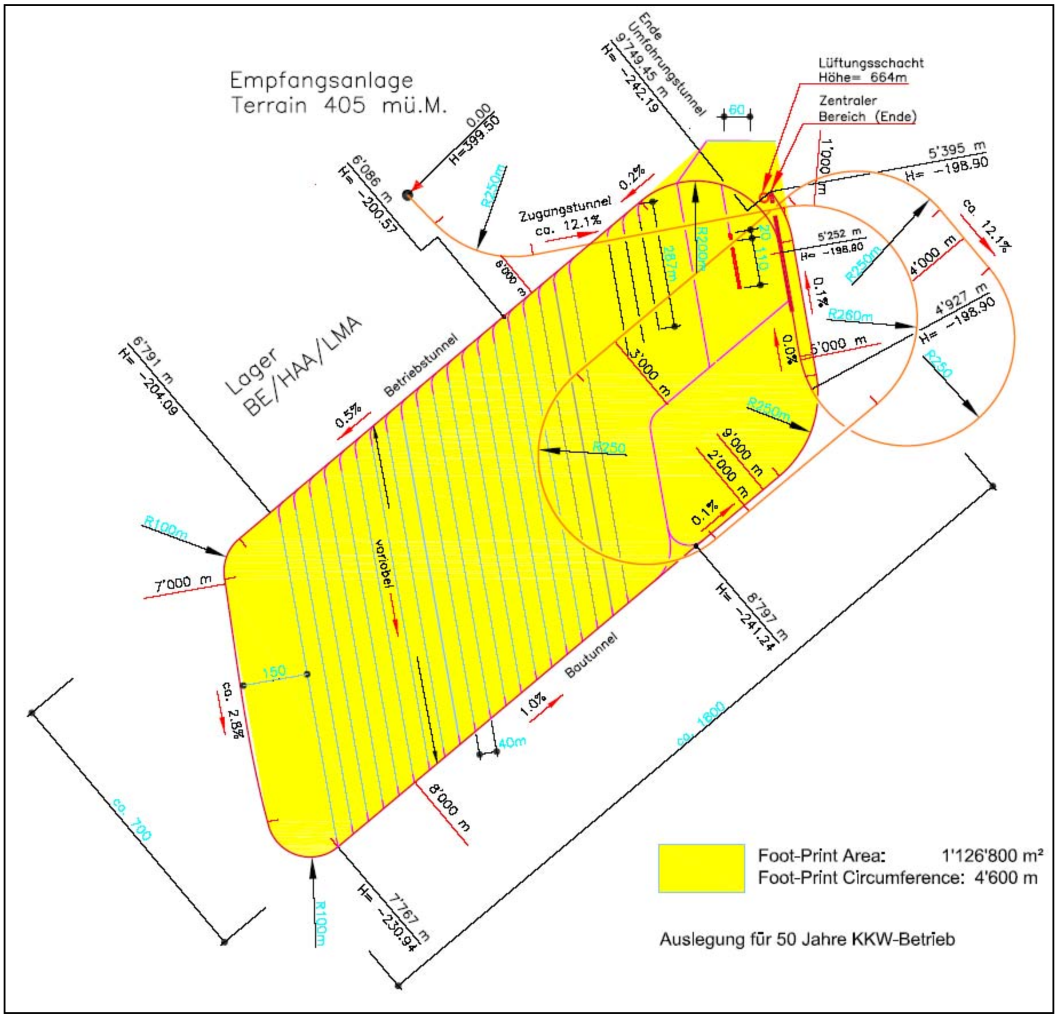

Figure 2. Plan view of the repository layout for SF/HLW/ILW in Opalinus Clay (after Nagra, 2006, NIB 06-07, 2006, Appendix 4).

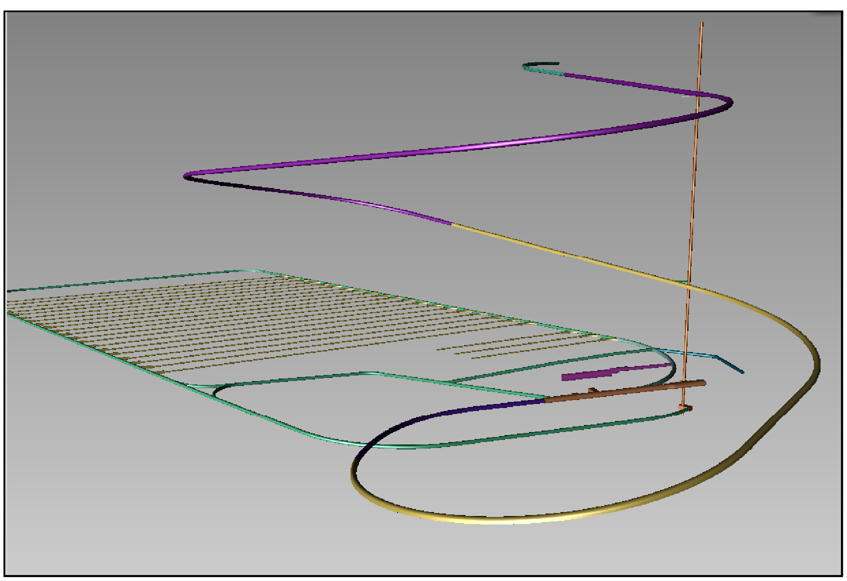

Figure 3. Three-dimensional view of the repository layout.

2.1.2 Functional Requirements Related to the Hydrogeologic Environment

The IFC development focuses on a model of the Opalinus Clay of the Zürcher Weinland as a potential host formation for a SF/HLW/ILW repository. The geological and hydrogeological environment is described in Nagra (2002b, NTB 02-05, Section 4.2). The Opalinus Clay is considered as a host rock mainly because of its hydrogeologic and geochemical homogeneity, tectonic stability, self-sealing capacity, low permeability, low natural resource potential, geochemical stability and retention capacity, and its favorable engineering properties. Some of these characteristics allow for a simplified treatment of the host rock and its hydrogeologic and geomechanical properties within the IFC. The functional requirements related to the hydrogeological environment are summarized in Table 2.

Table 2. Functional Requirements Related to the Hydrogeologic Environment

#	**Requirement**	**Comment/Reference**
R6	Represent relevant hydrogeologic features (stratigraphy and properties) of the repository host rock and confining units.	See Nagra (2002b, NTB 02-05, Tables 4.2-1 and 4.2-2; Figure 4.2-7).
R7	Represent the relevant regional hydrologic conditions.	See Nagra (2002b, NTB 02-05, Section 4.2.5, Figures 4.2-8 and 4.2-10, Table 4.2-3).

2.1.3 Functional Requirements Related to Accepted FEPs

Table 3 summarizes the functional requirements that result from the list of safety-relevant phenomena considered in the IFC. The list is a subset of all examined features, events and processes (FEPs). Only accepted FEPs related to environmental processes are considered in the IFC; FEPs related to radionuclide processes, the biosphere, and special issues are not considered. Moreover, FEPs related to short-term, transient effects after repository closure (e.g., resaturation of EDZ and backfill, radiation-related and thermal processes) are currently not considered. The FEP numbering follows that of Nagra (2006, NIB 06-07).

Table 3. Functional Requirements Related to the Accepted FEPs

#	**Requirement**	**Comment/Reference**
R8	Represent water flow through rock matrix	FEP 1.3.1; discontinuities on a scale less than one meter (referred to as fissures) are considered to be part of the rock matrix
R9	Represent water flow through transmissive discontinuities in host rock	FEP 1.3.2; transmissive discontinuities include fractures and fracture zones; in Opalinus Clay, fractures are hydraulically active only under certain stress conditions.
R10	Represent gas/water flow through EDZ	FEP 1.3.4; consider gas channeling effects in highly heterogeneous EDZ; EDZ properties may be time dependent.
R11	Represent gas/water flow through sealing zones	FEP 1.3.5; includes bentonite seal and sealing-zone EDZ.
R12	Represent gas/water flow through concrete backfill between emplacement tunnel and operation tunnel	FEP 1.3.6; concrete plugs and associated EDZ in ILW facility.
R13	Represent water flow in confining units	FEP 1.3.7; by definition, the model domain is bounded by regional aquifers, which are considered the compliance boundary and are thus excluded from the IFC; however, the upper and lower confining units may contain local aquifers (Nagra, 2002b, NTB 02-05, Figure 7.4-1).
R14	Represent resaturation of cementitious backfill	FEP 1.3.10; considered safety-relevant for ILW facility.
R15	Represent gas generation by anaerobic corrosion of metals, microbial degradation, radiolysis, and decay	FEP 1.3.11; dependence of gas generation rate on water availability is not considered safety-relevant.
R16	Represent water consumption by gas generation	FEP 1.3.13.
R17	Represent gas dissolution/degassing	FEP 1.3.14.
R18	Represent formation of gas phase and gas pressure build-up	FEP 1.3.15.
R19	Represent gas-induced porewater displacement	FEP 1.3.16; see Nagra (2002b, NTB 02-05, Figure 7.4-7)
R20	Represent gas transport by advection and diffusion of dissolved gas	FEP 1.3.17; see Nagra (2004, NTB 04-06, Figure 3.1-1, Illustration 1).

Table 3 (cont.) Functional Requirements Related to the Accepted FEPs

#	Requirement	Comment/Reference
R21	Represent gas transport by two-phase flow	FEP 1.3.18; see Nagra (2004, NTB 04-06, Figure 3.1-1, Illustration 2).
R22	Represent gas transport by dilatant gas pathway formation	FEP 1.3.19; see Nagra (2004, NTB 04-06, Sections 3.1 and 4.2, Figure 3.1-1, Illustration 3).
R23	Represent gas accumulation in confining units	FEP 1.3.21.
R24	Represent rock mechanical evolution of EDZ	FEP 1.4.1; specifically post-closure evolution of EDZ properties.
R25	Represent tunnel convergence	FEP 1.4.3; potentially safety-relevant for ILW facility (Nagra, 2002b, NTB 02-05, Sections 5.3.3.1 and 5.4.3).
R26	Represent increase of hydraulic conductivity by uplift/erosion	FEP 1.4.7; see Nagra (2002b, NTB 02-05, Section 5.2.2.3).
R27	Represent effects of chemical/mineralogical alteration of bentonite	FEP 1.5.2; increase in permeability due to reduction in bentonite swelling pressure.
R28	Represent sealing effect of high-pH plume in host rock	FEP 1.5.4; potential development of skin zone in host rock around ILW facility.
R29	Represent sealing effect of high-pH plume in tunnel backfill	FEP 1.5.11; sealing effect on sand / bentonite backfill of operation tunnels in ILW facility.

2.2 Interface Requirements

The IFC has to be able to exchange input parameters and output variables with other components of the IRRC (see Figure 1). Moreover, the code needs to be designed such that it can be embedded as a module into a system-level modeling tool such as GoldSim (GoldSim Technology Group, `http://www.goldsim.com`). These interface requirements are summarized in Table 4.

Table 4. Interface Requirements

#	Requirement	Comment/Reference
R30	Provide interfaces for the exchange of parameters and variables with other IRRC modules.	Model calculating gas generation rates, STMAN, and RTC.
R31	Provide interfaces for the integration of IFC into a system-level modeling tool.	E.g., GoldSim (see Nagra, 2007b, Order 960.09, p. 3).

2.3 Performance Requirements

Since the IFC will be called multiple times during a probabilistic analysis using Monte-Carlo simulations, it is essential that the code runs efficiently and in a robust manner for a large set of representative parameter combinations and scenarios. These performance requirements are summarized in Table 5.

Table 5. Performance Requirements

#	Requirement	Comment
R32	Perform a large number of IFC simulations within an acceptable clock time	The acceptable clock time is affected by CPU time and load; the acceptable CPU time depends on the number of processes that can be run in parallel; the manageable model size depends on single-CPU performance.
R33	Perform IFC simulations in a robust manner	Successful completion of individual IFC runs cannot be predicted or guaranteed, requiring the implementation of an acceptable error recovery strategy.

3. Software Design

This section discusses the general design of the IFC and describes how each of the requirements identified in Section 2 is implemented into the numerical code. The model representing the repository system and geosphere (i.e., the IFC model) is described in Section 4.

3.1 General Approach

As mentioned in Section 1 and in accordance with Nagra (2007b, Order 960.09, p. 1), the IFC is developed based on the assumption that most FEPs as well as elements of the repository are to be implemented into the PSA concept using a (simplified) process model. Issues of scenario selection and uncertainty propagation analysis are outside the scope of the IFC.

Since the IFC is intended to be a site-specific prediction model tailored to the design of a SF/HLW/ILW repository located in Opalinus Clay, IFC development is not only concerned with software design, but also with the development of a conceptual model for the repository and tunnel system, and the representation of safety-relevant processes and phenomena. The implementation of the requirements outlined in Section 2 follows an approach that is aimed at (1) providing sufficient flexibility that allows for the potential adaptation of the conceptual model, (2) taking advantage of the well-defined scope of the IFC's intended application, making it computationally efficient, and (3) minimizing software development and testing.

These goals are achieved by basing the IFC on the well-established, general-purpose two-phase flow and transport simulator TOUGH2 (Pruess et al., 1999; `http://www-esd.lbl.gov/TOUGH2`). The code will be modified to account for FEPs that are specific to the Swiss nuclear waste disposal concept. These modifications are implemented in the inverse modeling code iTOUGH2 (Finsterle, 2007abc; 2004; `http://www-esd.lbl.gov/iTOUGH2`), which provides a framework for calling the TOUGH2 forward simulator using different parameter sets and for easily extracting certain performance measures. Moreover, iTOUGH2 has the capability to perform Monte Carlo simulations in parallel (Finsterle, 1998), should such an option become desirable. Finally, it has been demonstrated (Zhang et al., 2007) that TOUGH2 (and iTOUGH2) can be linked to the GoldSim system-level modeling tool. Developing the IFC based on iTOUGH2 rather than TOUGH2 may have the disadvantage that the massively-parallel version of TOUGH2 (Wu et al., 2002; Zhang et al., 2003) cannot be utilized. However, should multiple processors be available for PSA calculations, they would most likely be used for the "embarrassingly parallel" task of running multiple Monte Carlo simulations simultaneously. In what follows, we refer to the simulator simply as "TOUGH2", implying that it is the forward model used within the iTOUGH2 framework.

Many of the required processes and phenomena are directly addressed by the capabilities of the standard version of TOUGH2 (see Section 3.2). The site- and repository-specific requirements (specifically R22, R24, R25, R26, R27, R28, and R29) are incorporated by simplified parametric models or by interpolation from look-up tables created by more sophisticate process models. It is beyond the scope of the IFC to develop, examine, or justify these parametric models; references to supporting documentation will be given, if available. Formal testing of the correct implementation of these submodels in iTOUGH2-IFC will be presented in Section 6; however, validation of the submodels (i.e., demonstration of their adequacy for the intended use) may require extensive analyses.

As mentioned above, the IFC consists of (1) a simulation code (i.e., a customized version of a specific iTOUGH2 module), and (2) a site-specific conceptual model of the repository system in the Opalinus Clay. Development of the iTOUGH2-IFC code is discussed in the remainder of this section; the conceptual model development is documented in Section 4.

3.2 Standard TOUGH2 Simulation Capabilities

Table 6 summarizes some of the simulation capabilities that are provided by the standard version of TOUGH2; they are available without the need for code modifications. If invoked by a proper conceptual model, these built-in capabilities address a substantial number of the IFC requirements identified in Section 2. The capabilities are described in detail in Pruess et al. (1999).

The TOUGH2 suite of simulators consists of multiple modules of varying sophistication and complexity (Pruess et al., 1999; Pruess, 2004; Finsterle et al., 2008). While one of the simplest modules will be used for the IFC (e.g., the equation-of-state (EOS) module No. 5 for two-phase flow of water and hydrogen), the more advanced capabilities (which may include density-driven liquid flow, multiple gas species, radionuclide transport, and coupled geomechanical and biogeochemical process simulations) are available for validation studies or to provide input for a suitable abstraction within the IFC.

Table 6. Simulation Capabilities of Standard TOUGH2 and iTOUGH2

#	Capability	Requirement Addressed	Comment
1	Simulation of two-phase (gas and liquid) flow through porous media; handles single- and two-phase conditions, including phase-state changes	R8, R9, R10, R11, R12, R13, R14, R15, R18, R19, R21, R23	Two-phase flow through porous materials is simulated using the extended version of Darcy's law; phase properties (density, viscosity) are calculated internally; phase interference is described by capillary pressure and relative permeability functions.
2	Simulation of two components (water and a non-condensible gas); both components exist in both phases	R17, R18, R20	The two-phase, two-component formulation allows for the simulation of evaporation and dissolution effects, appearance and disappearance of a gas phase, and component diffusion in each of the phases; for the IFC, a single gas component (hydrogen) is chosen.
3	Representation of heterogeneity (zonal or local; above the scale of an individual grid block)	R8, R9, R10, R11, R12, R13	Provided that two-phase flow is appropriately represented by Darcy's law, multiple materials (including matrix, fractures, fracture zones, EDZ, bentonite, concrete, seals, plugs, etc.) can be simulated.
4	Formulations of fractured systems using double-porosity, dual permeability, effective continuum model, Active Fracture Model	R8, R10	Allows for inclusion of fissures, dense fracture networks, or other bi-modal systems; the Active Fracture Model (Liu et al., 1998) may be used to represent gas channeling and gas piping effects. Accounts for pressure-dependent porosity changes.
5	Integral finite difference method with unstructured grids	R1, R2, R3, R4, R5, R6, R7, R9	Enables flexible discretization of complex geometry, and allows for "non-geometric" representation of abstracted repository elements.
6	Capability to handle nonlinearities	R22, R24, R25, R27, R28, R29, R33	Nonlinearities are inherent in all two-phase flow processes; the code's capability to handle these inherent nonlinearities will allow the inclusion of additional nonlinear effects to represent certain FEPs
7	iTOUGH2 framework	R30, R31	Provides convenient interfaces to other modules and programs

3.3 Implementation of Relevant Processes

This subsection describes in more detail those processes that are specific to the IFC, or that required code modifications.

3.3.1 Representation of Resaturation Process

Resaturation of cementitious backfill material into the initially air-filled portions of the ILW facility (R14; FEP 1.3.10) affects the storage volume for gas generated in the repository and thus the related pressure build-up. The effect can be simulated in the IFC using an appropriate discretization of the ILW emplacement tunnels and by specifying a non-zero initial gas saturation. Since the IFC only considers a single gas component (i.e., hydrogen), the initial gas in the IFC needs to be modeled also as hydrogen, rather than air. Resaturation is then simulated using the standard modeling capabilities of TOUGH2. See also the discussion on initial conditions in Sections 3.4 and 9.3.1, and on multi-component gases in Section 9.1.1.

3.3.2 Representation of Gas Generation

Rate of gas generation (R15; FEP 1.3.11) for the SF/HLW/ILW facilities will be provided externally as time-dependent source terms. They are expected to be consistent with the values given in Nagra (2002c, NTB 02-06, Table 4.3-1). Gas generation will cease after about 170,000 years. While waste is emplaced with a 3 m spacing between the 2 m long HLW and 4.6 m long SF canisters, gas generation is modeled as a line source along the emplacement tunnels. If considered relevant, water consumption (R16; FEP 1.3.13) as a result of gas generation could be invoked as a component- or phase-specific sink term that is proportional to the gas generation rate. However, the limitation of gas generation by lack of water is not considered significant (Nagra, 2007a, AN 07-115, FEP 1.3.12); therefore, no water sink terms are specified in the current base-case model.

3.3.3 Representation of Pathway Dilation

The creation of dilatant gas pathways (R22; FEP 1.3.19) is discussed in detail in Nagra (2004, NTB 04-06; Sections 3.1 and 4.2). This microfracturing process is initiated as the gas pressure approaches the minimum principal stress. The threshold pressure for dilatant gas flow is considered a material- and depth-dependent property and is also related to the local stress field. Pressure-dependent pathway dilation leads to increased permeability and reduced capillary strength. Pathway dilation is implemented in the IFC as follows (Nagra, AN 08-320, 2008):

- Calculate the depth-dependent threshold pressure p_d [Pa] for dilatant gas flow:

$$p_d(z) = d \cdot (f - z) - e \qquad (1)$$

where:

z	: elevation [m.a.s.l.]
d	: lithostatic pressure gradient [Pa m^{-1}]
e	: empirical parameter [Pa]
f	: surface elevation [m.a.s.l.]

- Calculate the vertical permeability k_v [m^2] as a function of p_d and pore pressure p:

$$k_v(p,z) = \begin{cases} k_{v,0} & p \le p_d(z) \\ k_{v,0} + b \cdot (p - p_d(z))^a & p > p_d(z) \end{cases} \qquad (2)$$

where:

$k_{v,0}$	: undisturbed vertical permeability [m^2]
p	: absolute pore pressure [Pa]
a	: empirical exponent [-]
b	: empirical coefficient [m^2 Pa^{-a}]

- Calculate the anisotropy ratio A [-] as a function of k_v:

$$A(k_v) = \frac{k_h}{k_v} = 5^{(k_{v,0}/k_v)^c} \tag{3}$$

where:

c	: empirical exponent [-]

- Calculate the horizontal permeability k_h [m^2] as a function of A:

$$k_h(A) = A \cdot k_v \tag{4}$$

- Calculate the capillary-strength parameter $1/\alpha$ [Pa] as a function of k_h using Leverett scaling:

$$\frac{1}{\alpha} \sim \frac{1}{\alpha_0}\sqrt{\frac{k_h}{k_{h,0}}} \tag{5}$$

where:

$1/\alpha_0$	: undisturbed capillary-strength parameter [Pa]
$k_{v,0}$	: undisturbed horizontal permeability [m^2]

- Porosity and the parameters of the characteristic curves (except the capillary-strength parameter) are considered constant.
- Single- and two-phase flow within dilatant pathways will be calculated using the standard TOUGH multi-phase process description.

Different parametric models describing pressure-dependent changes in Opalinus Clay properties can be implemented to evaluate conceptual model uncertainty.

3.3.4 Representation of Mechanical Processes

No geomechanical process simulations are performed within the IFC. However, the impacts of geomechanical processes on hydrogeologic properties are accounted for in an abstracted way by externally provided functions. Potential feedback mechanisms (i.e., coupled hydrologic-mechanical processes) are ignored.

FEP 1.4.1, R24: EDZ Self-Sealing

Self-sealing of the EDZ results in a reduction in permeability, which is implemented as an externally provided, time-dependent permeability-reduction factor $f_{kEDZ}(t)$ applied to all elements representing the EDZ.

$$k_{EDZ} = k_{EDZ,0} \cdot f_{kEDZ}(t) \tag{6}$$

Here, $k_{EDZ,0}$ is the initial permeability of the EDZ; $f_{kEDZ}(t)$ is provided as a look-up table. Corresponding changes in two-phase flow parameters (e.g., increase in capillary strength) are ignored, but could be implemented analogous to Section 3.3.3.

Similarly, the porosity of the EDZ is also reduced as a result of self-sealing. Again, a time-dependent porosity-reduction factor $f_{\phi EDZ}(t)$ is provided as a user-specified look-up table. Since porosity also changes as a function of pore pressure, the effect is implemented in the IFC by calculating a time-dependent rate of porosity change due to self-sealing (rather than a time-dependent porosity itself), which is then added to the porosity change due to pore compressibility $\Delta\phi_c$ to arrive at the new porosity:

$$\Delta\phi_{EDZ} = \phi_{EDZ,0}\left(f_{\phi EDZ}(t+\Delta t) - f_{\phi EDZ}(t)\right) \tag{7}$$

$$\phi_{EDZ}(t+\Delta t) = \phi_{EDZ}(t) + \Delta\phi_c + \Delta\phi_{EDZ} \tag{8}$$

Here, $\phi_{EDZ,0}$ is the initial EDZ porosity. Note that a reduction in porosity leads to expulsion of the phase mixture present in the pore space of each element.

FEP.1.4.3, R25: Tunnel Convergence

In the ILW facility, creep of the host rock leads to tunnel convergence, which results in a pore-volume reduction in the repository and potentially in pore-water expulsion. As before, a look-up table provides a time-dependent porosity-reduction factor $f_{\phi LMA}(t)$, which is then used to calculate the porosity change:

$$\Delta\phi_{ILW} = \phi_{LMA,0}\left(f_{\phi ILW}(t+\Delta t) - f_{\phi ILW}(t)\right) \tag{9}$$

$$\phi_{ILW}(t+\Delta t) = \phi_{ILW}(t) + \Delta\phi_c + \Delta\phi_{ILW} \tag{10}$$

Corresponding changes in two-phase flow parameters (e.g., increase in capillary strength) could be implemented analogous to Section 3.3.3. The change in bulk volume and repository geometry will be ignored. Note that TOUGH2 provides for the calculation of a pore-pressure-dependent porosity change $\Delta\phi_c$.

Specifying a time-dependent porosity reduction without considering coupled hydro-mechanical effects may lead to unrealistic effects. For example, it is unlikely that tunnel convergence proceeds at a rate that is independent of whether the pore space is gas filled or fully liquid saturated. Prescribing a porosity reduction in a fully water saturated, tight formation may lead to abrupt and excessive pressure increases due to the small water compressibility. To avoid this unrealistic behavior and the associated numerical difficulties, tunnel convergence is limited to elements that contain gas. Despite the significantly higher gas compressibility, pressures in the ILW increase and the gas-water mixture will be expulsed due to tunnel convergence.

FEP 1.4.7, R26: Uplift

Decompaction of the Opalinus Clay due to erosion and uplift leads to an increase in permeability, which is represented by a look-up table of permeability modifiers

$$k_{OPA} = k_{OPA,0} \cdot f_{k,Uplift}(t) \tag{11}$$

Here, $k_{OPA,0}$ is the initial permeability of the Opalinus Clay.

3.3.5 Representation of Chemical Processes

No biogeochemical processes will be performed within the IFC. However, the impact of biogeochemical processes on hydrogeologic properties will be accounted for in an abstracted manner by externally provided functions. Potential feedback mechanisms (i.e., coupled hydrologic-biogeochemical processes) are ignored.

Chemical and mineralogical alterations of bentonite (R27; FEP 1.5.2) may lead to a change in permeability. Moreover, high-pH plumes from cement in the ILW facility may cause changes in the porewater composition and mineralogical alterations in sealing zones and in the host rock (R28, FEP 1.5.4; R29, FEP 1.5.11), most likely resulting in the development of a skin zone. The abstraction of these geochemical effects is described in Kosakowski et al. (2008); their implementation into the IFC is discussed in this subsection.

Permeability reduction due to geochemical sealing occurs in a thin skin zone, in which the pore space is locally clogged. Only flow perpendicular to the skin zone, which develops along the interface between two geochemically active materials, is affected by geochemical sealing processes. A local-scale porosity for this skin zone is calculated as a function of time:

$$\phi(t) = \begin{cases} \phi_0 \exp\left(-l(t/t_c)^m\right) - \left(\phi \exp(-l) - \phi_c\right)\dfrac{t}{t_c} & t \le t_c \\ \phi(t) = \phi_c & t > t_c \end{cases} \tag{12}$$

Parameters l and m are provided by the user for each material interface that leads to geochemical sealing. The clogging time t_c is calculated as a function of liquid saturation:

$$t_c = T_c / S_l \tag{13}$$

where T_c is the user-provided clogging time under fully saturated conditions. The clogging porosity ϕ_c is inversely calculated (using a bisection method) from the minimal clogging permeability (see below).

The skin-zone permeability is calculated from the local-scale porosity using the Kozeny-Carman relationship:

$$k(\phi) = k_0 \left(\frac{\phi(t)}{\phi_0}\right)^3 \left(\frac{1-\phi_0}{1-\phi(t)}\right)^2 \tag{14}$$

The clogging permeability is given as a fraction of the initial permeability:

$$k(\phi_c) = \kappa \cdot k_0 \tag{15}$$

The effective permeability used to calculate flow across an interface between two geochemically active materials is then calculated as the harmonic mean of the unaffected permeability and the time-dependent skin-zone permeability of a user-specified thickness.

3.4 Initial Conditions and Simulation Period

Resaturation, gas generation, the associated flow processes, and other safety-relevant processes are inherently time-dependent. Consequently, the IFC will simulate the transient evolution of the flow field around the repository. However, neither the transient effects during repository construction, operation, and sealing phases are likely to be simulated. Given the expected long lifetime of the waste canisters (Nagra, 2004, NTB 04-06, Table 2.3-1), gas generation is not considered to be significant (with exception of the initial corrosion of construction and tunnel-support materials) during the early period immediately after repository closure. The choice for an appropriate starting time for the IFC simulations (determining initial conditions) will be determined and justified. The corresponding initial conditions for the IFC simulations can either be pre-calculated, or—should they depend on the parameters varied during the Monte Carlo simulation—updated within the IFC.

Gas generation is expected to last for approximately 170,000 years (Nagra 2002c, NTB 02-06, Table 4.3-1). Simulations will be performed for 1 million years.

3.5 Addressing Interface Requirements

Interfaces to the TOUGH2 and iTOUGH2 simulators consist of standard ASCII text files. These text files could be directly used as the interfaces to the upstream and downstream models providing input to or using output from the IFC. In addition, iTOUGH2 provides a convenient interface for varying TOUGH2 input parameters and for selecting TOUGH2 outputs. Finally, experience with linking (i)TOUGH2 to the GoldSim system-level model show that input parameters and output variables of the process simulator can be shared with the system-level simulator.

Appropriate pre- and post-processing routines may need to be developed, depending on the interface requirements of the upstream and downstream models. An interface will be developed that allows for a seamless integration of the code into the PSA framework (R31).

3.6 Replicating Reference Waste Emplacement Tunnel

In response to requirement R32, it is essential to reduce the model size by exploiting inherent symmetries. Specifically, the regular geometry of the array of waste emplacement tunnels exhibits multiple local symmetry planes (i.e., the vertical planes along the tunnel axes, and the vertical midplanes between tunnels; details are discussed in Section 4). This means that the tunnel array can be approximated by a single representative waste emplacement tunnel. However, since there is no global symmetry of the entire repository system and the surrounding host rock, the representative emplacement tunnel submodel has to be multiplied and appropriately connected to the geosphere model. This is accomplished by the following procedure:

(1) A global model is generated, consisting of the geosphere and the non-symmetric underground openings.

(2) The region of the waste emplacement tunnel array is cut out from the model and left void, drastically reducing the total number of grid blocks.

(3) A representative waste emplacement tunnel submodel (RWETS) is generated; it represents half of a single tunnel and the surrounding host formation to the midpoint between neighboring tunnels.

(4) The RWETS is connected to the global model; note that it only occupies a small fraction of the void space created in Step (2).

(5) The system-state variables calculated at the connection between the RWETS and the global model are extracted and copied to internal, Dirichlet-type boundary elements at the interface between the void and the global model.

iTOUGH2 has been modified to allow replicating primary and secondary variables from parent elements (i.e., each element at the interface between the RWETS and the global model) to one or multiple daughter boundary elements (at the corresponding internal boundary elements between the void space and the global model). Dynamically prescribing the system state as time-dependent Dirichlet-type boundary conditions at these internal boundary elements ensures that gas and liquid that flow from the representative waste emplacement tunnel to the global model are multiplied, entering the global model at the appropriate location.

4. IFC Representation of Repository System

4.1 Model Domain and Dimensionality

The system to be modeled by the IFC consists of the host rock (Opalinus Clay) and all relevant engineered components embedded in it (such as emplacement tunnels, access tunnels, operations tunnels, ventilation tunnels, construction tunnels, observation tunnels, ventilation shafts, test and pilot facilities, plugs and seals; these subsurface structures are backfilled and are surrounded by an EDZ). In addition, the surrounding geosphere needs to be represented, specifically the clay-rich confining units that may contain local aquifers (Wedelsandstein and Sandsteinkeuper aquifers). Regional aquifers (Malm aquifer and Muschelkalk aquifer) are considered to define the compliance boundary, i.e., they do not assume a barrier function (Nagra, 2002b, NTB 02-05, Section 4.2), and flow and transport processes within these aquifers do not need to be simulated within the IFC.

Given the geometry of the system and the expected direction of driving forces, the system to be modeled is inherently three-dimensional. Moreover, the scales to be considered—even if lumping pore- and small-scale features and processes into a continuum representation—span several orders of magnitude, from decimeters (e.g., the thickness of the EDZ) to kilometers (e.g., flow in the local aquifers). Given the constraints on computational efficiency (R32), an accurate, three-dimensional casting of the repository system is not feasible. Consequently, the conceptual model of the repository system for the IFC needs to exploit inherent symmetries, and—if justifiable—compromise on accuracy, fidelity, and transparency for the sake of computational efficiency. The simplifications proposed below appear reasonable, but may need to be formally justified by comparison with detailed process simulations, sensitivity, and impact analyses.

4.2 Representation of Key Model Components

4.2.1 Representation of Far Field

Figure 4 shows a hydrogeological framework model for a repository in the Opalinus Clay of the Zürcher Weinland. It indicates the following flow regimes (see also Nagra, 2002b, NTB 02-05, Section 4.2):

- Horizontally layered stratigraphy; subvertical, transmissive discontinuities are not shown, but may be present.
- Predominantly vertical flow (and diffusion) in the host rock.
- Predominantly horizontal flow in the local aquifers; potential flow distance to discharge boundaries is large compared to repository footprint.
- Predominantly vertical flow in upper and lower confining units.

While this conceptual model of flow in the far field is predominantly one- or two-dimensional, it is inherently three-dimensional, specifically when considering the gas-release pattern from the engineered system. A three-dimensional model is therefore set up to represent the far field—sensitivity analyses could be performed to evaluate the impact of lower-dimensional models, should computational constraints require the reduction of the number of grid blocks.

Constant pressure boundaries are applied at the top and bottom of the geosphere model, based on measurements from the Benken borehole (Nagra, 2002b, NTB 02-05, Figure 4.2-8) or related information. No-flow boundaries can be applied along the vertical sides, with exception of the layers representing the local aquifers, where a horizontal hydraulic gradient will be imposed based on head measurements. Given the predominantly vertical flow direction within the host rock and the confining layers, the lateral extent of the model (along the direction of the gradient in the local aquifers) can be limited.

Larger, steeply dipping discontinuities (e.g., faults) can be included using discrete elements, accounting for their actual position relative to the repository. Currently, the presence of a single, vertical high-transmissivity zone is accounted for in the mesh design (see Section 4.3.2 for details). Hydrogeologic properties of the geosphere are summarized in Nagra (2004, NTB 04-06, Tables 3.3-1, 3.3-2, and 3.3-3); the properties used in the IFC base-case model are discussed in Section 4.4.

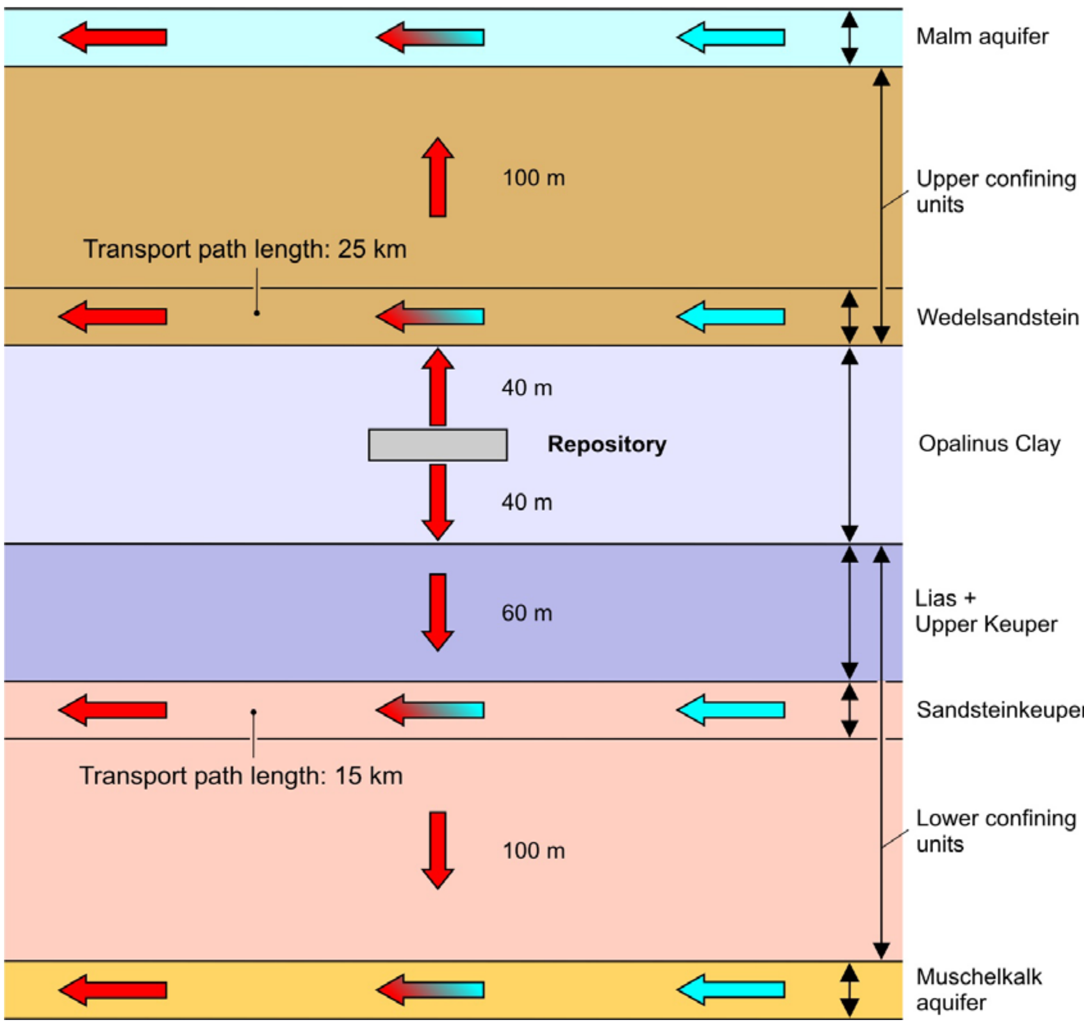

Figure 4. Hydrogeological framework model of a repository in the Opalinus Clay of the Zürcher Weinland (Nagra, 2002c, NTB 02-06, Figure 3.5-1)

4.2.2 Representation of Waste Emplacement Tunnels

Gas generation by anaerobic corrosion of metals, microbial degradation, radiolysis, and decay originates mainly in the waste emplacement tunnels. The creation of a free gas phase is expected to impact the pressure and flow fields within the backfilled tunnels and the near field, in turn affecting potential radionuclide transport pathways and velocities (to be calculated by the RTC). Moreover, pressure build-up and gas- and liquid-phase transport are affected by the ability of gas to escape the emplacement tunnels, either directly into the surrounding host rock, or along the buffer and backfill materials and EDZ to the operations tunnel and other connected, backfilled cavities. The appropriate representation of the array of emplacement tunnels is therefore a crucial element of the IFC. Different representations are needed for the SF/HLW, pilot, and ILW facilities.

The repository layout is shown in Figure 2 above. The SF/HLW facility consists of an array of twenty-seven, 800 m long, parallel emplacement tunnels with a diameter of 2.5 m, dipping at an average slope of approximately 4.2% from the operations tunnel in the north towards the construction tunnel in the south; the spacing between tunnels is 40 m. Operations and construction tunnels have a slope of approximately 0.5%; the access ramp dips at approximately 12.1%. A pilot facility (consisting of three emplacement tunnels) is located in the north-eastern corner of the main facility. The ILW facility consists of two short emplacement tunnels, referred to as LMA-1 (110 m) and LMA-2 (60 m). Several seals (R11; FEP 1.3.5) and plugs (R12; FEP 1.3.6) will be installed during closure of the facility. The repository is located at a depth of approximately 600 m below ground surface, in the mid-plane of the 105–115 m thick Opalinus Clay. The repository has a footprint of approximately 1 km^2. Details about the geometry of the emplacement tunnels are summarized in Nagra (2007, NIB 06-07).

The layout and geometry of the SF/HLW emplacement tunnels and the pilot facility exhibits the following approximate symmetries:

(1) Vertical symmetry plane along axis of emplacement tunnel.

(2) Vertical symmetry plane, halfway between (i.e., 20 m from) and parallel to axes of emplacement tunnels.

These symmetry planes ignore repository edge effects and local heterogeneities. Moreover, it is assumed that the gas conditions in a single emplacement tunnel are not significantly affected by the conditions along the construction and operation tunnels. These conditions are non-uniform as gas accumulates along these tunnels in a cumulative fashion along the prevalent flow direction. The magnitude and behavior of gas flow within the operation, construction, and access tunnels critically determine the validity of this conceptualization. If these fluxes are small and conditions in the tunnels are approximately uniform, only 1/2 of a single emplacement tunnel (i.e., only about 2.5% of the entire emplacement tunnel array) needs to be represented in the IFC. The connection of the emplacement tunnel to the construction and operation tunnels is described in Section 4.2.3. The end sections of the emplacement tunnels, where no waste will be stored, as well as seals, locks, and turn-out sections will be explicitly included (R5).

Perpendicular to the tunnel axis, discretization will allow for the representation of the canister (as the gas source), the backfilled tunnel, the EDZ, and the host rock. Hydrogeologic properties for the engineered materials and geologic formations are summarized in Section 4.4). According to the calculations presented in Nagra (2004, NTB 04-06, Figure 4.2-5), isobars become essentially horizontal at a distance of about 10 m above and below the tunnel axis. The vertical extent of this zone is also expected to contain the 13 MPa isobar, which corresponds to the threshold pressure for dilatant gas flow (see Section 3.3.3). It seems appropriate to connect the near-field submodel of the waste emplacement drift to the far-field geosphere model (see Section 4.2) at elevations of ±10 m from the elevation of the repository axis.

The ILW emplacement tunnels are implemented explicitly due to a lack of symmetry.

4.2.3 Representation of Other Backfilled Underground Structures

Escape of gas along the backfilled tunnel system (R4) is one of the main gas transport variants described in Nagra (2004, NTB 04-06, Section 4.3, Table 4.3-1). The tunnel system includes the access ramp, construction tunnel, operations tunnel, observation tunnels, detour tunnel, central area, ventilation shaft and other backfilled underground openings. Waste emplacement tunnels are connected to the operations tunnel in the north and construction tunnel in the south. The ILW facility is connected to the tunnel system in the north-eastern corner of the repository, and a construction and ventilation shaft is present in the north-eastern corner of the repository (see Figure 2). Several seals are in place along the tunnel system. This configuration does not exhibit an obvious symmetry.

To accurately represent this potentially significant gas-release pathway, the tunnel system is represented in full. While the detailed geometry of the tunnel segments is simplified, the connectivity, relative position, and interaction with the geosphere are observed.

The various tunnel cross sections are represented in a simplified manner, reflecting flow-relevant geometrical properties (specifically, cross-sectional area). Each tunnel segment is surrounded by an EDZ (R3 and R11, FEP 1.3.5), and connected to the host rock. Plugs and seals (R5) are represented accordingly, using hydrogeologic properties of the backfill material.

The single, representative waste emplacement tunnel and the near-field host rock surrounding it (see Section 4.2.2) will be connected to the operations and/or construction tunnel at a single location (e.g., that of the central emplacement tunnel). To represent the interaction between the entire SF/HLW facility and the operations and construction tunnels, special elements allowing for time-dependent Dirichlet boundary conditions are attached along the operations and construction tunnels; the pressures and saturations (or hydrogen-mass fraction) specified for these special boundary elements are taken (at each time step) from those elements of the representative emplacement tunnel that are connected to the operations tunnel. Again, this assumes that the conditions in the center emplacement tunnel (connected to the operations tunnel) are representative of all emplacement tunnels. This approach allows for a reasonable representation of the impact of the emplacement tunnels on flow conditions within the tunnel system.

Similarly to the treatment of the emplacement tunnels, potential gas releases from the tunnel system to the host rock and confining layers are enabled by connecting the tunnel system vertically to the far-field model described in Section 4.2. Furthermore, the access ramp is directly connected to the Wedelsandstein aquifer (R23; FEP 1.3.21) to accommodate one of the gas-release scenario described in Nagra (2004, NTB 04-06, Section 4.3).

4.2.4 Equivalent Conceptual Repository Model

The complex repository layout shown in Figure 2 is simplified to be able to account for approximate symmetries, and to make the model conceptually and computationally tractable. An Equivalent Conceptual Repository Model (ECRM) was developed by Nagra; it is shown in Figure 5. It preserves essential geometrical aspects of the actual repository layout, specifically tunnel lengths and footprint area. The ECRM is the basis for generating a computational grid, as discussed in Section 4.3.

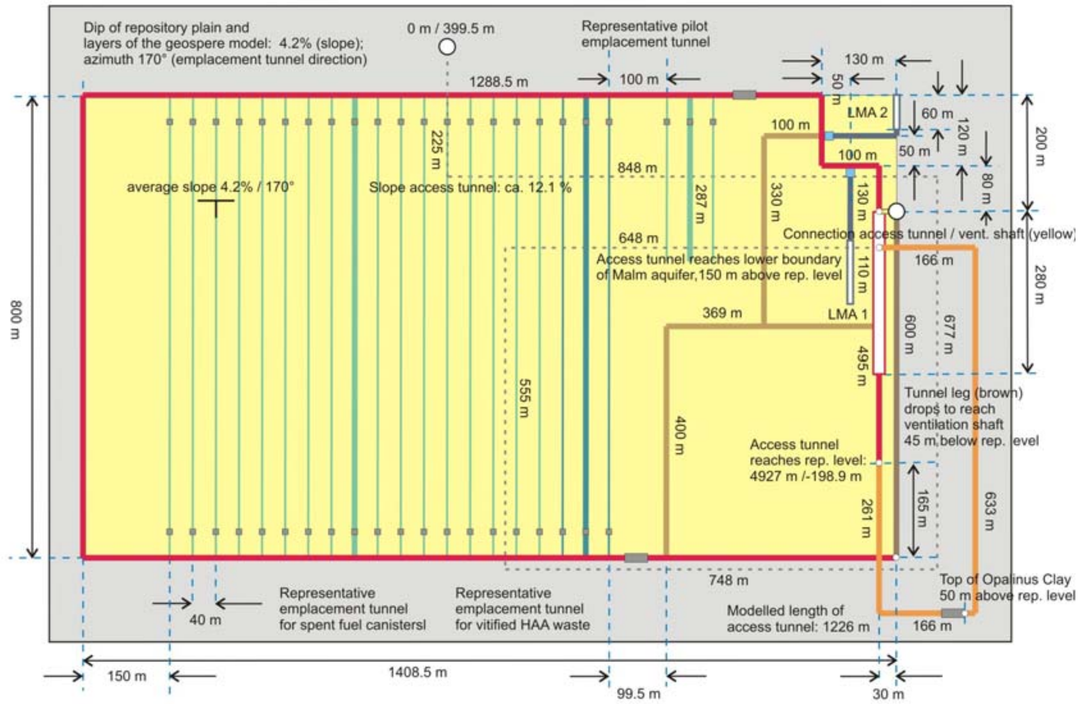

Figure 5. Equivalent conceptual repository model

4.3 Mesh Generation

4.3.1 General Approach

A computational mesh for the integral finite differences code iTOUGH2-IFC is generated, properly representing the geometry and properties of all key features of the geologic framework model (see Figure 4) and the simplified repository system (see Figure 5). Mesh generation occurs in several steps, where submeshes are generated separately (using a combination of internal mesh generation capabilities of iTOUGH2-IFC, Fortran routines for mesh manipulation, and Unix script files); the resulting submeshes are eventually linked together. The following submeshes are generated:

- Host rock and confining units
- Local aquifers (Wedelsandstein and Sandsteinkeuper aquifers)
- High-transmissivity zone
- Representative emplacement tunnel for SF/HLW facility
- Representative emplacement tunnel for pilot facility
- Emplacement tunnel for long-lived intermediate-level wastes, LMA-1
- Emplacement tunnel for long-lived intermediate-level wastes, LMA-2
- Operations tunnel
- Construction tunnel

- All other backfilled tunnels (i.e., access tunnel, connecting tunnel, detour tunnel, control tunnel, central area, shaft)

The generation of each of these submeshes is described in the following subsections. For details, the reader is referred to the supporting Unix script files (see Appendix A2) and Fortran programs (see Appendix A3) used to generate the IFC mesh. Figure 6 shows the submeshes in a three-dimensional depiction; plan views are shown in Figure 7. Note that the submeshes of the waste emplacement tunnels (shown in red) contain the waste, backfill material, EDZ, and the host rock in the immediate vicinity of the tunnels (see Sections 4.3.3 and 4.3.4 for details); the construction and operations tunnels (shown in green) include the backfilled tunnels, associated EDZ, and the surrounding host rock, which extends in horizontal direction from starter and turn-out tunnels (i.e., the respective connections of the construction and operation tunnels to the waste emplacement tunnels) to the outer (northern and southern) edges of the model (see Section 4.3.5 for details); the remaining underground structures (shown in blue) only represent the backfilled structure and associated EDZ in a simplified manner (see Section 4.3.6 for details).

The mesh has a total of approximately 36,000 grid blocks and 112,000 connections between them. Two equations (one for the component water, one for hydrogen) are set up for each grid block, resulting in a system of nonlinear equations with approximately 72,000 unknowns to be solved at each time step. Approximately 10,000 time steps need to be solved to reach the intended simulation time of 1,000,000 years. Time stepping is automatically adjusted; thus, the number of time steps and total CPU time may considerably depend on the parameter set.

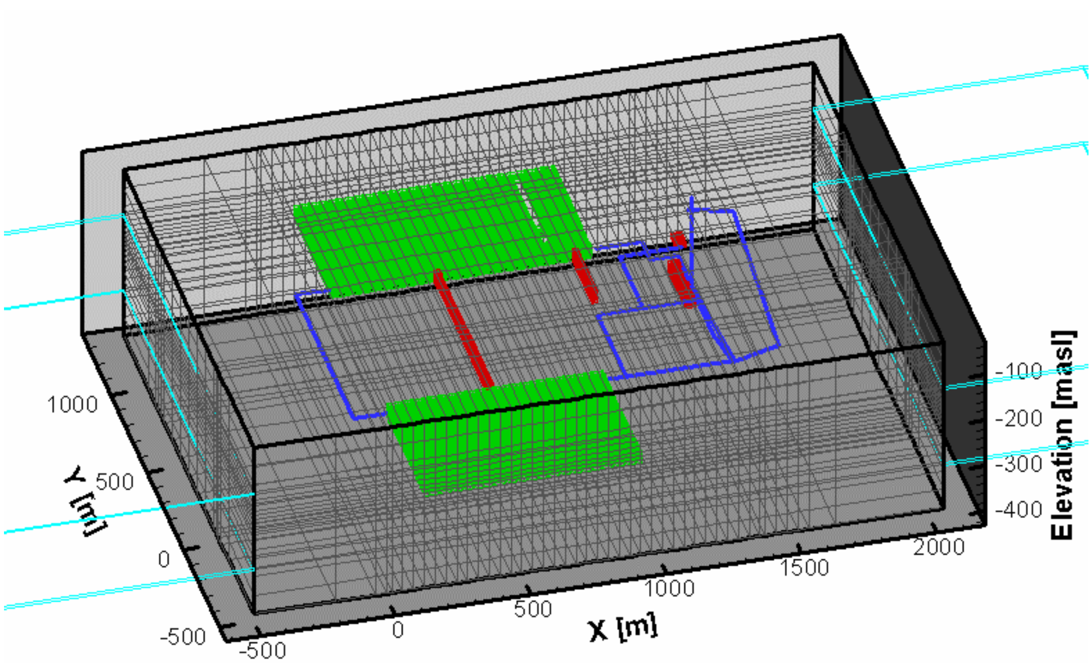

Figure 6. Three-dimensional view of computational mesh of IFC model; submesh of geosphere (gray), local aquifers (cyan), representative waste emplacement tunnels (red), operations and construction tunnels (green), and other backfilled tunnels (blue).

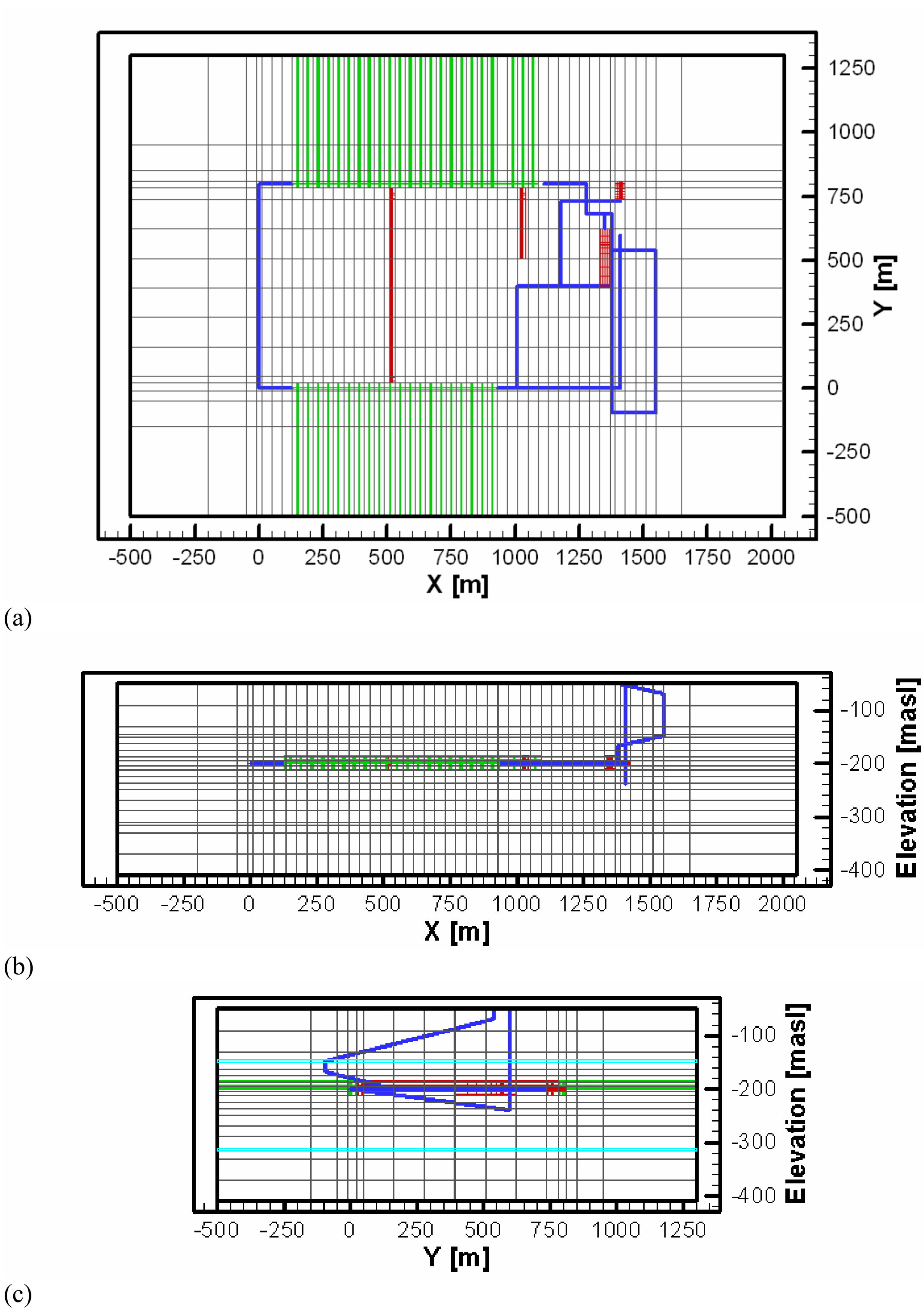

Figure 7. (a) XY-, (b) XZ-, and (c) YZ-views of computational mesh of IFC model; submesh of geosphere (gray), waste emplacement tunnels (red), operations and construction tunnel submesh (green), and other backfilled tunnels (blue)

4.3.2 Submesh Geosphere

The geosphere mesh comprises the host rock and surrounding confining units and local aquifers. The repository submeshes will be embedded into the geosphere mesh. The basic geosphere mesh is a cube of dimensions 2050 m × 1800 m × 360 m. The horizontal cross section of this cube extends 500 m beyond each side of the repository footprint. The top of the cube is at an elevation of -48.9 m.a.s.l., representing the base of the Malm; the bottom of the geosphere mesh is at an elevation of -408.9 m.a.s.l., representing the top of the Muschelkalk. The repository horizon is at an elevation of -198.9 m.a.s.l. The vertical stratification and discretization is shown in Figure 7b and c and summarized in Table 7.

Table 7. Vertical stratification of geosphere model

Elevation [m.a.s.l.]	Thickness [m]	Material name	Stratigraphic unit	Element name
-48.9	-	bMALM	Malm	T-g 1
-48.9 -143.9	95.0	DOGGE	Dogger	A2... A4...
-143.9 -148.9	5.0	WEDEL	Wedelsandstein (local aquifer)	A5...
-148.9 -248.9	100.0	OPALI	Opalinus Clay	A6... AE...
-248.9 -308.9	60.0	LIAS	Lias and Upper Keuper	AF... AH...
-308.9 -313.9	5.0	SANDS	Sandsteinkeuper (local aquifer)	AI...
-313.9 -408.9	95.0	KEUPE	Lower confining unit	AJ... AL...
-408.9	-	bMUSC	Muschelkalk	B-g 1

At the left (approximately south-west) and right (approximately north-east) sides of the model at elevations of -146.4 and -311.4 m.a.s.l., four one-dimensional, horizontal submeshes are attached to represent the Wedelsandstein and Sandsteinkeuper These two local aquifers extend 25 km and 15 km downstream to their respective compliance boundaries. The length of the upstream branches of the local aquifers is 10 km.

Provisions are made to introduce a vertical, high-transmissivity zone through the center of the repository in east-western direction at Y = 392.5 m. The vertical extent of the 1-m thick zone (discretization too small to be visible in Figure 7) can be adjusted by providing appropriate fault properties within the zone for each stratigraphic layer as listed in Table 7. (See also discussion of Table 17 in Section 4.4).

After generation of the geosphere base mesh, all elements within the repository footprint at the elevation of the repository horizon are removed to make room for the representative waste emplacement tunnel meshes (for spent fuel and high level waste, for the pilot facility, and for the two long-lived intermediate level waste facilities). Averaging planes and Dirichlet boundary elements are attached to the internal faces of the cut-out regions. The averaging planes are used to connect the representative waste emplacement tunnels to the geosphere model at their representative locations; the internal Dirichlet boundary elements are used to provide the replicated state variables where virtual tunnels are located.

4.3.3 Submesh Representative Emplacement Tunnels

A single waste emplacement tunnel is discretized to represent the twenty tunnels for the disposal of spent fuel and high-level waste. The submesh of the representative emplacement tunnel is embedded into the geosphere mesh and connected to the operations and construction tunnel submeshes (see Section 4.3.5) at a representative location (i.e., the central tunnel at X=510 m, see Figure 7a). The conditions calculated at the submodel boundaries are then replicated to all interfaces between virtual emplacement tunnels and the surrounding submeshes.

The domain of the representative emplacement tunnel submodel extends in X-direction from the center of the tunnel to the midpoint between two tunnels (i.e., a length of 20.0 m); in Y direction from the starter tunnel near the construction tunnel (at Y=22.0 m) to the lock near the operations tunnel (at Y=783.0 m)—the starter and turn-off tunnels are not part of the emplacement tunnel submesh; they belong to the construction and operations tunnel submeshes, respectively. Vertically, the submesh is 26.0 m thick, centered at the elevation of the tunnel axis (Z=-198.9 m.a.s.l.).

The model domain is discretized such that the different elements of the emplacement tunnels are approximately represented using a Cartesian grid. These elements include:

- Waste
- Backfilled emplacement drift
- Lock
- Abutment
- Seal
- EDZ
- Opalinus Clay

A three-dimensional view of the mesh is shown in Figure 8.

The two YZ-planes that intersect the tunnel axis and the mid-plane between emplacement tunnels are symmetry planes and thus no-flow boundaries. The XZ-planes at end faces of the tunnel are connected to three averaging planes at each side (the construction and operations tunnel sides). The three averaging planes average the conditions in the backfilled tunnel, the surrounding EDZ, and the host rock.

Starting with the XZ averaging planes near the construction tunnel, individual tunnel sections are discretized. The horizontal planes at the top and bottom of the submodel are averaged to match the discretization of the geosphere model.

The discretization in Z-direction approximately captures the varying geometries of the tunnel cross sections and their respective EDZs, specifically the higher lock on the operations tunnel side of the model.

The discretization of the representative tunnel of the pilot facility is identical to that of the northern section (Y > 508.0 m) of the representative emplacement tunnel for spent fuel and high-level waste, with the exception that all elements start with the letter “p”.

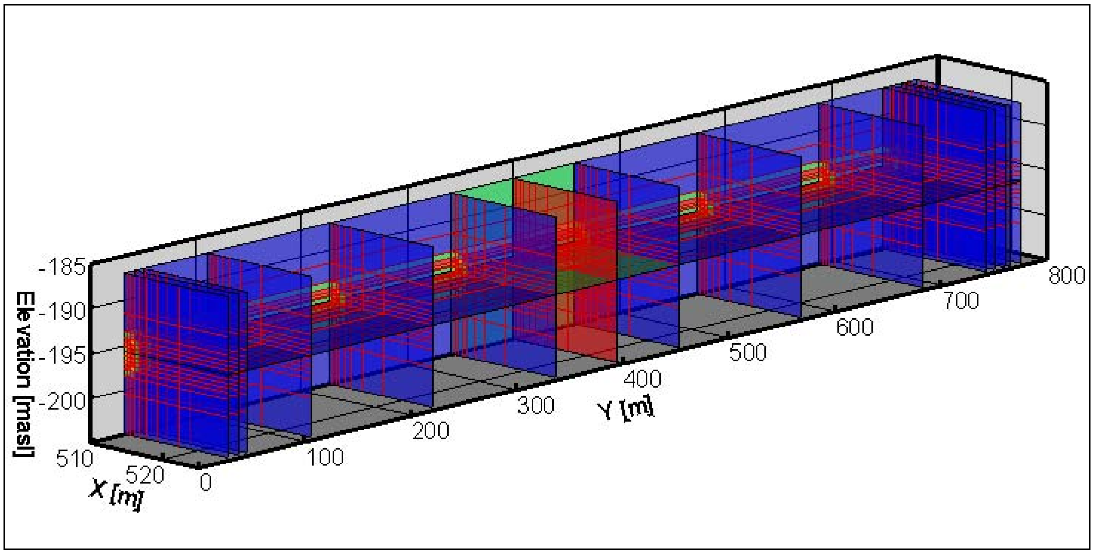

Figure 8. Three-dimensional view of representative waste emplacement tunnel model

4.3.4 Submesh Intermediate-Level Waste Facility

Two submeshes representing the two intermediate-level waste facilities are created and inserted into the geosphere model as local grid refinements. Figure 9 shows the discretization of the first facility. Multiple averaging elements are attached at the six sides of the model to facilitate the connection to the coarser geosphere model.

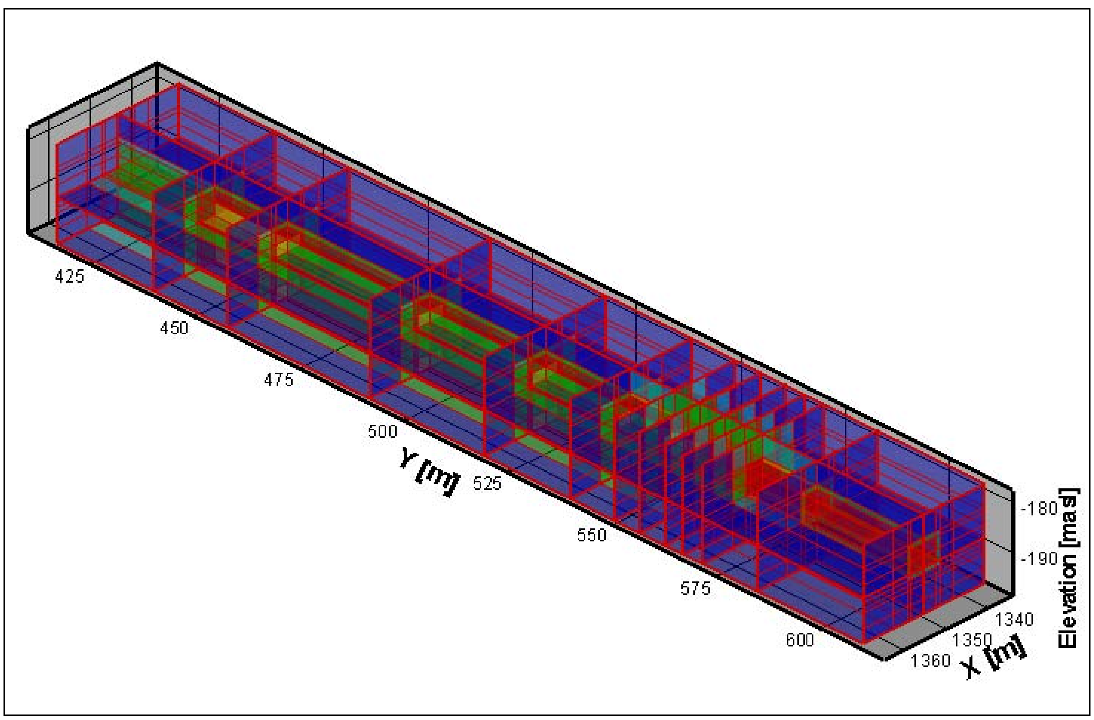

Figure 9. Three-dimensional view of intermediate-level waste facility

4.3.5 Submesh Operations and Construction Tunnels

Submeshes with relatively high resolution are constructed for the operations and construction tunnels to be able to provide the connections (turn-out and starter tunnels) to the 17 waste emplacement tunnels for spent fuel, the three tunnels for high-level wastes, and the three tunnels of the pilot facility. Moreover, EDZs of the various openings with different diameter have to be accommodated. A three-dimensional view of a section of the operations tunnel mesh in the vicinity of the representative waste emplacement tunnel is shown in Figure 10. Recall that the single representative waste emplacement tunnel mesh is fully connected to the operations tunnel mesh, whereas the (19) virtual emplacement tunnels are connected through internal Dirichlet boundary elements attached to the operations tunnel mesh; the system state calculated at the connection between the representative emplacement tunnel and the operations tunnel is prescribed at these internal boundary elements to achieve the desired replication effect.

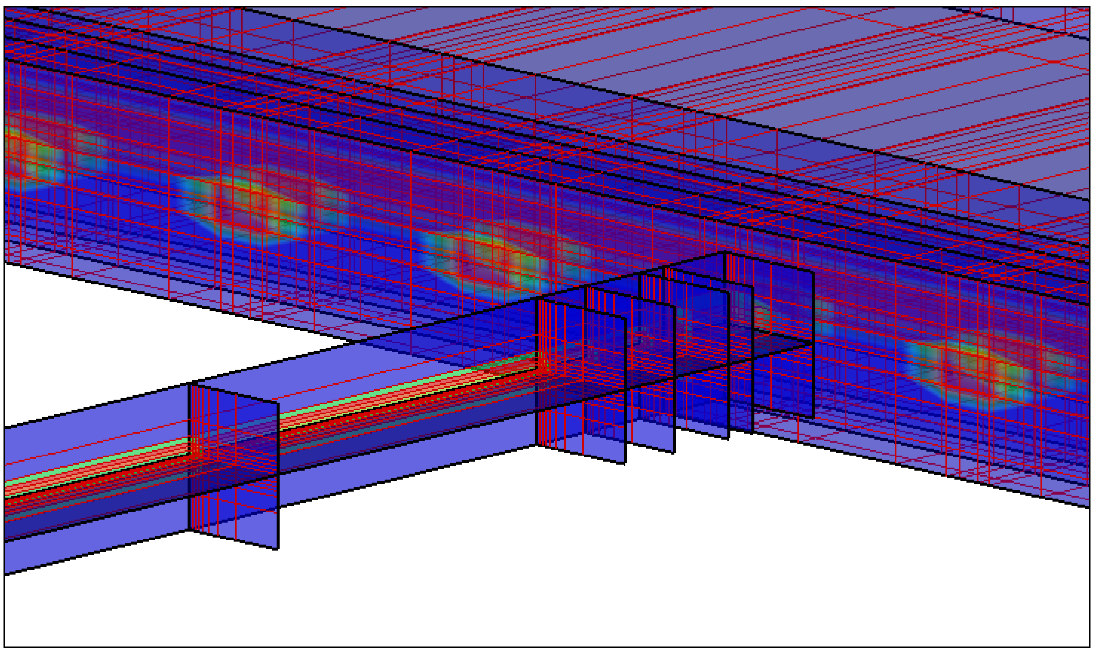

Figure 10. Three-dimensional view of connection between representative waste emplacement tunnel and operations tunnel

4.3.6 Submesh Backfilled Underground Structures

With the exception of the waste emplacement tunnels as well as the operations and construction tunnels, all the other backfilled underground structures (i.e., access tunnel, central area, connection tunnel between operations and construction tunnel, the shaft, connection tunnel between construction tunnel and shaft, the detour and control tunnels, and other minor tunnel sections; see blue lines in Figure 6 and Figure 7) are discretized in the following, simplified manner. The backfilled tunnel and surrounding EDZ are represented by two concentric, cylindrical elements that are inserted into each quadrilateral elements of the geosphere model that is intersected by the respective tunnel segment. While this simplified approach allows for buoyancy-driven gas flow along inclined tunnels and their EDZs, buoyancy effects within the tunnel cross section are ignored.

4.4 Hydrogeologic Properties

Hydrogeologic properties need to be specified for the various natural and man-made materials in the IFC model. While many of these parameters are uncertain and thus varied as part of a probabilistic assessment of the repository performance, a base-case parameter set is given here as a reference. The hydrogeologic parameter sets summarized in Table 8 through Table 16 can be used for testing and initial sensitivity analyses. The source of each value is indicated, if available. Assumed values are considered reasonable. The iTOUGH2-IFC input file corresponding to these property values is shown in Figure A - 3.

Table 8. Material Properties, EDZs

Symbol	Description	Value	Units	Reference/Comment
k	Permeability $EDZ_{SF/HLW/Pilot}$ EDZ_{LMA} $EDZ_{seal/plug}$ $EDZ_{all\ tunnels}^{*}$ EDZ_{shaft}	 1×10^{-19} 1×10^{-19} 5×10^{-20} 1×10^{-19} 1×10^{-19}	m^2	 NTB 02-03, Table 9.4-5 AN 08-173, Table 4.2 AN 08-173, Table 4.2 assumed assumed
ϕ	Porosity	0.22	-	NTB 02-03, Table 9.4-5 AN 08-173, Table 4.2
c_ϕ	Pore compressibility	2.3×10^{-11}	1/Pa	Derived from porosity and specific storage coefficient (10^{-6}; corrected value from AN 07-159, Table. 2): $c_\varphi = S_s \frac{1}{\rho g \varphi} - c_w$
$1/\alpha$	Gas-entry value	3.0	MPa	NTB 04-06, Table 3.3-1 AN 07-173, Table 4.2
n	Pore-size distribution index	1.67	-	same as Opalinus Clay as given in AN 07-325
S_{lr}	Residual liquid saturation	0.0	-	same as Opalinus Clay as given in AN 07-325
S_{gr}	Residual gas saturation	0.0	-	same as Opalinus Clay as given in AN 07-325
* "all tunnels" includes: operations tunnel, construction tunnel, access tunnel, detour tunnel, connection tunnel, control tunnel, central area				

Table 9. Material Properties, Backfill and Sealing Materials

Symbol	Description	Value	Units	Reference/Comment
k	*Permeability* S/B 1[*] S/B 2[&] S/B 3[%] Bentonite[#] Backfill[@]	 1×10^{-16} 1×10^{-18} 1×10^{-19} 1×10^{-20} 1×10^{-17}	m^2	AN 07-159, Tables 2 and 3
ϕ	*Porosity* S/B 1[*] S/B 2[&] S/B 3[%] Bentonite[#] Backfill[@]	 0.30 0.30 0.30 0.40 0.25	-	AN 07-159, Tables 2 and 3
c_ϕ	*Pore compressibility* S/B 1[*] S/B 2[&] S/B 3[%] Bentonite[#] Backfill[@]	 0.00 0.00 0.00 0.00 0.00	1/Pa	Derived from porosity and specific storage coefficient (10^{-6}; from AN 07-159, Table. 2): $c_\varphi = S_s \frac{1}{\rho g \varphi} - c_w$ results in negative pore compressibility → set to zero
$1/\alpha$	*Gas-entry value* S/B 1[*] S/B 2[&] S/B 3[%] Bentonite[#] Backfill[@]	 0.10 1.00 3.00 10.00 0.30	MPa	assumed
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0.25	-	assumed
S_{gr}	Residual gas saturation	0.01	-	assumed

* S/B 1: Sand/Bentonite-80/20 moderately compacted; applied to access tunnel, central area, operations tunnel, pilot facility, turn out, construction tunnel, control tunnel, detour tunnel, connection tunnel

& S/B 2: Sand/Bentonite-80/20 highly compacted; applied to shaft

% S/B 3: Sand/Bentonite-70/30; applied to seals in access tunnel

\# Bentonite; applied in shaft seal

@ Backfill; applied to SF/HLW/Pilot emplacement tunnels, LMA1/LMA2 emplacement tunnels

Table 10. Material Properties, Opalinus Clay

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	 1×10^{-20} 2×10^{-21}	m^2	NTB 02-03, Table 9.4-2 horizontal vertical
ϕ	Porosity	0.12	-	NTB 02-03, Table 9.4-1
c_ϕ	Pore compressibility	8.05×10^{-9}	1/Pa	Derived from porosity and specific storage coefficient (10^{-5}) from NTB 02-03, Table 9.4-2 $c_\varphi = S_s \frac{1}{\rho g \varphi} - c_w$
$1/\alpha$	Gas-entry value	1.80	MPa	AN 07-325 Table 3
n	Pore-size distribution index	1.67	-	AN 07-325 Table 3
S_{lr}	Residual liquid saturation	0.00	-	AN 07-325 Table 3
S_{gr}	Residual gas saturation	0.003	-	AN 07-325 Table 3

Table 11. Material Properties, Steeply Dipping Discontinuity

Symbol	Description	Value	Units	Reference/Comment
k	Transmissivity	1×10^{-10}	m^2/s	NTB 02-03, Table 9.4-4c
ϕ	Porosity	0.10	-	assumed
c_ϕ	Pore compressibility	1×10^{-8}	1/Pa	assumed
$1/\alpha$	Gas-entry value	0.10	MPa	assumed
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0.20	-	assumed
S_{gr}	Residual gas saturation	0.01	-	assumed

Table 12. Material Properties, Dogger

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	1×10^{-19}	m^2	assumed
ϕ	Porosity	0.20	-	assumed
c_ϕ	Pore compressibility	1×10^{-8}	1/Pa	assumed
$1/\alpha$	Gas-entry value	10.00	MPa	assumed
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0.20	-	assumed
S_{gr}	Residual gas saturation	0.01	-	assumed

Table 13. Material Properties, Lias and Upper Keuper

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	5×10^{-21}	m^2	NTB 02-03, Table 9.4-4a
ϕ	Porosity	0.10	-	assumed
c_ϕ	Pore compressibility	2.6×10^{-9}	1/Pa	Derived from porosity and specific storage coefficient (3×10^{-6}) from AN 07-325, Table 2 $c_\varphi = S_s \frac{1}{\rho g \varphi} - c_w$
$1/\alpha$	Gas-entry value	1.00	MPa	AN 07-325, Table 3
n	Pore-size distribution index	2.00	-	AN 07-325, Table 3
S_{lr}	Residual liquid saturation	0.25	-	AN 07-325, Table 3
S_{gr}	Residual gas saturation	0.01	-	AN 07-325, Table 3

Table 14. Material Properties, Lower Keuper

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	5×10^{-21}	m^2	assumed
ϕ	Porosity	0.10	-	assumed
c_ϕ	Pore compressibility	1.0×10^{-9}	1/Pa	assumed
$1/\alpha$	Gas-entry value	1.00	MPa	assumed
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0.25	-	assumed
S_{gr}	Residual gas saturation	0.01	-	assumed

Table 15. Material Properties, Wedelsandstein Aquifer

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	5×10^{-17}	m^2	NTB 02-03, Table 9.4-4a
ϕ	Porosity	0.10	-	assumed
c_ϕ	Pore compressibility	1×10^{-8}	1/Pa	assumed
$1/\alpha$	Gas-entry value	0.20	MPa	NTB 04-06, Table 3.3-3
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0. 90	-	assumed to obtain gas accessible porosity of 0.001 given in NTB 04-06, Table 3.3-3
S_{gr}	Residual gas saturation	0.01	-	assumed

Table 16. Material Properties, Sandsteinkeuper Aquifer

Symbol	Description	Value	Units	Reference/Comment
k	Permeability	2×10^{-15}	m^2	NTB 02-03, Table 9.4-4a
ϕ	Porosity	0.05	-	NTB 02-03, Table 9.4-4a
c_ϕ	Pore compressibility	1×10^{-8}	1/Pa	assumed
$1/\alpha$	Gas-entry value	0.10	MPa	assumed
n	Pore-size distribution index	2.00	-	assumed
S_{lr}	Residual liquid saturation	0. 90	-	assumed to obtain gas accessible porosity of 0.001 given in NTB 04-06, Table 3.3-3
S_{gr}	Residual gas saturation	0.01	-	assumed

Table 17 contains a list of all five-character material names used in the `ROCKS` block of the iTOUGH2-IFC model. Material names starting with a "`b`" are boundary elements. Material names starting with a "`F`" followed by the material name in lower-case characters are elements within the fault zone of that material; to introduce the steeply dipping continuity, assign fault properties (see Table 11 or material "`FAULT`") to all these materials; otherwise, the properties should be identical to those of the corresponding stratigraphic layer. Material names starting with "`EDZ`" refer to the excavation-disturbed zones around specific tunnel segments. Material names starting with "`WA`" represent the gas-generating waste. Material names starting with "`SEAL`" refer seals and plugs. Material names starting with "`ET`" refer to backfilled waste emplacement tunnels. Material names starting with "T" refer to various backfilled tunnel segments. The `ROCKS` block of a complete iTOUGH2-IFC input file can be found in Figure A - 3.

Table 17. Material Names and Description

Name	Material
OPALI	Opalinus Clay
Fopal	Potential fault zone in Opalinus Clay
bOPAL	Opalinus Clay boundary element
FAULT	Generic fault (not used; copy to all bXXXX materials if needed)
bFAUL	Fault boundary elements
bMALM	Malm (upper boundary)
DOGGE	Dogger
Fdogg	Potential fault in Dogger
WEDEL	Wedelsandstein aquifer
Fwede	Potential fault in Wedelsandstein aquifer
bWEDE	Wedelsandstein aquifer boundary elements
LIAS	Lias and Keuper
Flias	Potential fault in Lias and Keuper
SANDS	Sandsteinkeuper aquifer
Fsand	Potential fault in Sandsteinkeuper aquifer
bSAND	Sandsteinkeuper aquifer boundary elements
KEUPE	Lower Keuper
Fkeup	Potential fault in Lower Keuper
bMUSC	Muschelkalk aquifer (lower boundary)
EDZsf	EDZ around waste emplacement tunnels (spent fuel and high-level waste)
EDZpi	EDZ around pilot facility
EDZco	EDZ around construction tunnel
EDZop	EDZ around operations tunnel
EDZac	EDZ around access tunnel
EDZvt	EDZ around connection tunnel between operations and construction tunnels
EDZca	EDZ around central area
EDZkt	EDZ around control tunnel
EDZdt	EDZ around detour tunnel
EDZsh	EDZ around shaft
EDZl1	EDZ around intermediate-level waste facility 1
EDZl2	EDZ around intermediate-level waste facility 2
EDZse	EDZ around seals
bEDZs	Internal boundary elements for EDZ around waste emplacement tunnels for spent fuel and high-level waste
bEDZp	Internal boundary elements for EDZ around pilot facility
WAsf	Waste (spent fuel and high-level waste)
WApil	Waste in pilot facility
WAlm1	Waste in intermediate-level waste facility 1
WAlm2	Waste in intermediate-level waste facility 2
SEAL	Seal emplacement tunnel (S/B 80/20, highly compacted)
SEALa	Seal access tunnels (S/B 70/30)[#]
SEALs	Seal shaft (compacted bentonite and gravel)
ABUTM	Abutment (gravel)
ETsf	Emplacement tunnel for spent fuel and high-level waste, backfilled with compacted bentonite

Table 17 (cont.). Material Names and Description

`ETpil`	Pilot facility backfilled with compacted bentonite
`ETlm1`	Emplacement tunnel of intermediate-level waste facility 1, backfilled with mortar
`ETlm2`	Emplacement tunnel of intermediate-level waste facility 2, backfilled with mortar
`TURNO`	Turn-out from spent fuel, high-level waste, and pilot facility into operations tunnel
`bTURN`	Internal boundary elements connecting to turn-outs from spent fuel, high-level waste, and pilot facilities into operations tunnel
`START`	Starter tunnel off the construction tunnel to spent fuel, high-level waste, and pilot facilities
`bSTAR`	Internal boundary elements connecting to starter tunnels off the construction tunnel to spent fuel, high-level waste, and pilot facilities
`LOCK`	Lock, backfilled with (S/B 70/30)
`Tshaf`	Shaft above Opalinus Clary Shaft, backfilled with gravel
`TacCO`	Access tunnel, backfilled with crushed Opalinus Clay
`Tacce`	Access tunnel (S/B 70/30)
`Tconn`	Connection tunnel between operations and construction tunnels (S/B 70/30)
`Tcons`	Construction tunnel (S/B 70/30)
`Tcont`	Control tunnel (S/B 70/30)
`Tdeto`	Detour tunnel (S/B 70/30)
`Toper`	Operations tunnel (S/B 70/30)
`Tcent`	Central area (S/B 70/30)
`Tlma1`	Connection to intermediate-level facility 1 (S/B 70/30)
`Tlma2`	Connection to intermediate-level facility 2 (S/B 70/30)
# Percentages of sand and bentonite in backfill mixture	

4.5 Parameters of Geomechanical and Geochemical FEPs

Table 18 shows the base-case parameter set for the geomechanical and geochemical FEPs discussed in Sections 3.3.3 through 3.3.5. The corresponding `IFS` block of the iTOUGH2-IFC input file is shown in Figure A - 3.

Table 18. Parametric Models for Special FEPs and Related Coefficients

FEP	Description	Parametric Model/ Coefficients/ Reference/Comment
1.3.19	*Pathway dilation:* Parametric model describing change in absolute permeability as a function of gas pressure and coefficients	AN 07-002, p. 4 $k_v(p,z) = \begin{cases} k_{v,0} & p \le p_d(z) \\ k_{v,0} + b(p - p_d(z))^a & p > p_d(z) \end{cases}$ $k_h(k_v) = k_v / A(p)$ $A(p,z) = \begin{cases} 5 & p \le p_d(z) \\ 5^{(k_{v,0}/k_v(p,z))^c} & p > p_d(z) \end{cases}$ $p_d(z) = d \cdot (f - z) - e$ Coefficients: a = 3.0 (1 ≤ a ≤ 8) b = 1×10^{-21} m^2 Pa^{-a} c = 0.25 (0 < c < 1) d = 2.5×10^4 Pa/m e = 2.0×10^6 Pa f = 399.5 m.a.s.l. Apply to Opalinus Clay only
	Parametric model describing change in porosity as a function of permeability or gas pressure	No change
	Parametric model describing change in gas-entry value as a function of permeability, porosity, or gas pressure	AN 07-002, p. 5 Leverett scaling for capillary strength $\frac{\alpha(p,z)}{\alpha_0} \sim \sqrt{\frac{k(p,z)}{k_0}}$

Table 18 (cont.): Parametric Models for Special FEPs and Related Coefficients

FEP	Description	Parametric Model/ Coefficients/ Reference/Comment
1.4.1	*Self-sealing of EDZ:* Parametric model describing change in absolute permeability of EDZ as a function of time	AN 07-002, p. 6 $k_{EDZ} = k_{EDZ,0} f_{EDZ,k}(t)$ $f_{EDZ,k}(t)$ provided as look-up table or coefficients of a polynomial, separate for individual EDZs
	Parametric model describing change in porosity as a function of permeability or time	AN 07-002, p. 6 $\phi_{EDZ} = \phi_{EDZ,0} f_{EDZ,\phi}(t)$ $f_{EDZ,\phi}(t)$ provided as look-up table or coefficients of a polynomial, separate for individual EDZs
	Parametric model describing change in gas-entry value as a function of permeability, porosity, or time	no change
1.4.3	*Tunnel convergence:* Parametric model of L/ILW porosity as a function of time and pressure	AN 07-002, p. 7 $\phi_{BF} = \phi_{BF,0} f_{\phi BF}(t)$ $f_{\phi BF}(t)$ provided as look-up table or coefficients of a polynomial, applied to porosity of backfill material in intermediate-level waste facility $\phi_{BF,0} = 0.25$
1.4.7	*Uplift:* Parametric model of material-dependent absolute permeability as a function of time (and depth)	AN 07-002, p. 7 Option A: $k_{OPA} = k_{OPA,0} f_{k,Uplift}(t)$ $f_{k,Uplift}(t)$ provided as look-up table or coefficients of a polynomial; applied to Opalinus Clay only Option B: Same as FEP 1.3.19, with a time- (and depth-) dependent threshold pressure p_d provided by a look-up table of surface elevations.

Table 18 (cont.): Parametric Models for Special FEPs and Related Coefficients

FEP	Description	Parametric Model/ Coefficients/ Reference/Comment
1.5.2, 1.5.4, 1.5.11	*Chemical alteration effects*: Abstraction methodology and corresponding parametric model of changes in material properties of bentonite and skin zone.	AN-44-08-02, AN 08-238 Block-scale porosity remains unchanged *Minimal local-scale porosity:* $\phi(t) = \phi_0 \exp\left(l - (t/t_c)^m\right) - \left(\phi \exp(-l) - \phi_c\right)\frac{t}{t_c} \quad t \le t_c$ $\phi(t) = \phi_c \quad t > t_c$ $t_c = T_c / S_l$ (AN 07-238, p. 5) *Porosity-permeability relationship:* $\frac{k(\phi)}{k_0} = \left(\frac{\phi(t)}{\phi_0}\right)^3 \left(\frac{1-\phi_0}{1-\phi(t)}\right)^2$ *Coefficients*: Sealing layer thickness: 1 mm (AN 08-238, p. 4) Cement-OPA (AN-44-08-02, Table 2) $l = 1.0$ $m = 0.4$ $T_c = 100$ years ($40 \le T_c \le 750$) $\phi_c \leftarrow k(\phi_c) = \kappa \cdot k_0$ $\kappa = 0.01$ (AN 07-238, p. 5) Cement-tunnel backfill (AN-44-08-02, Table 1) $l = 1.0$ $m = 0.45$ $T_c = 200$ years ($100 \le T_c \le 2000$) $\phi_c \leftarrow k(\phi_c) = \kappa \cdot k_0$ $\kappa = 0.01$ (AN 07-238, p. 5)

4.6 Initial and Boundary Conditions

The calculated pressure and flow fields are determined by (among other factors) the conditions applied at the model boundaries. Constant pressures are prescribed at the top and bottom of the model (inducing vertical upflow), and on the eastern and western end points of the two local aquifers (Wedelsandstein and Sandsteinkeuper), providing a regional, horizontal flow field within these aquifers. No-flow conditions are prescribed elsewhere; details can be found in Table 19.

Gas production in the waste emplacement tunnels are prescribed as time-dependent mass generation rates per tunnel length (for spent fuel and high-level waste) or volume of waste (for intermediate-level waste). The values are given in Table 20 and Table 21. The gas generation rates shown in Table 21 were derived from Nagra (2002c, NTB 02-06, Table 4.3-1), assuming a hydrogen density under standard conditions of 0.089 kg m^{-3}, and a total waste volume in both intermediate-level waste facilities of 6000 m^3. The waste volume is that of the IFC model grid, which was constructed based on the drawings of Nagra (2006, NIB 06-07, Beilage 11 and Profile O (for LMA1) and Beilage 4 and Profile L (for LMA2)). The iTOUGH2-IFC GENER block implementing the rates of Table 20 and Table 21 are shown in Figure A - 3.

The entire model domain is assumed to be initially fully liquid saturated. The initial pressure distribution (i.e., prior to gas generation) is calculated by running the model to steady state using the Dirichlet boundary condition discussed above and summarized in Table 19. To improve computational efficiency, the steady-state simulation performed to obtain initial conditions is conducted in two steps, where the first step uses homogeneous material properties throughout the model domain.

Should the boundary pressures be considered uncertain and varied during a PSA calculation (as anticipated in Table 22 below), the pre-gas-generation steady-state run has to be included in the simulation.

Table 19. Boundary Conditions in Aquifers

	Description	Value	Units	Reference/ Comment
P_{top}	Absolute pressure at top of IFC model (i.e., base Malm aquifer, 150 m above repository horizon)	4.50	MPa	Assuming hydrostatic pressure distribution with ρ_w=1000 kg m^{-3}, and g=9.81 m^2 s^{-1}. Surface elevation (399.5 m.a.s.l.) and base Malm aquifer (-48.9 m.a.s.l.) from AN 08-173, Table 2
P_{bot}	Absolute pressure at bottom of IFC model (i.e., top of Muschelkalk aquifer, 210 m below repository horizon)	8.03	MPa	Assuming hydrostatic pressure distribution with ρ_w=1000 kg m^{-3}, and g=9.81 m^2 s^{-1}. Surface elevation (399.5 m.a.s.l.) and top Muschelkalk aquifer (-408.9 m.a.s.l.) from AN 08-173, Table 2
i_{Wedel}	Hydraulic gradient in Wedelsandstein aquifer	0.001	m/m	NTB 02-03, Tab. 9.4.4a Absolute pressure at center of Wedelsandstein aquifer: 4.82 MPa, i.e., -62 m head difference, NTB 02-03, Figure 4.61; Surface elevation (399.5 m.a.s.l.) and base Malm aquifer (-146.4 m.a.s.l.) from AN 08-173, Table 2
$p_{,Wedel,u}$	Upstream pressure Wedelsandstein	4.9331	MPa	11.275 km upstream of model center with gradient i_{Wedel}
$p_{,Wedel,d}$	Downstream pressure Wedelsandstein	4.5648	MPa	26.275 km downstream of model center with gradient i_{Wedel}
i_{Sand}	Hydraulic gradient in Sandsteinkeuper aquifer	0.005	m/m	NTB 02-03, Tab. 9.4.4a Absolute pressure at center of Sandsteinkeuper aquifer: 7.70 MPa, i.e., +61 m head difference, NTB 02-03, Figure 4.61 Surface elevation (399.5 m.a.s.l.) and base Malm aquifer (-311.9 m.a.s.l.) from AN 08-173, Table 2
$p_{Sand,u}$	Upstream pressure Sandsteinkeuper	8.2499	MPa	11.275 km upstream of model center with gradient i_{Sand}
$p_{,Sand,d}$	Downstream pressure Sandsteinkeuper	6.8986	MPa	16.275 km downstream of model center with gradient i_{Sand}

Table 20. Neumann Boundary Conditions (Gas Generation Rates)

	Description	Value	Units	Reference/ Comment
$q_{SF,HLW}$	Gas generation rates (kg/s per meter of SF or HLW emplacement tunnel) as a function of time	4.88×10^{-11} for 0 < t < 200,000 years	kg s^{-1} m^{-1}	AN 08-173, Tab. 5 NTB 02-06, Tab. 4.3-1
q_P	Gas generation rates (kg/s per meter of pilot facility tunnel) as a function of time	4.88×10^{-11} for 0 < t < 200,000 years	kg s^{-1} m^{-1}	AN 08-173, Tab. 5 NTB 02-06, Tab. 4.3-1
q_{LMA1}	Table of gas generation rates (kg/s per m^3 of LMA 1 waste) as a function of time	see Table 21	kg s^{-1} m^{-3}	Derived from NTB 02-06, Tab. 4.3-1
q_{LMA2}	Table of gas generation rates (kg/s per m^3 of LMA 2 waste) as a function of time	see Table 21	kg s^{-1} m^{-3}	Derived from NTB 02-06, Tab. 4.3-1

Table 21. Time-Dependent Gas Generation Rate for LMA1 and LMA2 in Kilograms per Second and Cubic-Meter of Waste

Time [years]	Gas Generation Rate [kg s^{-1} m^{-3}]
0	3.27×10^{-10}
3	3.18×10^{-10}
10	5.21×10^{-11}
30	5.21×10^{-11}
100	4.65×10^{-11}
300	3.74×10^{-11}
1000	2.13×10^{-11}
3000	9.48×10^{-12}
10000	4.74×10^{-12}
30000	2.40×10^{-12}
100000	9.48×10^{-13}
170000	0.0
1000000	0.0

4.7 Parameters Potentially Varied in PSA Calculations

As part of a probabilistic performance assessment calculation, many of the input parameters are varied to examine the impact of parameter uncertainty on model predictions. Unique designations for each *potentially* varied parameter are given in Table 22. These parameters include a set of hydrogeologic properties for each material listed in Table 17, parameters of the geomechanical and geochemical FEPs (see Table 18), as well as certain boundary conditions (see Table 19 through Table 21).

Potential statistical correlations among the uncertain parameters must be generated by the sampling procedure

Aspects of the conceptual model may also be changed during a PSA analysis. Some of these conceptual choices are invoked by setting appropriate flags in the iTOUGH2-IFC input file; however, they are not listed here, because these flags are not numerical values sampled from a probability distribution function.

Table 22. Parameters Potentially Varied in PSA Calculations

Parameter Designation	**Parameter Description**	**Units**
	Hydrogeologic Parameters[&]	
*MMMMM*_POR	porosity ϕ	-
*MMMMM*_PERX	absolute permeability in x direction k_x	m^2
*MMMMM*_PERY	absolute permeability in y direction k_y	m^2
*MMMMM*_PERZ	absolute permeability in z direction k_z	m^2
*MMMMM*_COM	pore compressibility c_ϕ	1/Pa
*MMMMM*_TORTX	tortuosity factor for binary diffusion τ	-
*MMMMM*_GK	Klinkenberg parameter b	1/Pa
*MMMMM*_RP_Slrk	residual liquid saturation for relative permeability functions S_{lrk}	-
*MMMMM*_RP_Sgr	residual gas saturation S_{gr}	-
*MMMMM*_CP_Srlc	residual liquid saturation for capillary pressure function S_{lrc}	-
*MMMMM*_CP_n	van Genuchten parameter n	-
*MMMMM*_CP_1/a	van Genuchten parameter $1/\alpha$	Pa
*MMMMM*_CP_m	van Genuchten parameter m	-
*MMMMM*_CP_g	van Genuchten active fracture model parameter γ	-

[&] Hydrogeologic parameters are specified for each material defined in the ROCKS block (see Figure A - 3) of the IFC model. The variable *MMMMM* in the parameter designation is to be replaced with the five-character material name listed in the first column of Table 17; a description of the material is also given in Table 17. The base-case values of these parameters are given in Table 8 through Table 16, with k_x=k_y, S_{lrk} = S_{lrc}, m=1-1/n, and b=0.

Table 22 (cont.) Parameters Potentially Varied in PSA Calculations

Parameter Designation	**Parameter Description**	**Units**
	Pathway Dilation	
OPALI_PD_a	Pathway dilation model Eq. (2), parameter *a*	-
OPALI_PD_b	Pathway dilation model Eq. (2), parameter *b*	$m^2 Pa^{-a}$
OPALI_PD_c	Pathway dilation model Eq. (3), parameter *c*	-
OPALI_PD_d	Pathway dilation model Eq. (1), parameter *d*	Pa/m
OPALI_PD_e	Pathway dilation model Eq. (1), parameter *e*	Pa
OPALI_PD_f	Pathway dilation model Eq. (1), parameter *f*	m.a.s.l.
	EDZ Self-Sealing[$]	
EDZ*MM*_SS_KT_i	Time of table entry i of permeability modification factor due to self-sealing of EDZ *MM*	s
EDZ*MM*_SS_K_i	Permeability modification factor due to self-sealing of EDZ *MM* at time index i	-
EDZ*MM*_SS_KC_i	ith coefficient of polynomial describing permeability modification factor due to self-sealing of EDZ *MM*	-
EDZ*MM*_SS_PT_i	Time of table entry i of porosity modification factor due to self-sealing of EDZ *MM*	s
EDZ*MM*_SS_P_i	Porosity modification factor due to self-sealing of EDZ *MM* at time index i	-
EDZ*MM*_SS_PC_i	ith coefficient of polynomial describing porosity modification factor due to self-sealing of EDZ *MM*	-
[$] Permeability and porosity reduction factors due to self-sealing (as well as tunnel convergence and uplift) can be provided either as look-up tables of time vs. factor, or as coefficients of a polynomial; see Section 5.2 for details.		
	Tunnel Convergence	
*MMMMM*_TC_PT_i	Time of table entry i of porosity modification factor due to tunnel convergence of LMA backfill material *MMMMM*	s
*MMMMM*_TC_P_i	Porosity modification factor due to tunnel convergence of LMA backfill material *MMMMM* at time index i	-
*MMMMM*_TC_PC_i	ith coefficient of polynomial describing porosity modification factor due to tunnel convergence of LMA backfill material *MMMMM*	-
	Uplift	
OPALI_UL_KT_i	Time of table entry i of permeability modification factor or surface elevation due to uplift	s
OPALI_UL_K_i	Permeability modification factor or surface elevation due to uplift at time index i	-
OPALI_UL_KC_i	ith coefficient of polynomial describing permeability modification factor or surface elevation due to uplift	-

Table 22 (cont.) Parameters Potentially Varied in PSA Calculations

Parameter Designation	Parameter Description	Units
	Geochemical Sealing#	
*MMMMM-NNNNN*_GS_t	Clogging time (Eq. 13), T_c	s
*MMMMM-NNNNN*_GS_l	Geochemical sealing model (Eq. 12) parameter *l*	-
*MMMMM-NNNNN*_GS_m	Geochemical sealing model (Eq. 12) parameter *m*	-
*MMMMM-NNNNN*_GS_k	Geochemical sealing model (Eq. 15) parameter κ	-
*MMMMM-NNNNN*_GS_d	Thickness of sealing layer	m
# Geochemical sealing is applied to all connections of an interface *MMMMM-NNNNN*, where *MMMMM* and *NNNNN* are two material names from the list in Table 17 defining an interface.		
	*Generation Rates**	
*SSSSS*_T_i	Time of gas generation table entry i for sink/source *SSSSS*	s
*SSSSS*_T_i	Gas generation rate i for sink/source *SSSSS*	kg/s
* Gas (or liquid) generation rates are given as tables of time vs. mass rate in block GENER of the iTOUGH2-IFC input file (see Figure A - 3)		
	Dirichlet Boundary Conditions@	
*EEEEE*_P	Boundary pressure for element *EEEEE*	Pa
@ In the IFC model, constant pressures are applied at the top boundary (element T-g 1) and the bottom boundary (element B-g 1). The gradient in the Wedelsandstein aquifer is defined by boundary pressures specified in the westernmost and easternmost elements WAw 1 and WAe11, respectively; the gradient in the Sandsteinkeuper aquifer is defined by boundary pressures specified in the westernmost and easternmost elements SAw 1 and SAe11, respectively. If boundary pressures are considered uncertain and varied during a PSA analysis, a steady-state simulation has to be performed to obtain appropriate initial conditions (see		

5. Input Formats

As iTOUGH2-IFC is based on TOUGH2-EOS and iTOUGH2, the standard manuals (Pruess et al., 1999; Finsterle, 2007abc; downloadable from `http://www-esd.lbl.gov/TOUGH+/manuals.html`) apply. This section discusses the input commands and formats that were added to the standard code, providing the additional parameters and controls needed to invoke the special capabilities discussed in Sections 3.3.3, 3.3.4, 3.3.5, and 3.6. This input is provided in the forward (i.e., TOUGH2) input file using keywords and formatted input if parameters and options. There are three new keywords: (1) "`COPY `" for replicating the system state (see Section 5.1), (2) "`IFC  `", followed by input to address geomechanical and geochemical FEPs (see Section 5.2), and (3) "`PICNIC`" to identify the interface between IFC and PICNIC-TD cross sections (see Section 5.3).

5.1 Replicating System States to Boundary Elements

As discussed in Section 3.6, the system state (i.e., pressure and gas saturation or hydrogen mass fraction)—calculated at the interface between the representative waste emplacement tunnel and the global geosphere model—needs to be copied to internal Dirichlet-type boundary elements to multiply the gas and liquid flows exiting or entering the emplacement tunnel array at specific locations.

An element whose system state is to be copied is referred to as the parent element. The primary variables of the parent element will be copied to one or more daughter elements, which are Dirichlet-type boundary elements with a large volume. Note that the boundary element can be connected to multiple elements of the global mesh, thus effectively reducing the number of internal boundary elements and the amount of replication needed.

The input is provided in the forward (i.e., TOUGH2) input file following the line with the keyword "`COPY `". The parameters and input format are as follows:

COPY	Keyword introducing information on replicating element system states
Record COPY.1	
	Format (I5,5X,A3,I2) NDaughter, Parent
NDaughter	Number of daughter elements
Parent	Parent element name (five-character code name, where the first three characters are arbitrary, and the last two characters are integers)
Record COPY.2	
	Format (8(A3,I2,5X) (Daughter (I),I=1,NDaughter)
Daughter	Daughter element names (five-character code names, where the first three characters are arbitrary, and the last two characters are integers)
Record COPY.3	A blank record closes the COPY data block

Figure 11 shows an example, where the pressure and saturation calculated for parent element `s-o 1` is copied to one daughter boundary element (named `S-o 1`), and the system state of parent element `h-g 1` is copied to four daughter elements (`H-g 1` through `H-g 4`).

```
COPY ----1----*----2----*----3----*----4
    1     s-o 1
S-o 1
    4     h-g 1
H-g 1     H-g 2     H-g 3    H-g 4
   ..     .....
.....
```

Figure 11. Excerpt of TOUGH2 block showing input format for replicating system state from parent to daughter elements.

5.2 Geomechanical and Geochemical Processes

The added geomechanical process capabilities include pathway dilation (Section 3.3.3), as well as EDZ self-sealing, tunnel convergence, and uplift (Section 3.3.4). The input is provided in the forward (i.e., TOUGH2) input file following the line with the keyword "`IFC  `". The parameters and input format are as follows:

IFC Keyword introducing information on geomechanical and geochemical FEPs in the following order:

1. FEP 1.3.19 Pathway dilation
2. FEP 1.4.1 EDZ self-sealing
3. FEP 1.4.3 Tunnel convergence
4. FEP 1.4.7 Uplift
5. FEPs 1.5.2, 1.5.4, and 1.5.11 Geochemical sealing

Record IFC.1 Start input related to FEP 1.3.19, pathway dilation

Format (I5)
NPD

NPD Number of parameters needed in pathway dilation model. The currently implemented model, see Equations (1)–(3), contains 6 parameters, so NPD should be set to 6. Set to zero to ignore pathway dilation effects.

Record IFC.2

Format (6E10.4))
(PDPar(I),I=1,NPD)

PDPar Parameters of pathway dilation model:

PDPar(1) = a : Exponent in Eq. (2) (typically $1 \le a \le 8$)
PDPar(2) = b : Coefficient in Eq. (2) (typically 10^{-21} m^2)
PDPar(3) = c : Exponent in Eq. (3) (typically $0 < c < 1$)
PDPar(4) = d : Lithostatic pressure gradient, Eq. (1) (typically 2.5×10^4 Pa/m)

PDPar(5) = e : Empirical parameter, Eq. (1) (typically 2.0×10^6 Pa)
PDPar(6) = f : Surface elevation, Eq. (1) (for IFC: 399.5 m.a.s.l.)

Record IFC.3 — Start input related to FEP 1.4.1, EDZ self-sealing

Format (I5)
NSSEDZFlag

NSSEDZFlag — Flag indicating whether FEP 1.4.1 (EDZ self-sealing) shall be invoked

- < 0 : Do not invoke EDZ self-sealing, and do not read additional input regarding this FEP (i.e., go to Record IFC.9)
- 0 : Continue reading input, but do not invoke EDZ self-sealing
- 1 : Reduce porosity and permeability due to EDZ self-sealing
- 2 : Reduce permeability due to EDZ self-sealing
- 3 : Reduce porosity due to EDZ self-sealing

Record IFC.4 — (only if NSSEDZFlag > 0)

Format (I5)
NEDZ

NEDZ — Number of EDZ types; each EDZ type (defined by one or more material names) will have its own parameter set describing self-sealing processes

Record IFC.5

Format (I5)
NMatEDZ(I)

NMatEDZ(I) — Number of materials comprising EDZ type I

Record IFC.6

Format (A5)
(CMatEDZ(I,J),J=1,NMatEDZ(I))

CMatEDZ(I,J) — NMatEDZ(I) lines containing the five-character names of the materials that belong to EDZ type I.

Record IFC.7 — (only if NSSEDZFlag = 1 or 2)

Format (A)
FileName

FileName — Name of file containing polynomial coefficients or look-up table of permeability modifiers. If file name is "this", continue reading on following lines in the current TOUGH2 input file.

The format of the look-up table is as follows:

Format(*)
NfkEDZ(I)

NfkEDZ(I) — If positive, NfkEDZ(I) is the number of data points in permeability-modifier look-up table for EDZ type I; the look-up table itself is read in the following format:

Format(*)
(Time(J), PermMod(J), J = 1, NfkEDZ(I))

Time(J)	Time in seconds
PermMod(J)	Permeability modifier (dimensionless) at time Time(J)

If negative, -NfkEDZ(I) is the number coefficients in a polynomial of degree -NfkEDZ(I)-1, providing permeability modifiers as a function of time for EDZ type I; the coefficients are read in the format:

Format(*)
(Coefficient(J), J = 0, -NfkEDZ(I)-1)

Coefficient(J)	Coefficients of polynomial

<u>Record IFC.8</u> — (only if NSSEDZFlag = 1 or 3)

Format (A)
FileName

FileName — Name of file containing polynomial coefficients or look-up table of porosity modifiers. If file name is “this”, continue reading on following lines in the current TOUGH2 input file.

The format of the look-up table is as follows:

Format(*)
NfpEDZ(I)

NfpEDZ(I) — If positive, NfpEDZ(I) is the number of data points in porosity-modifier look-up table for EDZ type I; the look-up table is read in the following format:

Format(*)
(Time(J), PorMod(J), J = 1, NfpEDZ(I))

Time(J)	Time in seconds
PorMod(J)	Porosity modifier (dimensionless) at time Time(J)

If negative, -NfpEDZ(I) is the number coefficients in a polynomial of degree -NfpEDZ(I)-1, providing porosity modifiers as a function of time for EDZ type I; the coefficients are read in the following format:

Format(*)
(Coefficient(J), J = 0, -NfpEDZ(I)-1)

Coefficient(J)	Coefficients of polynomial

Repeat Records 5 through 8 NEDZ times for each EDZ type.

<u>Record IFC.9</u> — Start input related to FEP 1.4.3, ILW tunnel convergence

Format (I5)

NLMAFlag

NLMAFlag — Flag indicating whether FEP 1.4.3 (tunnel convergence) shall be invoked

< 0 : Do not invoke tunnel convergence, and do not read additional input regarding this FEP (i.e., go to Record IFC.13)

0 : Continue reading input, but do not invoke tunnel convergence

> 0 : Reduce porosity due to tunnel convergence

<u>Record IFC.10</u> (only if NLMAFlag > 0)

Format (I5)
NMatLMA

NMatLMA — Number of materials defining ILW backfill material subject to tunnel convergence

<u>Record IFC.11</u>

Format (A5)
(CMatLMA(J), J=1,NMatLMA)

CMatLMA(J) — NMatLMA lines containing the five-character names of the materials that are subject to tunnel convergence.

<u>Record IFC.12</u>

Format (A)
FileName

FileName — Name of file containing polynomial coefficients or look-up table of porosity modifiers. If file name is "this", continue reading on following lines in the current TOUGH2 input file.

The format of the look-up table is as follows:

Format(*)
NfpLMA

NfpLMA — If positive, NfpLMA is the number of data points in porosity-modifier look-up table for tunnel convergence; the look-up table is read in the following format:

Format(*)
(Time(J), PorMod(J), J = 1, NfpLMA)

Time(J) — Time in seconds
PorMod(J) — Porosity modifier (dimensionless) at time Time(J)

If negative, -NfpLMA is the number coefficients in a polynomial of degree -NfpLMA-1, providing porosity modifiers for tunnel convergence; the coefficients are read in the following format:

Format(*)
(Coefficient(J), J = 0, -NfpLMA-1)

Coefficient(J) — Coefficients of polynomial

PorMod(J) Porosity modifier (dimensionless) at time Time(J)

Record IFC.13 Start input related to FEP 1.4.7, uplift

Format (I5)
NUpliftFlag

NUpliftFlag Flag indicating whether FEP 1.4.7 (uplift) shall be invoked.

- < 0 : Do not invoke uplift, and do not read additional input regarding this FEP (i.e., go to Record IFC.15)
- 0 : Continue reading input, but do not invoke uplift
- 1 : Increase permeability due to uplift by providing time-dependent permeability modification factor
- 2 : Increase permeability due to uplift by providing time-dependent surface elevation to be applied in pathway dilation model

Record IFC.14 (only if NUpliftFlag > 0)

Format (A)
Filename

FileName Name of file containing polynomial coefficients or look-up table of permeability modifiers or surface elevation. Permeability change will affect all elements representing Opalinus Clay (i.e., elements with material names `OPALI` or `bOPAL`). If file name is "this", continue reading on following lines in the current TOUGH2 input file.

The format of the look-up table is as follows:

Format(*)
NfkUplift

NfkUplift If positive, NfkUplift is the number of data points in permeability-modifier (if NUpliftFlag=1) or surface elevation (if NUpliftFlag=2) look-up table for uplift; the look-up table is read in the following format:

Format(*)
(Time(J), PermMod(J), J = 1, NfkUplift)

Time(J) Time in seconds
PermMod(J) Permeability modifier (dimensionless) at time Time(J)

If negative, -NfkUplift is the number coefficients in a polynomial of degree -NfpLMA-1, providing permeability modifiers (if NUpliftFlag=1) or surface elevation (if NUpliftFlag=2) for uplift; the coefficients are read in the following format:

Format(*)
(Coefficient(J), J = 0, -NfkUplift-1)

Coefficient(J) Coefficients of polynomial

<u>Record IFC.15</u> Start input related to geochemical FEPs 1.5.2, 1.5.4, and 1.5.11, sealing effects at backfill-host rock interfaces

Format (I5)
NChemFlag

NChemFlag Flag indicating whether geochemical FEPs shall be invoked.

< 0 : Do not invoke geochemical FEPs, and do not read additional input regarding this FEP

0 : Continue reading input, but do not invoke geochemical FEPs

> 0 : Invoke geochemical FEPs

<u>Record IFC.16</u> Interface

Format (I5)
NChemFlag

NChemFlag Flag indicating whether geochemical FEPs shall be invoked.

<u>Record IFC.17</u> (only if NChemFlag > 0)

Format (I5)
NChem

NChem Number of geochemical interface types; each type (defined by one or more material names) will have its own parameter set describing geochemical sealing processes

<u>Record IFC.18</u>

Format (I5)
NMatChem(I)

NMatChem(I) Number of materials comprising geochemical interface type I

<u>Record IFC.19</u>

Format (A5,5X,A5)
(CMatChem(I,J,1),CMatChem(I,J,2),J=1,NMatChem(I))

CMatChem(I,J,1) NMatChem(I) lines containing two five-character names of the materials that define geochemical interface type I.

<u>Record IFC.20</u>

Format (*)
XClogTime(I), XLChem(I), XMChem(I), XKappaChem(I), SealThickness(I)

XClogTime(I) T_c : Clogging time under fully saturated conditions, see Eq. (13), for geochemical interface type I

XLChem(I) l : Parameter l, see Eq. (12), for geochemical interface type I

XMChem(I) m : Parameter m, see Eq. (12), for geochemical interface type I

XKappaChem(I) κ : Fraction of permeability defining minimum permeability and clogging porosity, see Eq. (15), for geochemical interface type I

SealThickness(I) d : Thickness of sealing layer (typically, 0.001 m), for geochemical interface type I

Figure 12 shows an example of the IFC block in which all look-up tables are provided directly in the TOUGH2 input file.

```
IFC  ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    A         B         C         D         E         F          FEP 1.3.19
       3.0   1.0E-21      0.25     2.5E4     2.0E6     399.5
    1                            EDZ self-sealing                       FEP  1.4.1
    2                            Number of EDZ types
    2                            Number of materials in EDZ type 1, LMA
EDZl1
EDZl2
this                             File name containing permeability modifier look-up table
    2                            Number of data points in permeability modifier look-up table
       0.0       1.0
   1.57788E11   0.01
this                             File name containing porosity modifier look-up table
    2                            Number of data points in porosity modifier look-up table
       0.0       1.0
   1.57788E11   0.10
    3                            Number of materials in EDZ type 2
EDZsf
EDZhl
EDZpi
this                             File name containing permeability modifier look-up table
    2                            Number of data points in permeability modifier look-up table
       0.0       1.0
   1.57788E10   0.01
this                             File name containing porosity modifier look-up table
    2                            Number of data points in porosity modifier look-up table
       0.0       1.0
   1.57788E10   0.10
    1                            LMA tunnel convergence                 FEP  1.4.3
    4                            Number of materials defining LMA backfill material
ETlm1
ETlm2
WAlm1
WAlm2
this                             File name containing porosity modifier look-up table
    2                            Number of data points in permeability modifier look-up table
       0.0       1.0
   1.57788E10   0.80
    1                            Uplift                                 FEP  1.4.7
this                             File name containing permeability modifier look-up table
    2                            Number of data points in permeability modifier look-up table
       0.0       1.0
   3.15576E13  100.0
    1                            Geochemical sealing       FEPs 1.5.2, 1.5.4, 1.5.11
    1                            Number of geochemical interface types
    3                            Number of material pairs for 1st interface type
ETsf      EDZsf                  Materials defining interface with geochemical sealing
ABUTM     EDZsf
LOCK      EDZsf

 3.15576E09                      Clogging time
 1.0                             Parameter l
 0.4                             Parameter m
 0.01                            Parameter kappa
 0.001                           Sealing layer thickness
```

Figure 12. Excerpt of TOUGH2 block `IFC` showing input format for geomechanical and geochemical FEPs.

5.3 IFC-PICNIC Interface

The 3D flow fields calculated by iTOUGH2-IFC will be used as input to PICNIC-TD, which calculates radionuclide transport in a network of 1D stream tubes. Fluxes at selected cross sections will be extracted from the 3D flow fields and entered into the corresponding 1D stream tubes. The interface between IFC and PICNIC is defined by a list of quadrilateral cross sections. The average of liquid flow across this cross section, as well as porosity and liquid saturation, will be calculated at each time step, and written to three output files (one each for low rate, porosity, and saturation). These files will then be passed on to PICNIC-TD. The definition of cross sections is provided in the forward (i.e., TOUGH2) input file following the line with the keyword “`PICNIC`”.

The procedure of mapping IFC results to PICNIC legs is a follows. iTOUGH2-IFC will loop through all TOUGH connections. If a connection (i.e., the line segment connecting two grid blocks) intersects the quadrilateral defining the cross section of a PICNIC (note that the quadrilateral can have any orientation in space, but should be planar), the flow rate along this connection (or, alternatively, the component of this flow rate normal to the quadrilateral PICNIC cross section) will be assigned to the corresponding PICNIC leg. Flow is considered positive if in the direction of the normal vector to the quadrilateral according to the right-hand rule. Multiple TOUGH connections can contribute to the total flow entering a PICNIC leg. The flow rate from each TOUGH connection intersecting the PICNIC leg is weighted by the relative contribution of its cross-sectional area to the cross-sectional area of the quadrilateral. It is recommended that the PICNIC leg is chosen such that the cross-sectional area of the quadrilateral and the sum of all intersecting TOUGH cross-sectional areas are identical or match closely. Porosity and liquid saturation for the PICNIC leg is calculated as the area-weighted sum of the porosities and saturations of the elements intersected by the quadrilateral.

The parameters and input format are as follows:

PICNIC Keyword introducing information on the IFC-PICNIC interface

<u>Record PICNIC.1</u>

Format (I5)
NPicnicFlag

NPicnicFlag
- 0 : Ignore IFC-PICNIC interface information
- 1 : Take total fluid flow across interface
- 2 : Only take normal component to cross section

<u>Record PICNIC.2</u>

Format (A)
FileName

FileName Name of file containing cross section definition. If file name is “this”, read on following lines in the current TOUGH2 input file.

<u>Record PICNIC.3</u> (or external file)

Format (A20)
LegName(I)

LegName(I) Name of PICNIC leg No. *I*.

Record PICNIC.4 (or external file)

Format (*)
(LegAreaVertex(I,J,K),J=1,4,K=1,3)

LegAreaVertex Four sets of X, Y, and Z coordinates, defining a planar, convex quadrilateral (e.g., a square, rectangle, parallelogram, trapezium, or any other convex quadrilateral). This quadrilateral is the cross section of PICNIC leg No. *I*. Flow is considered positive if in the direction of the normal vector to the quadrilateral according to the right-hand rule.

Repeat Records PICNIC.3 and PICNIC.4 to define a total number of NLegs quadrilaterals representing PICNIC cross sections. The PICNIC block should be closed with an empty line.

```
PICNIC --1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1                              Assign total flow to cross section
this                               Read cross sectional information from this file
Repository footprint above         Name used to identify 1. cross section/PICNIC leg
    130.00      0.00   -100.00     X, Y, and Z coordinate of 1. point of quadrilateral
    130.00    800.00   -100.00     X, Y, and Z coordinate of 2. point of quadrilateral
    930.00    800.00   -100.00     X, Y, and Z coordinate of 3. point of quadrilateral
    930.00      0.00   -100.00     X, Y, and Z coordinate of 4. point of quadrilateral
Emplacement tunnel @ CT
    509.00     22.50   -199.90
    509.00     22.50   -197.90
    511.00     22.50   -197.90
    511.00     22.50   -199.90
                                   Use empty line to close PICNIC block
```

Figure 13. Excerpt of TOUGH2 block `PICNIC` showing input format for IFC-PICNIC interface.

Figure 14 shows an excerpt of the iTOUGH2-IFC output file related to the definition of PICNIC interfaces. For each cross section (in this example, only two legs are defined), it shows the coordinates of the quadrilaterals and a list of TOUGH2 connections that intersect the cross section. The coordinates of the intersection point and the reduced areal contribution of the connection are also printed. The sum of all areal contributions is equal to the area of the quadrilateral.

Figure 15 is an excerpt of file IFC_q.dat, which contains the liquid flow rates at the specified PICNIC cross sections as a function of time. The identical format is used in files IFC_p.dat and IFC_s.dat, which contain the average porosity and saturation values, respectively. The information in these three files is transferred to PICNIC and used for radionuclide transport simulations.

```
INTERFACE TO PICNIC
+++++++++++++++++++

The full flux will be assigned to cross sections.
The following  2 cross sections are defined for exporting IFC results to PICNIC.

==========================================================================================
Leg No.   Name                Vertex No.           X           Y           Z        Area
------------------------------------------------------------------------------------------
      1   Repository footprint above    1       130.00        0.00     -100.00   640000.00
                                        2       130.00      800.00     -100.00
                                        3       930.00      800.00     -100.00
                                        4       930.00        0.00     -100.00

Number of connections intersecting cross section:        220
Connection  Connection ID  Elem 1  Elem 2   Intersected    X         Y         Z       Area
------------------------------------------------------------------------------------------
         1          20721  A24 8   A34 8    A34 8     150.00      6.25  -100.00    1268.29
         2          20774  A25 8   A35 8    A35 8     150.00     34.75  -100.00     956.10
         3          20827  A26 8   A36 8    A36 8     150.00    104.50  -100.00    4487.80
         4          20880  A27 8   A37 8    A37 8     150.00    219.50  -100.00    4487.80
         5          20933  A28 8   A38 8    A38 8     150.00    334.50  -100.00    4487.80
       ...          .....  .....   .....     .....    ......    ......  .......    .......
       219          38022  A2D27   A3D27     A3D27    910.00    760.25  -100.00    1736.59
       220          38077  A2E27   A3E27     A3E27     910.00   796.25  -100.00    1073.17


==========================================================================================
Leg No.   Name                Vertex No.           X           Y           Z        Area
------------------------------------------------------------------------------------------
      2   Emplacement tunnel @ CT       1      509.00       22.50     -199.90        4.00
                                        2      509.00       22.50     -197.90
                                        3      511.00       22.50     -197.90
                                        4      511.00       22.50     -199.90

Number of connections intersecting cross section:         30
Connection  Connection ID  Elem 1  Elem 2   Intersected    X         Y         Z       Area
------------------------------------------------------------------------------------------
         1              4  s-c 2   s52 1    s52 1     510.08     22.50  -198.32       0.13
         2              5  s-c 2   s62 1    s62 1     510.08     22.50  -198.48       0.13
         3              6  s-c 1   s72 1    s72 1     510.14     22.50  -198.48       0.13
         4              7  s-c 1   s82 1    s82 1     510.14     22.50  -198.76       0.13
         5              8  s-c 1   s92 1    s92 1     510.14     22.50  -199.04       0.13
        ..           ....  .....   .....     .....    ......    ......  .......    .......
        29           1986  s-c 2   sA2 4    sA2 4     510.58     22.50  -199.15       0.13
        30           1987  s-c 2   sB2 4    sB2 4     510.58     22.50  -199.32       0.13

No PICNIC-IFC interface errors detected.
Results on files IFC_q.dat, IFC_p.dat, and IFC_s.dat.
```

Figure 14. Excerpt of TOUGH2 output file showing information about IFC-PICNIC interface.

```
# IFC-PICNIC interface for: flow [m^3/year]
# Title: Gas release
# Date:  10-JAN-09  13:20
     Time [yr]      Repository footprint  Emplacement tunnel @
-3168777.09332        -0.2731856880E-03      0.3472797345E-05
-3168713.71714        -0.2576938298E-03      0.3522137854E-05
-3168586.96479        -0.2353636700E-03      0.3540346696E-05
-3168333.46009        -0.2102361356E-03      0.3551546349E-05
-3167826.45068        -0.1912826119E-03      0.3558121300E-05
-3166812.43187        -0.1845193430E-03      0.3561407310E-05
-3164784.39425        -0.1877533270E-03      0.3559415353E-05
-3160728.31901        -0.1946183775E-03      0.3552449094E-05
-3152616.16853        -0.2008622243E-03      0.3536692015E-05
-3136391.86757        -0.2065915057E-03      0.3516524360E-05
-3103943.26565        -0.2119470749E-03      0.3501468952E-05
-3039046.06180        -0.2155947985E-03      0.3496608039E-05
-2909251.65412        -0.2174387992E-03      0.3500075988E-05
-2649662.83875        -0.2183853751E-03      0.3507587480E-05
-2130485.20800        -0.2189805712E-03      0.3516097472E-05
-1092129.94651        -0.2193942913E-03      0.3524164802E-05
       0.00000        -0.2196887133E-03      0.3531255877E-05
       0.27500        -0.2196887133E-03      0.3533397398E-05
       0.55000        -0.2196887134E-03     -0.4784615881E-03
       1.00000        -0.2196887135E-03     -0.3210506247E-03
       1.99000        -0.2196887137E-03     -0.1575628135E-03
       3.00000        -0.2196887134E-03     -0.1148094647E-03
       3.30553        -0.2196887132E-03     -0.2560945152E-03
       3.91658        -0.2196887125E-03     -0.1513015149E-03
       4.52763        -0.2196887110E-03     -0.1374751082E-03
       5.13868        -0.2196887081E-03     -0.1232044076E-03
       5.74973        -0.2196887033E-03     -0.1169859994E-03
       6.97183        -0.2196886751E-03     -0.4377550507E-04
       8.19393        -0.2196886123E-03     -0.3799301106E-04
       9.41603        -0.2196884936E-03     -0.2900414053E-04
      10.00000        -0.2196884216E-03     -0.9631774958E-04
      ........        .................     .................
```

Figure 15. Excerpt of file IFC_q.dat, created by iTOUGH2-IFC, providing flow rates at cross section to PICNIC.

6. Testing of Code Modifications

As outlined above, iTOUGH2-IFC is based on the TOUGH2 simulator and iTOUGH2 optimization software. Both codes are well established and have been extensively verified and validated. Specifically, TOUGH2 and iTOUGH2 have been verified for use within the Yucca Mountain project. The following subsections present simulation cases that were developed to test the correct implementation of code modifications needed to address the specific requirements of the IFC.

6.1 Replicating System States to Boundary Elements

To test the correct implementation of the replication capability, a one-dimensional model was set up, simulating water displacement due to constant-pressure gas injection. The system is represented using two approaches. In the reference case (Figure 16a), water displacement is simulated in elements of equal size; in the test case (Figure 16b), the first element is replaced with a smaller element (mimicking a representative waste emplacement tunnel); its volume *V* and cross-sectional area *A* are only one-tenth of the respective values in the reference case. The dynamic system state of this representative element is then copied to a boundary element that is connected to the second element. The TOUGH2 input files for the reference and test model is shown in Figure 17. The input file for the test case (Figure 18) contains the new input block `COPY`. The system state calculated for element `A11  1` is copied after completion of each time step to the dummy boundary element `DUM  1`. The two systems are expected to yield consistent simulation results. Slight differences between the model results are anticipated, because the system state in the boundary element lags behind by one time step. As demonstrated in Figure 19, this error is insignificant, even for a highly transient simulation with fast changes in flow rates and saturations. The correct implementation of the system state replication feature into iTOUGH2-IFC is thus considered verified.

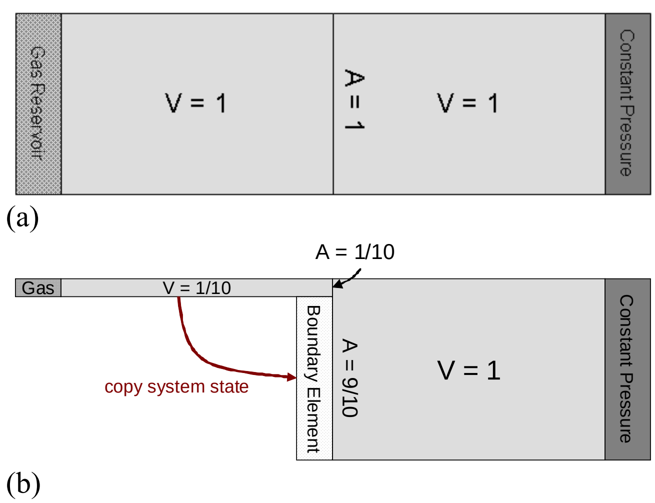

Figure 16. Set-up of test case to verify implementation of replication feature; (a) reference case; (b) test case

```
TOUGH2-IFC input file for testing replication feature; reference model
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    0     2650.     .3500 1.000E-13                          2.51      920.
bOPAL    0     2650.     .9900 1.000E-13                          2.51   100000.

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3      0.200E+00 0.050E+00
    1      0.000E+00 0.000E+00 1.000E+00
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   22500      1010000090000000400006000
 0.000E+00 6.000E+03 0.100E+00 1.000E+00
    1.0E-7
 100000.000000000000    0.00000000000000  20.000000000000000
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    2    6
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1          OPALI .1000E-03
A11 2          OPALI .1000E-03
IN             bOPAL
OUT            bOPAL

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN   A11 1                   1 .1000E-10 .5000E-02 .1000E-01
A11 1A11 2                   1 .5000E-02 .5000E-02 .1000E-01
A11 2OUT                     1 .5000E-02 .1000E-10 .1000E-01

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN
 120000.000000000000  1.0000000000000000  20.000000000000000
OUT 0
 100000.000000000000 10.5000000000000000  20.000000000000000

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 17. TOUGH2-IFC input file for testing the replication feature; reference case

```
TOUGH2-IFC input file for testing replication feature; test case (includes COPY)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    0     2650.     .3500 1.000E-13                          2.51      920.
bOPAL    0     2650.     .9900 1.000E-13                          2.51   100000.

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3      0.200E+00 0.050E+00
    1      0.000E+00 0.000E+00 1.000E+00
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   22500     100100000900000000400006000
 0.000E+00 6.000E+03 0.100E+00 1.000E+00
    1.0E-7
 100000.000000000000    0.00000000000000  20.000000000000000
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    2    6
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1          OPALI .1000E-04
A11 2          OPALI .1000E-03
IN             bOPAL
OUT            bOPAL
DUM 1          bOPAL

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN   A11 1                   1 .1000E-10 .5000E-02 .1000E-02
A11 1A11 2                   1 .5000E-02 .5000E-02 .1000E-02
A11 2OUT                     1 .5000E-02 .1000E-10 .1000E-01
DUM 1A11 2                   1 .5000E-02 .5000E-02 .9000E-02

COPY ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1     A11 1
DUM 1

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN
 120000.000000000000  1.0000000000000000  20.000000000000000
OUT
 100000.000000000000 10.5000000000000000  20.000000000000000

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 18. TOUGH2-IFC input file for testing the replication feature; test case

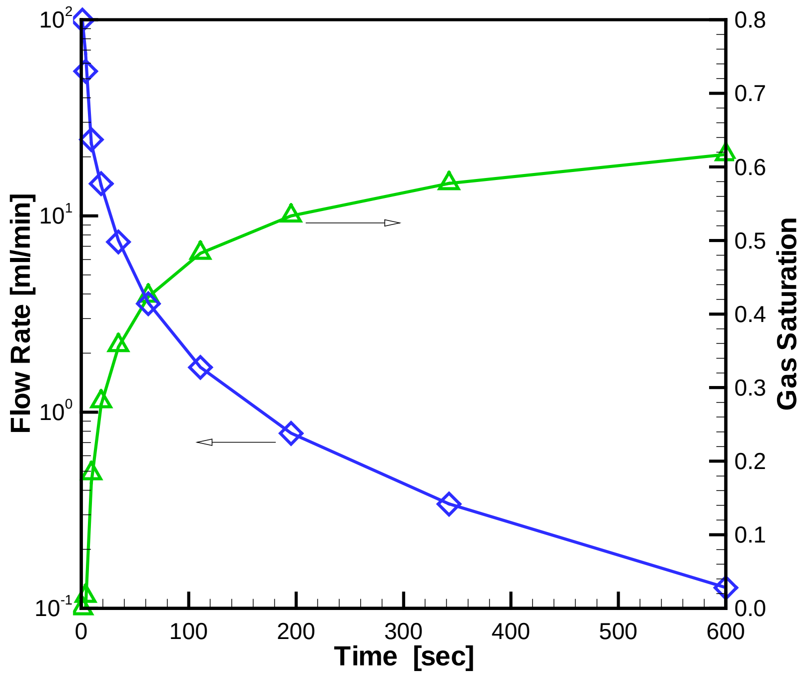

Figure 19. Comparison between reference case (symbols) and test case (lines) for verification of replication feature.

6.2 Flowpath Dilation

If gas pressure exceeds a certain depth-dependent threshold pressure, pathway dilation leads to an anisotropic increase in absolute permeability and a reduction in capillary strength (see Section 3.3.3 for details). Verification of the correct implementation of this process is done by a simple inspection of the horizontal and vertical permeabilities and the van Genuchten $1/\alpha$ parameter in a gridblock (belonging to the material type `OPALI`) that exceeds the threshold pressure due to gas injection. The values calculated by TOUGH2-IFC are compared to a simple hand calculation of the pathway dilation model described by Eqs. (1)–(5).

The TOUGH2-IFC input file is shown in Figure 20. Excerpts from the TOUGH2-IFC output file are shown in Figure 21, with relevant values highlighted in grey. Gas is injected into a single element, which is at an elevation of -200 m.a.s.l. Initial horizontal and vertical permeabilities are 1×10^{-20} m^2 and 2×10^{-21} m^2, respectively; the initial capillary-strength parameter is 18 MPa. The parameters of the pathway dilation model are given in block `IFC.2` (and reproduced in the header of the output file); they include a lithostatic pressure gradient of 0.0025 MPa/m, an empirical parameter *e* of 2 MPa, and a surface elevation of 400 m.a.s.l.

Pathway dilation is initiated in an element if gas injection leads to an excess pressure that exceeds the threshold pressure p_d, Eq. (1)). For the input parameters of the test problem, the threshold pressure is:

$$p_d = 0.0025 \cdot (400 - (-200)) - 2.0 = 13 \text{ MPa}$$

Once this threshold pressure is exceeded (which occurs at the sixth time step), hydrogeologic properties are changed according to Eqs. (2)–(5). Specifically, the pressure in the test element after six time steps is 15,571,633 Pa, which is correctly reported as 2.571633 MPa above the threshold pressure. Vertical permeability is calculated using Eq. (2):

$$k_v = 2\times10^{-21} + 1\times10^{-21}\cdot(15.571633 - 13.0)^3 = 1.90\times10^{-20}\ \text{m}^2$$

Given k_v, the horizontal permeability is calculated using Eqs. (3) and (4):

$$k_h = 1.90\times10^{-20}\cdot 5^{(2/19)^{0.25}} = 4.75\times10^{-20}\ \text{m}^2$$

Finally, the capillary-strength parameter is calculated using Eq. (5):

$$\frac{1}{\alpha} = 1.8\times10^{6}\sqrt{\frac{1\times10^{-20}}{4.75\times10^{-20}}} = 8.26\times10^{6}\ \text{Pa}$$

All these hand-calculated values are identical to those reported in the TOUGH2-IFC output file (see Figure 21). The correct implementation of the pathway dilation model into iTOUGH2-IFC is thus considered verified.

```
Test for IFC implementation of pathway dilation
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    2     2650.     .1200 1.000E-20 1.000E-20 2.000E-21               1000.

   11           0.50     0.003                         0.02
   11           1.67  18.0E+06    1.0E30
bOPAL    0     2650.     .1200 1.000E-20 1.000E-20 2.000E-21              -1000.

PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1   6       6000000900000000400003000
 0.000E+00 2.000E+03 1.000E-00
    1.0E-5
 100000.000000000000   10.50000000000000  20.000000000000000
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
s64 1          OPALI0.1125E+01                       470.25     44.75   -200.00

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
s64 1
 6000000.00000000000   0.000000000000000  20.000000000000000

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
s64 1SF  1                   0     COM2      0.001

IFC  ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    A         B         C         D         E         F         FEP 1.3.19
       3.0    1.0E-21      0.25     2.5E4     2.0E6     400.0
   -1                       EDZ self-sealing                         FEP  1.4.1
   -1                       LMA tunnel convergence                   FEP  1.4.3
   -1                       Uplift                                   FEP  1.4.7
   -1                       Geochemical sealing

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 20. TOUGH2-IFC input file for testing pathway dilation

```
       @@@@@   @@   @  @   @@@  @  @   @@       @@@  @  @   @  @  @  @      @@   @@@@@  @   @@   @   @     @@@   @  @  @   @
         @    @  @  @  @  @     @  @  @  @     @     @  @@ @@  @  @  @     @  @    @    @  @  @  @@  @     @  @  @  @  @@  @
         @    @  @  @  @  @ @@  @@@@    @       @@   @  @ @ @  @  @  @     @@@@    @    @  @  @  @ @ @     @@@   @  @  @ @ @
         @    @  @  @  @  @  @  @  @   @          @  @  @   @  @  @  @     @  @    @    @  @  @  @  @@     @ @   @  @  @  @@
         @     @@    @@    @@@  @  @  @@@@     @@@   @  @   @   @@   @@@@  @  @    @    @   @@   @   @     @  @   @@   @   @


                  TOUGH2 IS A PROGRAM FOR MULTIPHASE MULTICOMPONENT FLOW IN PERMEABLE MEDIA, INCLUDING HEAT FLOW.
         IT IS A MEMBER OF THE MULKOM FAMILY OF CODES, DEVELOPED BY KARSTEN PRUESS AT LAWRENCE BERKELEY NATIONAL LABORATORY.

                                COPYRIGHT (C) 1999, THE REGENTS OF THE UNIVERSITY OF CALIFORNIA.

                         ********************************************************************************
                         ********************  THIS TOUGH2 RUN WAS CALLED BY iTOUGH2  *******************
                         ***********  iTOUGH2 V6.3 (DECEMBER, 2008) FOR LINUX, S. FINSTERLE  ************
                         ********************      EQUATION OF STATE MODULE:  5       *******************
                         ********************    TODAY'S DATE:   10-Jan-09  10:16     *******************
                         ********************************************************************************


=====================================================================================================================================

 UNIX COMMAND LINE: /home/finster/bin/itough2 -tough2 FEP_PD IFC
 PROBLEM TITLE    :  Test for IFC implementation of pathway dilation

*************************************************************************************************************************************

 REFERENCE CONDITIONS
 --------------------

 GAS PRESSURE              = 0.101300E+06 PA
 TEMPERATURE               = 0.300000E+02 DEG-C
 SATURATED VAPOR PRESSURE  = 0.424149E+04 PA
 WATER DENSITY             = 0.995753E+03 KG/M^3
 WATER VISCOSITY           = 0.797231E-03 PA-S
 WATER COMPRESSIBILITY     = 0.445935E-09 1/PA

*************************************************************************************************************************************

...
```

```
I N T E G R A T E D   F L O W   C O D E
*****************************************

FEP 1.3.19: Pathway Dilation
============================

Pathway dilation considered in Opalinus Clay
Number of parameters specified           :    6
Vertical permeability increase:
    kv(P) = kv0              if  P < Pd
    kv(P) = kv0+B*(P-Pd)^A   if  P > Pd
       where:                A =  0.3000E+01 [-]
                             B =  0.1000E-20 [-]

Horizontal permeability increase:
    kh(P) = kv/An

Anisotropy ratio:
    An(P) = 5^[(kv0/kv(P))^C]
       where:                C =  0.2500E+00 [-]

Threshold Pressure as a function of elevation z:
    Pd(z) = D*(F-z) - E
       where:                D =  0.2500E+05 [Pa/m]
                             E =  0.2000E+07 [Pa]
                             F =  0.4000E+03 [masl]


FEP 1.4.1: EDZ Self-Sealing
===========================
EDZ self-sealing NOT considered.

FEP 1.4.3: Emplacement Tunnel Convergence
=========================================
Tunnel convergence NOT considered.

FEP 1.4.7: Uplift
=================
Uplift effects NOT considered.

FEPs 1.5.2, 1.5.4, 1.5.11: Geochemical Sealing of Interfaces
============================================================
Geochemical sealing effects NOT considered.
```

```
...
*****************************************************************************************************************************************

 s64 1(    1,2) ST = 0.10000E+01 DT = 0.10000E+01 DX1= 0.16909E+05 DX2= 0.74196E-05 T =  30.000 P =  6016909. S = 0.00000E+00
 s64 1(    2,2) ST = 0.30000E+01 DT = 0.20000E+01 DX1= 0.33819E+05 DX2= 0.14839E-04 T =  30.000 P =  6050728. S = 0.00000E+00
 s64 1(    3,2) ST = 0.70000E+01 DT = 0.40000E+01 DX1= 0.67643E+05 DX2= 0.29677E-04 T =  30.000 P =  6118370. S = 0.00000E+00
 s64 1(    4,4) ST = 0.15000E+02 DT = 0.80000E+01 DX1= 0.95829E+06 DX2= 0.10000E+02 T =  30.000 P =  7076664. S = 0.36248E-03
 s64 1(    5,4) ST = 0.31000E+02 DT = 0.16000E+02 DX1= 0.59033E+07 DX2= 0.24677E-02 T =  30.000 P = 12979961. S = 0.28302E-02
 &&& VISCO &&&   P= 0.23739E+08 IS OUTSIDE THE RANGE ( -.10000E+06, 0.20000E+08)   &&&&&&&&&&
 +++++++++   CANNOT FIND PARAMETERS AT ELEMENT *s64 1*      XX(M) =  0.23743E+08  0.10007E+02  0.20000E+02
 +++++++++ REDUCE TIME STEP AT (    6, 1) ++++++++++++++++   NEW DELT = 0.800000E+01
 %%% IFC PATHWAY DILATION: ELEMENT WITH MAXIMUM OVERPRESSURE: s64 1;  MAXIMUM OVERPRESSURE:    2.571633 [MPa]
 s64 1(    6,3) ST = 0.39000E+02 DT = 0.80000E+01 DX1= 0.25917E+07 DX2= 0.10691E-02 T =  30.000 P = 15571633. S = 0.38993E-02

 CPU-TIME SINCE LAST OUTPUT:      0.02 SEC;   TOTAL CPU-TIME:      0.02 SEC

 Test for IFC implementation of pathway dilation

          OUTPUT DATA AFTER (    6, 3)-2-TIME STEPS                                                  THE TIME IS 0.123584E-05 YEARS
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC    KON        DX1M          DX2M          DX3M          MAX. RES.      NER    KER        DELTEX
  0.39000E+02      6      3     18      2       0.25917E+07  0.10691E-02  0.00000E+00    0.43253E-06       1      2       0.80000E+01
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM.  INDEX       P       SG     XHYDL       PCAP    DG       K(H)      K(V)   1/ALPHA  POROSITY      X        Y        Z MATERIAL
                  (PA)                         (PA) (KG/M^3)  (M^2)     (M^2)       (PA)              (M)      (M)      (M)

s64 1     1  15571633.  0.0039 0.241E-03  -.668E+06 12.482 0.475E-19 0.190E-19 0.826E+07  0.1200   470.25    44.75  -200.00   OPALI
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

Figure 21. Excerpt from TOUGH2-IFC output file, showing pathway dilation input parameters and results

6.3 EDZ Self-Sealing, Tunnel Convergence, and Uplift

With time, permeability and porosity of the EDZ are reduced as a result of geomechanical self-sealing, porosity is reduced in the ILW facility as a result of tunnel convergence, and permeability of the Opalinus Clay is increased as a result of uplift (see Section 3.3.4 for details). Verification of the correct implementation of these geomechanical processes is done by a simple inspection of the calculated permeabilities and porosities as a function of time. The values calculated by TOUGH2-IFC are compared to changes prescribed in look-up tables.

Figure 22 shows the TOUGH2-IFC input file. It consists of three unconnected elements, each associated with a material type that triggers either EDZ self-sealing, tunnel convergence, or uplift.

The temporal variation of porosities and permeabilities is specified through look-up tables in the IFC block of the input file. The prescribed curves for permeability and porosity are shown as solid lines in Figure 23 and Figure 24, respectively. The symbols are the discrete values calculated by iTOUGH2-IFC for each time step taken by the simulator; they track the prescribed curves, confirming the correct implementation of these abstracted geomechanical FEPs.

As noted in Section 3.3.4, porosity at any given location does not only change due to the FEPs addressed here, but also in response to elastic deformation caused by pore-pressure changes. As a result, the porosity at any given time may not be identical to that prescribed in the look-up tables, but slightly higher or lower, depending on whether the element is, respectively, at a higher or lower pressure compared to its initial pressure. Similarly, the permeability of elements in the Opalinus Clay affected by pathway dilation are also influenced by uplift; the combined effect is calculated in iTOUGH2-IFC, i.e., the permeability in these elements may be different from those expected by uplift alone, should the dilation threshold pressure be exceeded.

Finally, porosity in fully saturated EDZ and ILW backfill elements may not be reduced at the externally prescribed rate. Porosity reduction is limited as to avoid excessive overpressures caused by the very low compressibility of water combined with the formation’s low permeability, which results in a significantly reduced consolidation rate.

```
Test for IFC implementation of mechanical FEPs
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    0     2650.     .1200 1.000E-20 1.000E-20 2.000E-21              1000.
bOPAL    0     2650.     .1200 1.000E-20 1.000E-20 2.000E-21             -1000.
EDZsf    0     2650.     .2000 1.000E-19 1.000E-19 1.000E-19              1000.
bEDZs    0     2650.     .2000 1.000E-19 1.000E-19 1.000E-19             -1000.
ETlm1    0     2650.     .2500 1.000E-15 1.000E-15 1.000E-15              1000.
ETlm2    0     2650.     .2500 1.000E-15 1.000E-15 1.000E-15              1000.

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   11           0.25      0.01                         0.02
   11           2.00  -0.1E+06    1.0E30
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1  11       1100000900000000400003000
 0.000E+00 1.100E+02 1.000E+00 1.000E+00
    1.0E-5
 100000.000000000000   10.50000000000000  20.000000000000000
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
EDZ 1          EDZsf .1000E+01                                          -200.00
LMA 1          ETlm1 .1000E+01                                          -200.00
OPA 1          OPALI .1000E+01                                          -200.00

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

IFC  ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   -1                                                                FEP 1.3.19
    1                        EDZ self-sealing                        FEP  1.4.1
    1                        Number of EDZ types
    2                        Number of materials in EDZ type
EDZsf
bEDZs
this                         File name containing permeability look-up table
    3                        Number of data points in permeability look-up table
       1.0       1.0
       5.0       0.2
      10.0       0.1
this                         File name containing porosity look-up table
    3                        Number of data points in porosity look-up table
       1.0       1.0
       5.0      0.75
      10.0      0.60
    1                        LMA tunnel convergence                  FEP  1.4.3
    2                        Number of materials defining LMA backfill material
ETlm1
ETlm2
this                         File name containing porosity look-up table
    3                        Number of data points in porosity look-up table
       1.0       1.0
       5.0       0.6
      10.0       0.5
    1                        Uplift                                  FEP  1.4.7
this                         File name containing permeability look-up table
    3                        Number of data points in permeability look-up table
       1.0       1.0
       5.0      10.0
      10.0     100.0
   -1                        Geochemical FEPs

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 22. TOUGH2-IFC input file for testing pathway dilation

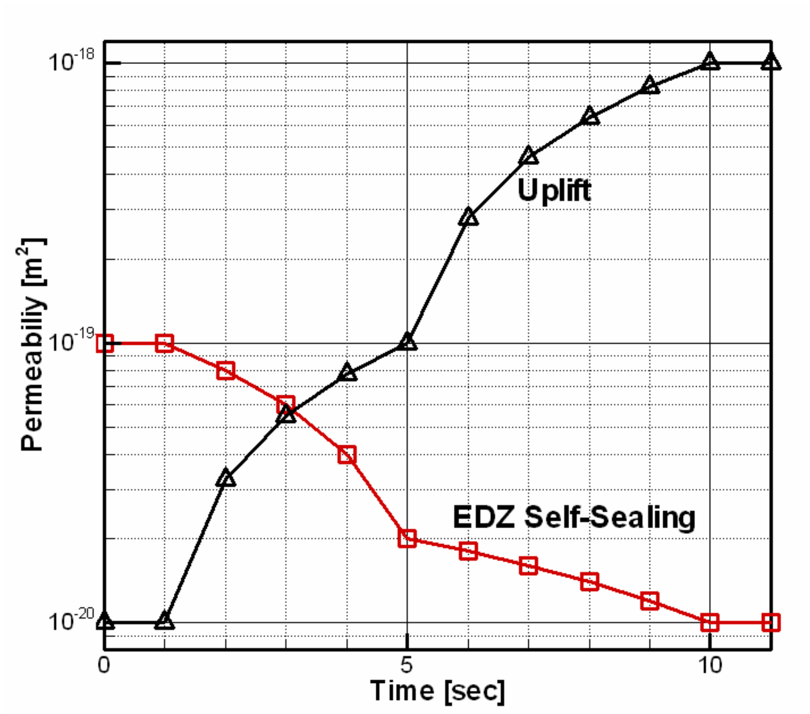

Figure 23. Comparison between prescribed (lines) and calculated (symbols) permeabilities in elements subject to EDZ self-sealing and uplift.

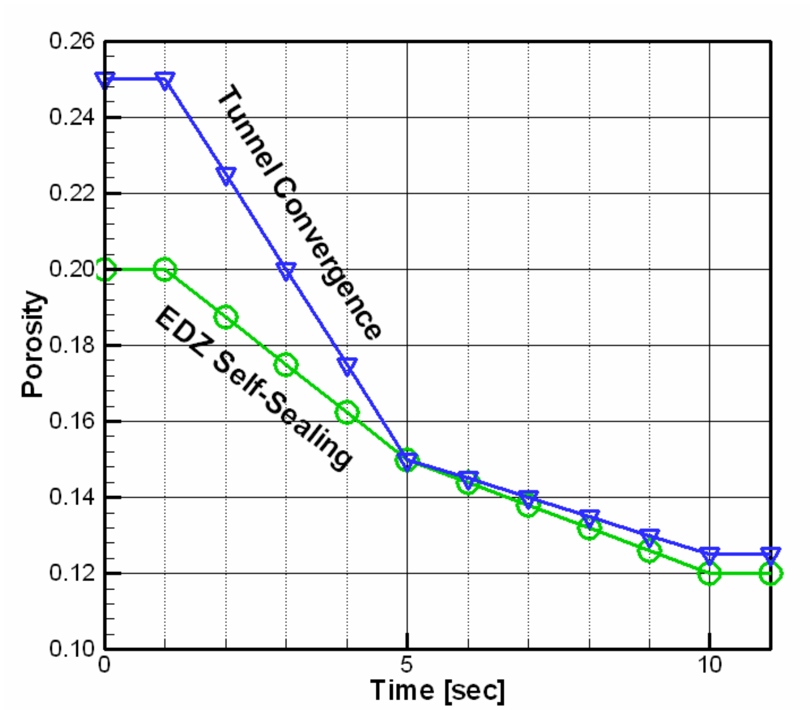

Figure 24. Comparison between prescribed (lines) and calculated (symbols) porosities in elements subject to EDZ self-sealing and tunnel convergence.

6.4 Geochemical Sealing

With time, a thin layer of mineral precipitates develops at the interface between cementitious backfill material and the host rock, leading to a reduction in the permeability perpendicular to this interface (see Section 3.3.5 for details). Verification of the correct implementation of this geochemical sealing process is done by a comparison of fluxes across in interface with a sealing layer, and the corresponding hand calculation of serial flow through a layered system.

A model of a simple test cell is developed (see Figure 25 for the corresponding TOUGH2_IFC input file). It consists of two 0.1 m long elements, one representing backfill material (element `ET    1`), the other the EDZ (element `EDZ  2`). A constant pressure gradient of 0.2 bar per 0.2 m is imposed. The IFC block indicates that the clogging time is set to 100 years, the sealing layer has a thickness of 0.01 m, and the permeability is maximally reduced to 0.1% of the undisturbed permeability (see Eq. (15)). The additional parameters (*l* and *m,* see Eq. (12)) determine the temporal evolution of the permeability reduction.

Darcy's law is used to calculate the expected flow rate Q [kg/s] in this heterogeneous system:

$$Q = A \cdot \bar{k} \cdot \frac{\rho}{\mu} \cdot \frac{\Delta P}{\Delta x} \tag{16}$$

Here, A [m^2] is the cross sectional area, $\bar{k}$ [m^2] is the effective permeability, ρ [kg m^{-3}] is water density, μ [Pa s] is dynamic viscosity, ΔP [Pa] is the imposed pressure difference, and Δx [m] is the flow distance. In the absence of geochemical sealing, the system considered consists of flow in series through two 0.1-m long layers with permeabilities of 10^{-17} and 10^{-19} m^2, respectively. The effective permeability for flow in series is calculated by the harmonic mean:

$$\bar{k}_0 = \frac{\Delta x}{\frac{b_1}{k_1} + \frac{b_2}{k_2}} = \frac{0.2}{\frac{0.1}{10^{-17}} + \frac{0.1}{10^{-19}}} = 1.98 \times 10^{-19} \text{ m}^2$$

With density and viscosity for water at 1 atm and 30°C (taken from the TOUGH2-IFC output file, see Figure 21), the flow rate is:

$$Q_0 = 1.0 \cdot 1.98 \times 10^{-19} \cdot \frac{995.75}{7.97 \times 10^{-4}} \cdot \frac{0.2 \times 10^5}{0.2} = 2.47 \times 10^{-8} \text{ kg s}^{-1}$$

Inserting a sealing layer of 0.01 m thickness and a permeability that is 0.1% of the unclogged permeability yields an effective permeability after maximum clogging of

$$\bar{k}_s = \frac{0.2}{\frac{0.19}{1.98 \times 10^{-19}} + \frac{0.01}{1.98 \times 10^{-22}}} = 3.96 \times 10^{-21} \text{ m}^2$$

and a steady-state flow rate of

$$Q_0 = 1.0 \cdot 3.96 \times 10^{-21} \cdot \frac{995.75}{7.97 \times 10^{-4}} \cdot \frac{0.2 \times 10^5}{0.2} = 4.95 \times 10^{-10} \text{ kg s}^{-1}$$

As shown in Figure 26, the flow rate calculated by TOUGH2-IFC transitions from the theoretical value for the unclogged system to that of the maximally clogged system within the specified clogging time of 100 years. The correct implementation of geochemical sealing under fully saturated conditions is thus considered verified. Recall, that the clogging time is dynamically adjusted to account for partial clogging under unsaturated conditions, yielding a smaller permeability reduction in the presence of gas.

```
Test for IFC implementation of geochemical sealing
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    0     2650.     .1200 1.000E-20 1.000E-20 2.000E-21              1000.
bOPAL    0     2650.     .1200 1.000E-20 1.000E-20 2.000E-21             -1000.
ETsf     0     2650.     .2500 1.000E-17 1.000E-17 1.000E-17              1000.
bETsf    0     2650.     .2500 1.000E-17 1.000E-17 1.000E-17             -1000.
EDZsf    0     2650.     .2000 1.000E-19 1.000E-19 1.000E-19              1000.
bEDZs    0     2650.     .2000 1.000E-19 1.000E-19 1.000E-19             -1000.

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   11           0.01      0.01                      0.02
   11           2.00  -0.1E+06    1.0E30
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2 300       110000090002000040000 3000
 0.000E+006.3115E+09 1.000E+05
    1.0E-7
 100000.000000000000    0.00000000000000  30.000000000000000
MOMOP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ET  1          ETsf 0.1000E+00                     1346.00    439.50   -196.40
EDZ 2          EDZsf0.1000E+00                     1347.00    439.50   -196.40
IN  0          bETsf0.0000E+00
OUT 3          bEDZs0.0000E+00

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN  0ET  1                  10.1000E-100.5000E-010.1000E+01
ET  1EDZ 2                  10.5000E-010.5000E-010.1000E+01
EDZ 2OUT 3                  10.5000E-010.1000E-100.1000E+01

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
IN  0
 120000.000000000000   0.000000000000000  30.000000000000000
OUT 3
 100000.000000000000   0.000000000000000  30.000000000000000

IFC  ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   -1                       Pathway dilation                          FEP 1.3.19
   -1                       EDZ self-sealing                          FEP  1.4.1
   -1                       LMA tunnel convergence                    FEP  1.4.3
   -1                       Uplift                                    FEP  1.4.7
    1                       Geochemical sealing
    1                       Number of geochemical interface types
    1                       Number of material pairs for 1st interface type
ETsf      EDZsf             Materials defining interface with geochemical
sealing
 3.15576E9                  Clogging time
 1.0                        Parameter l
 0.4                        Parameter m
 0.001                      Parameter kappa
 0.01                       Sealing layer thickness

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 25. TOUGH2-IFC input file for testing geochemical sealing

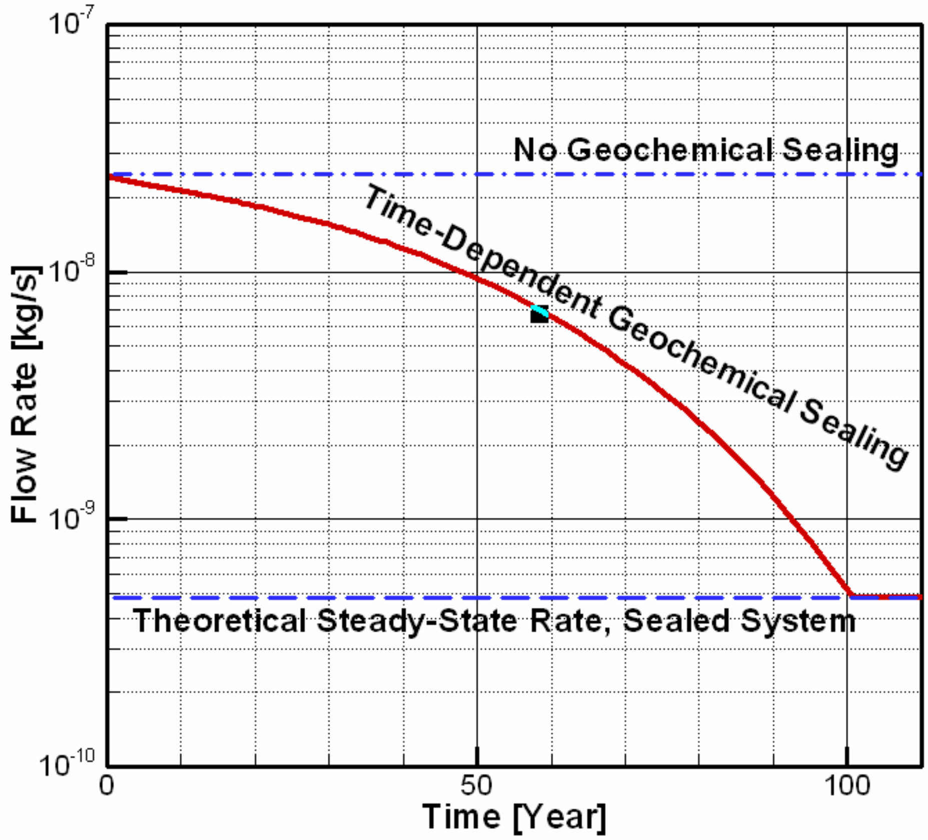

Figure 26. Flow rate through test cell with and without time-dependent geochemical sealing.

7. Test Simulation

A test simulation was performed using the iTOUGH2-IFC code and IFC model with the base-case parameter set as described in Section 4. The input file is shown in Figure A - 3. The purpose of this test run is to examine whether the simulation proceeds to the end time of 1 million years, and to get an indication of CPU time requirements. The simulation results are not discussed here.

A second simulation was conducted without inclusion of the FEPs described in Sections 3.3.3–3.3.5, i.e., without pathway dilation, EDZ self-sealing, tunnel convergence, uplift, and geochemical sealing.

The simulation was performed on a Dell laptop, Latitude D620, with an Intel© Corel™ 2 CPU T7600 @ 2.33 GHz and 2.00 GB of RAM, running under Microsoft Windows XP, Professional, Version 2002, Service Pack 3. The Fortran source code was compiled using the Intel® Visual Fortran Compiler 9.1.

The test simulation included three runs, where the first two generate the steady-state field that is used as the initial condition for the transient simulation in response to gas generation and imposed property changes (i.e., EDZ self-sealing, tunnel convergence, uplift, and geochemical alterations. The steady-state runs are not further described here.

Figure 27 shows the CPU time as a function of simulation time. Simulating the strong changes at early times with the initial expansion of the two-phase zone consumes a considerable fraction of the total CPU time. The difference in the computational demands for the simulations with and without the geomechanical and geochemical FEPs attests to the difficulties in resolving the nonlinearities and counteracting effects (specifically the early-time pressure increase due to high gas generation in the ILW facility combined with tunnel convergence, and the late-time transient effects imposed to account for uplift).

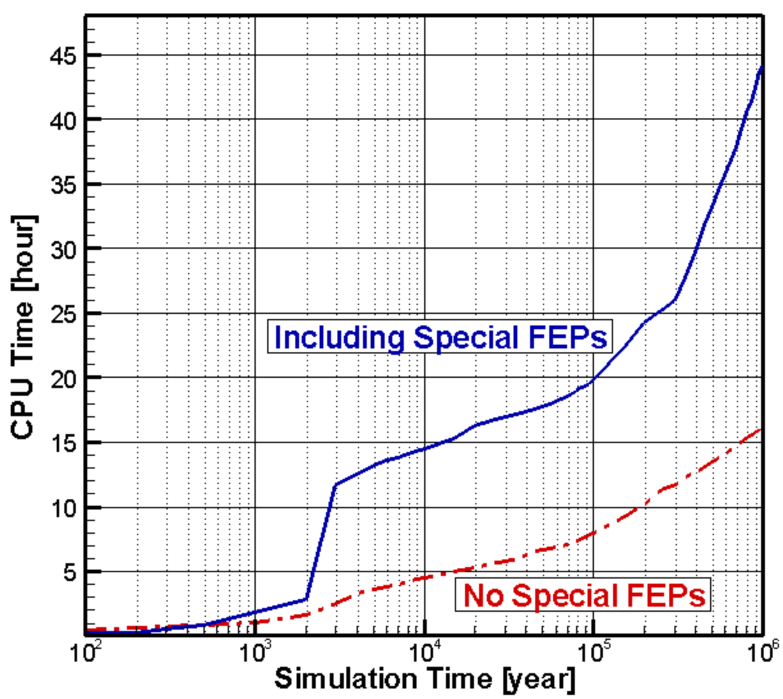

Figure 27. CPU time as a function of simulation time for a simulation with and without the inclusion of geomechanical and geochemical FEPs

Figure 28 shows an excerpt of the main iTOUGH2-IFC output file. After extensive header information, a list of element-related output variables is printed, including:

- Pressure [Pa]
- Gas saturation [m^3/m^3]
- Hydrogen mass fraction in the liquid phase [kg/kg]
- Capillary pressure [Pa]
- Gas density [kg/m^3]
- Horizontal and vertical absolute permeability [m^2]
- Capillary-strength parameter [Pa]
- Porosity [m^3/m^3]

In a second block, all connection-related output variables are printed, including:

- Total fluid mass flow rate [kg/s]
- Gas mass flow rate [kg/s]
- Liquid mass flow rate [kg/s]
- Gas phase velocity [m/s]
- Liquid phase velocity [m/s]
- Liquid relative permeability [-]
- Gas relative permeability [-]
- Permeability reduction fraction due to geochemical sealing [-]

The third block lists the specified gas generation rates, and the fourth block contains global mass and volume balances. Some information about the behavior of the geomechanical and geochemical FEPs is printed as needed.

```
1      @@@@@   @@   @  @   @@@  @  @   @@       @@@  @  @   @  @  @  @      @@   @@@@@  @  @@   @   @     @@@   @  @  @   @
         @    @  @  @  @  @     @  @  @  @     @     @  @@ @@  @  @  @     @  @    @    @ @  @  @@  @     @  @  @  @  @@  @
         @    @  @  @  @  @ @@  @@@@    @       @@   @  @ @ @  @  @  @     @@@@    @    @ @  @  @ @ @     @@@   @  @  @ @ @
         @    @  @  @  @  @  @  @  @   @          @  @  @   @  @  @  @     @  @    @    @ @  @  @  @@     @ @   @  @  @  @@
         @     @@    @@    @@@  @  @  @@@@     @@@   @  @   @   @@   @@@@  @  @    @    @  @@   @   @     @  @   @@   @   @


                    TOUGH2 IS A PROGRAM FOR MULTIPHASE MULTICOMPONENT FLOW IN PERMEABLE MEDIA, INCLUDING HEAT FLOW.
         IT IS A MEMBER OF THE MULKOM FAMILY OF CODES, DEVELOPED BY KARSTEN PRUESS AT LAWRENCE BERKELEY NATIONAL LABORATORY.

                                   COPYRIGHT (C) 1999, THE REGENTS OF THE UNIVERSITY OF CALIFORNIA.

                          ********************************************************************************
                          *********  THIS IS TOUGH2 RUN NO.    1 CALLED BY iTOUGH2 RUN NO.    1  *********
                          *************  iTOUGH2 V6.3 (DECEMBER, 2008) FOR PC, S. FINSTERLE  *************
                          ********************      EQUATION OF STATE MODULE: 55       *******************
                          ********************    TODAY'S DATE:   10-JAN-09  13:20     *******************
                          ********************************************************************************
 PROBLEM TITLE    :  Gas release

 ==================================================================================================================================
 PARAMETERS FOR FLEXIBLE DIMENSIONING OF MAJOR ARRAYS (SEE FILE maxsize.inc) ARE SUMMARIZED AT THE END.
 ==================================================================================================================================


 ====================================
           MESH IS 3-D XYZ
 ------------------------------------
 COORD.        MINIMUM        MAXIMUM
 ------------------------------------
   X      -0.25500E+05    0.12050E+05
   Y      -0.32500E+03    0.11250E+04
   Z      -0.12379E+04   -0.48400E+02
 ====================================
 ALL NCON = 111598 CONNECTIONS READ FROM FILE *MESH* REFERENCE KNOWN ELEMENTS, AND HAVE BEEN INITIALIZED TO THE DATA ARRAYS

 **********************************************************************************************************************************
 *                   EOS5: EQUATION OF STATE FOR WATER-HYDROGEN MIXTURES                                                          *
 **********************************************************************************************************************************
```

```
   OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (2,2,2,6)

                          NK  =  2   - NUMBER OF FLUID COMPONENTS
                          NEQ =  2   - NUMBER OF EQUATIONS PER GRID BLOCK
                          NPH =  2   - NUMBER OF PHASES THAT CAN BE PRESENT
                          NB  =  6   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN COMPONENT MASS FRACTIONS)


  AVAILABLE OPTIONS ARE: (NK,NEQ,NPH,NB) =                                            (2,2,2,6) - WATER AND H2

*******************************************************************************************************************************************

REFERENCE CONDITIONS
--------------------

GAS PRESSURE             = 0.101300E+06 PA
TEMPERATURE              = 0.300000E+02 DEG-C
SATURATED VAPOR PRESSURE = 0.424149E+04 PA
WATER DENSITY            = 0.995753E+03 KG/M^3
WATER VISCOSITY          = 0.797231E-03 PA-S
WATER COMPRESSIBILITY    = 0.445946E-09 1/PA

*******************************************************************************************************************************************

...

*****************************************
I N T E G R A T E D   F L O W   C O D E
*****************************************

GEOMECHANICAL FEPs
******************

FEP 1.3.19: Pathway Dilation
============================

Pathway dilation considered in Opalinus Clay
Number of parameters specified           :    6
Vertical permeability increase:
    kv(P) = kv0              if  P < Pd
    kv(P) = kv0+B*(P-Pd)^A   if  P > Pd
       where:                A =  0.3000E+01 [-]
```

```
                             B =  0.1000E-20 [-]

Horizontal permeability increase:
    kh(P) = kv/An

Anisotropy ratio:
    An(P) = 5^[(kv0/kv(P))^C]
       where:                C =  0.2500E+00 [-]

Threshold Pressure as a function of elevation z:
    Pd(z) = D*(F-z) - E
       where:                D =  0.2500E+05 [Pa/m]
                             E =  0.2000E+07 [Pa]
                             F =  0.3995E+03 [masl]


FEP 1.4.1: EDZ Self-Sealing
===========================

Number of EDZ types            :      2

EDZ type No.  1                :  EDZl1  EDZl2

Look-up table with permeability modification factors for EDZ type No.  1:   4 data points

   #             Time [sec]  Permeability Modifier
-----------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.157788E+12           0.100000E-01
   4           0.100000E+51           0.100000E-01

Look-up table with porosity modification factors for EDZ type No.  1:       4 data points

   #             Time [sec]      Porosity Modifier
-----------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.157788E+12           0.100000E+00
   4           0.100000E+51           0.100000E+00
```

```
EDZ type No.  2                :  EDZsf  EDZpi  EDZco  EDZop  EDZac  EDZvt  EDZce  EDZkt  EDZdt  EDZsh  EDZse  bEDZs  bEDZp

Look-up table with permeability modification factors for EDZ type No.  2:   4 data points

   #             Time [sec]  Permeability Modifier
--------------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.157788E+11           0.100000E-01
   4           0.100000E+51           0.100000E-01

Look-up table with porosity modification factors for EDZ type No.  2:       4 data points

   #             Time [sec]      Porosity Modifier
--------------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.157788E+11           0.100000E+00
   4           0.100000E+51           0.100000E+00


FEP 1.4.3: Emplacement Tunnel Convergence
=========================================

Materials affected :  ETlm1  ETlm2  WAlm1  WAlm2

Look-up table with porosity modification factors:   4 data points

   #             Time [sec]      Porosity Modifier
--------------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.157788E+11           0.800000E+00
   4           0.100000E+51           0.800000E+00
```

```
FEP 1.4.7: Uplift
=================


Look-up table with permeability modification factors:   4 data points

   #             Time [sec]  Permeability Modifier
--------------------------------------------------
   1          -0.100000E+51           0.100000E+01
   2           0.000000E+00           0.100000E+01
   3           0.315576E+14           0.100000E+03
   4           0.100000E+51           0.100000E+03

GEOCHEMICAL FEPs
++++++++++++++++

FEPs 1.5.2, 1.5.4, 1.5.11: Geochemical Sealing of Interfaces
============================================================

Geochemical sealing considered at  2 types of interfaces

Interface type No.  1                     :  ETsf   EDZsf
                                             ABUTM  EDZsf
                                             LOCK   EDZsf
                                             ETpil  EDZpi
                                             ABUTM  EDZpi
                                             LOCK   EDZpi
                                             SEAL   EDZse
                                             SEALa  EDZse
                                             ETlm1  EDZl1
                                             ETlm2  EDZl2
                                             Tconn  EDZvt
                                             Tcons  EDZco
                                             Toper  EDZop
                                             Tcent  EDZce
                                             Tacce  EDZac
                                             TacCO  EDZac
                                             Tcont  EDZkt
                                             Tdeto  EDZdt
                                             Tshaf  EDZsh
```

```
Clogging time                              :  0.1000000E+03 [y]
Minimum porosity function parameter l      :  0.1000000E+01 [-]
Minimum porosity function parameter m      :  0.4000000E+00 [-]
Minimum clogging permeability fraction     :  0.1000000E-01 [-]
Thickness of sealing layer                 :  0.1000000E-02 [m]

==================================================================================================================================
Interface type No.  2                      :  ETlm1  SEAL
                                              ETlm2  SEAL

Clogging time                              :  0.2000000E+03 [y]
Minimum porosity function parameter l      :  0.1000000E+01 [-]
Minimum porosity function parameter m      :  0.4500000E+00 [-]
Minimum clogging permeability fraction     :  0.1000000E-01 [-]
Thickness of sealing layer                 :  0.1000000E-02 [m]

==================================================================================================================================


INTERFACE TO PICNIC
+++++++++++++++++++

The full flux will be assigned to cross sections.
The following  2 cross sections are defined for exporting IFC results to PICNIC.


=================================================================================================================
Leg No.   Name                                     Vertex No.              X            Y            Z         Area
-----------------------------------------------------------------------------------------------------------------
      1   Repository footprint above         Name            1        130.00         0.00      -100.00    640000.00
                                                             2        130.00       800.00      -100.00
                                                             3        930.00       800.00      -100.00
                                                             4        930.00         0.00      -100.00

Number of connections intersecting cross section:          220
Connection  Connection ID  Element 1  Element 2   Intersected              X            Y            Z         Area
-----------------------------------------------------------------------------------------------------------------
         1          20759  A24 8      A34 8             A34 8         150.00         6.25      -100.00      1268.29
         2          20812  A25 8      A35 8             A35 8         150.00        34.75      -100.00       956.10
         3          20865  A26 8      A36 8             A36 8         150.00       104.50      -100.00      4487.80
         4          20918  A27 8      A37 8             A37 8         150.00       219.50      -100.00      4487.80
```

```
...
      215          37840  A2927      A3927              A3927          910.00      392.50     -100.00       39.02
      216          37895  A2A27      A3A27              A3A27          910.00      450.50     -100.00     4487.80
      217          37950  A2B27      A3B27              A3B27          910.00      565.50     -100.00     4487.80
      218          38005  A2C27      A3C27              A3C27          910.00      680.50     -100.00     4487.80
      219          38060  A2D27      A3D27              A3D27          910.00      760.25     -100.00     1736.59
      220          38115  A2E27      A3E27              A3E27          910.00      796.25     -100.00     1073.17


 =================================================================================================================
 Leg No.   Name                                     Vertex No.              X           Y           Z        Area
 -----------------------------------------------------------------------------------------------------------------
       2   Emplacement tunnel @ CT                           1         509.00       22.50     -199.90        4.00
                                                             2         509.00       22.50     -197.90
                                                             3         511.00       22.50     -197.90
                                                             4         511.00       22.50     -199.90

 Number of connections intersecting cross section:          16
 Connection  Connection ID  Element 1  Element 2   Intersected              X           Y           Z        Area
 -----------------------------------------------------------------------------------------------------------------
          1              4  s-c 2      s52 1              s52 1        510.92       22.50     -198.71        0.25
          2              5  s-c 2      s62 1              s62 1        510.92       22.50     -198.76        0.25
          3              6  s-c 1      s72 1              s72 1        510.47       22.50     -198.82        0.25
          4              7  s-c 1      s82 1              s82 1        510.47       22.50     -198.87        0.25
          5              8  s-c 1      s92 1              s92 1        510.47       22.50     -198.93        0.25
          6              9  s-c 1      sA2 1              sA2 1        510.47       22.50     -198.98        0.25
          7             10  s-c 2      sB2 1              sB2 1        510.92       22.50     -199.04        0.25
          8             11  s-c 2      sC2 1              sC2 1        510.92       22.50     -199.09        0.25
          9            663  s-c 2      s52 2              s52 2        510.97       22.50     -198.71        0.25
         10            664  s-c 2      s62 2              s62 2        510.97       22.50     -198.76        0.25
         11            665  s-c 1      s72 2              s72 2        510.53       22.50     -198.82        0.25
         12            666  s-c 1      s82 2              s82 2        510.53       22.50     -198.87        0.25
         13            667  s-c 1      s92 2              s92 2        510.53       22.50     -198.93        0.25
         14            668  s-c 1      sA2 2              sA2 2        510.53       22.50     -198.98        0.25
         15            669  s-c 2      sB2 2              sB2 2        510.97       22.50     -199.04        0.25
         16            670  s-c 2      sC2 2              sC2 2        510.97       22.50     -199.09        0.25

 No PICNIC-IFC interface errors detected.
 Results on files IFC_q.dat, IFC_p.dat, and IFC_s.dat.
```

```
     PRIMARY VARIABLES FROM   33 ELEMENTS WILL BE COPIED
     ===================================================

    1: PARENT ELEMENT: s-o 1         NUMBER OF DAUGHTER ELEMENTS:    1
       S-o 1

    2: PARENT ELEMENT: s-o 2         NUMBER OF DAUGHTER ELEMENTS:    1
       S-o 2

    3: PARENT ELEMENT: s-o 3         NUMBER OF DAUGHTER ELEMENTS:    1
       S-o 3
...

   29: PARENT ELEMENT: p-g71         NUMBER OF DAUGHTER ELEMENTS:    1
       P-g71

   30: PARENT ELEMENT: p-g80         NUMBER OF DAUGHTER ELEMENTS:    1
       P-g80

   31: PARENT ELEMENT: p-g81         NUMBER OF DAUGHTER ELEMENTS:    1
       P-g81

   32: PARENT ELEMENT: p-g90         NUMBER OF DAUGHTER ELEMENTS:    1
       P-g90

   33: PARENT ELEMENT: p-g91         NUMBER OF DAUGHTER ELEMENTS:    1
       P-g91

     *****************************************************************************************************************

     END OF INPUT DATA

     *****************************************************************************************************************
     *****************************************************************************************************************

 END OF TOUGH2 INPUT JOB --- ELAPSED TIME =     2.094 SECONDS

 *****************************************************************************************************************************
```

```
TOUGH2 Simulation No.    1.

...ITERATING...  AT [    1, 1] --- DELTEX = 0.100000E+10   MAX. RES. = 0.493818E+01  AT ELEMENT AI9 3  EQUATION   1
FILE *INDEX* EXISTS --- OPEN AS AN OLD FILE
L88 6(    1,2) ST = -.31688E+07 DT = 0.10000E+10 DX1= 0.17890E+04 DX2= 0.00000E+00 T =  30.000 P =  5963853. S = 0.00000E+00
...ITERATING...  AT [    2, 1] --- DELTEX = 0.200000E+10   MAX. RES. = 0.266816E-03  AT ELEMENT A2943  EQUATION   1
I43 7(    2,2) ST = -.31687E+07 DT = 0.20000E+10 DX1= 0.69628E+02 DX2= 0.00000E+00 T =  30.000 P =  5922662. S = 0.00000E+00
...ITERATING...  AT [    3, 1] --- DELTEX = 0.400000E+10   MAX. RES. = 0.266404E-03  AT ELEMENT I43 7  EQUATION   1
L68 6(    3,2) ST = -.31686E+07 DT = 0.40000E+10 DX1= 0.27533E+03 DX2= 0.00000E+00 T =  30.000 P =  5944946. S = 0.00000E+00
...ITERATING...  AT [    4, 1] --- DELTEX = 0.800000E+10   MAX. RES. = 0.725289E-03  AT ELEMENT L68 6  EQUATION   1
L86 6(    4,2) ST = -.31683E+07 DT = 0.80000E+10 DX1= 0.22728E+03 DX2= 0.00000E+00 T =  30.000 P =  5964758. S = 0.00000E+00
...ITERATING...  AT [    5, 1] --- DELTEX = 0.160000E+11   MAX. RES. = 0.201938E-03  AT ELEMENT o6220  EQUATION   1
...ITERATING...  AT [    5, 2] --- DELTEX = 0.160000E+11   MAX. RES. = 0.168128E-02  AT ELEMENT L64 6  EQUATION   1
I43 5(    5,3) ST = -.31678E+07 DT = 0.16000E+11 DX1= -.19556E+02 DX2= 0.00000E+00 T =  30.000 P =  5922673. S = 0.00000E+00
...ITERATING...  AT [    6, 1] --- DELTEX = 0.320000E+11   MAX. RES. = 0.186749E-03  AT ELEMENT o6220  EQUATION   1
L64 6(    6,2) ST = -.31668E+07 DT = 0.32000E+11 DX1= 0.14937E+01 DX2= 0.00000E+00 T =  30.000 P =  5945344. S = 0.00000E+00
...ITERATING...  AT [    7, 1] --- DELTEX = 0.640000E+11   MAX. RES. = 0.812378E-03  AT ELEMENT L64 6  EQUATION   1
L88 6(    7,2) ST = -.31648E+07 DT = 0.64000E+11 DX1= -.50906E+03 DX2= 0.00000E+00 T =  30.000 P =  5964425. S = 0.00000E+00
...ITERATING...  AT [    8, 1] --- DELTEX = 0.128000E+12   MAX. RES. = 0.163415E-02  AT ELEMENT L88 6  EQUATION   1
...ITERATING...  AT [    8, 2] --- DELTEX = 0.128000E+12   MAX. RES. = 0.566729E-02  AT ELEMENT L88 6  EQUATION   1
Ta 29(    8,3) ST = -.31607E+07 DT = 0.12800E+12 DX1= -.22680E+03 DX2= 0.00000E+00 T =  30.000 P =  4862581. S = 0.00000E+00
...ITERATING...  AT [    9, 1] --- DELTEX = 0.256000E+12   MAX. RES. = 0.170373E-02  AT ELEMENT o6232  EQUATION   1
...ITERATING...  AT [    9, 2] --- DELTEX = 0.256000E+12   MAX. RES. = 0.268438E-01  AT ELEMENT L77 6  EQUATION   1
L78 6(    9,3) ST = -.31526E+07 DT = 0.25600E+12 DX1= -.36184E+04 DX2= 0.00000E+00 T =  30.000 P =  5949308. S = 0.00000E+00
...ITERATING...  AT [   10, 1] --- DELTEX = 0.512000E+12   MAX. RES. = 0.784867E-02  AT ELEMENT o6232  EQUATION   1
...ITERATING...  AT [   10, 2] --- DELTEX = 0.512000E+12   MAX. RES. = 0.899062E-01  AT ELEMENT L78 6  EQUATION   1
L75 6(   10,3) ST = -.31364E+07 DT = 0.51200E+12 DX1= -.50791E+04 DX2= 0.00000E+00 T =  30.000 P =  5944225. S = 0.00000E+00
...ITERATING...  AT [   11, 1] --- DELTEX = 0.102400E+13   MAX. RES. = 0.279109E-01  AT ELEMENT o6232  EQUATION   1
...ITERATING...  AT [   11, 2] --- DELTEX = 0.102400E+13   MAX. RES. = 0.181113E+02  AT ELEMENT Ta 24  EQUATION   1
...ITERATING...  AT [   11, 3] --- DELTEX = 0.102400E+13   MAX. RES. = 0.804119E-02  AT ELEMENT Ta 24  EQUATION   1
L75 6(   11,4) ST = -.31039E+07 DT = 0.10240E+13 DX1= -.45163E+04 DX2= 0.00000E+00 T =  30.000 P =  5939709. S = 0.00000E+00
...ITERATING...  AT [   12, 1] --- DELTEX = 0.204800E+13   MAX. RES. = 0.771945E-01  AT ELEMENT o6232  EQUATION   1
...ITERATING...  AT [   12, 2] --- DELTEX = 0.204800E+13   MAX. RES. = 0.142500E+00  AT ELEMENT L85 6  EQUATION   1
L86 6(   12,3) ST = -.30390E+07 DT = 0.20480E+13 DX1= -.24413E+04 DX2= 0.00000E+00 T =  30.000 P =  5947063. S = 0.00000E+00
...ITERATING...  AT [   13, 1] --- DELTEX = 0.409600E+13   MAX. RES. = 0.174657E+00  AT ELEMENT o6232  EQUATION   1
...ITERATING...  AT [   13, 2] --- DELTEX = 0.409600E+13   MAX. RES. = 0.521680E-01  AT ELEMENT L88 6  EQUATION   1
L88 6(   13,3) ST = -.29093E+07 DT = 0.40960E+13 DX1= -.80206E+03 DX2= 0.00000E+00 T =  30.000 P =  5946264. S = 0.00000E+00
...ITERATING...  AT [   14, 1] --- DELTEX = 0.819200E+13   MAX. RES. = 0.345822E+00  AT ELEMENT o6227  EQUATION   1
...ITERATING...  AT [   14, 2] --- DELTEX = 0.819200E+13   MAX. RES. = 0.257881E-01  AT ELEMENT L68 6  EQUATION   1
L85 6(   14,3) ST = -.26497E+07 DT = 0.81920E+13 DX1= -.19162E+03 DX2= 0.00000E+00 T =  30.000 P =  5946068. S = 0.00000E+00
...ITERATING...  AT [   15, 1] --- DELTEX = 0.163840E+14   MAX. RES. = 0.634933E+00  AT ELEMENT o6227  EQUATION   1
```

```
 ...ITERATING...  AT [   15, 2] --- DELTEX = 0.163840E+14   MAX. RES. = 0.310771E-01  AT ELEMENT L77 6  EQUATION   1
 L74 6(   15,3) ST = -.21305E+07 DT = 0.16384E+14 DX1= -.59509E+02 DX2= 0.00000E+00 T =  30.000 P =  5936214. S = 0.00000E+00
 ...ITERATING...  AT [   16, 1] --- DELTEX = 0.327680E+14   MAX. RES. = 0.112020E+01  AT ELEMENT o6227  EQUATION   1
 ...ITERATING...  AT [   16, 2] --- DELTEX = 0.327680E+14   MAX. RES. = 0.351028E-01  AT ELEMENT Ta 29  EQUATION   1
 L74 6(   16,3) ST = -.10921E+07 DT = 0.32768E+14 DX1= -.31476E+02 DX2= 0.00000E+00 T =  30.000 P =  5936183. S = 0.00000E+00
 ...ITERATING...  AT [   17, 1] --- DELTEX = 0.344650E+14   MAX. RES. = 0.101778E+01  AT ELEMENT o6227  EQUATION   1
 ...ITERATING...  AT [   17, 2] --- DELTEX = 0.344650E+14   MAX. RES. = 0.499292E+01  AT ELEMENT Ta 24  EQUATION   1
 Ta 29(   17,3) ST = 0.00000E+00 DT = 0.34465E+14 DX1= -.16520E+01 DX2= 0.00000E+00 T =  30.000 P =  4862058. S = 0.00000E+00

 CPU-TIME SINCE LAST OUTPUT:    297.61 SEC;   TOTAL CPU-TIME:    297.61 SEC

 Gas release

          OUTPUT DATA AFTER (   17, 3)-2-TIME STEPS                                                      THE TIME IS 0.000000E+00 YEARS
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC    ITER  ITERC    KON        DX1M          DX2M          DX3M          MAX. RES.      NER    KER        DELTEX
  0.00000E+00     17       3     46      2       0.87967E+03  0.00000E+00  0.00000E+00    0.20300E-03    ****     1       0.34465E+14
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM.  INDEX       P        SG      XHYDL       PCAP    DG       K(H)      K(V)   1/ALPHA  POROSITY     X         Y         Z  MATERIAL
                  (PA)                           (PA) (KG/M^3)  (M^2)     (M^2)      (PA)               (M)       (M)       (M)

s22 1     1   5899219.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -189.90    OPALI
s32 1     2   5912995.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -194.40    OPALI
s42 1     3   5911093.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -196.40    OPALI
s52 1     4   5909818.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-18 0.100E-18 0.300E+07  0.2200  510.25    26.50  -197.15    EDZsf
s62 1     5   5914346.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-18 0.100E-18 0.300E+07  0.2200  510.25    26.50  -197.65    EDZsf
s72 1     6   5918985.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-15 0.100E-15 0.100E+06  0.4000  510.25    26.50  -198.15    ABUTM
s82 1     7   5923872.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-15 0.100E-15 0.100E+06  0.4000  510.25    26.50  -198.65    ABUTM
s92 1     8   5928758.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-15 0.100E-15 0.100E+06  0.4000  510.25    26.50  -199.15    ABUTM
sA2 1     9   5933644.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-15 0.100E-15 0.100E+06  0.4000  510.25    26.50  -199.65    ABUTM
sB2 1    10   5938255.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-18 0.100E-18 0.300E+07  0.2200  510.25    26.50  -200.15    EDZsf
sC2 1    11   5942735.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-18 0.100E-18 0.300E+07  0.2200  510.25    26.50  -200.65    EDZsf
sD2 1    12   5939792.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -201.40    OPALI
sE2 1    13   5934863.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -203.40    OPALI
sF2 1    14   5944666.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    26.50  -207.90    OPALI
s23 1    15   5875503.  0.0000 0.000E+00  0.000E+00  0.000 0.100E-19 0.200E-20 0.180E+08  0.1200  510.25    36.50  -189.90    OPALI
...

0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
 1         Gas release
```

```
                                                                                                    KCYC =    17  -  ITER =    3  -  TIME = 0.00000E+00
 ELEM1  ELEM2  INDEX        FLOF     FLO(GAS)    FLO(LIQ.)      V(GAS)    V(LIQ.)   KRL_1   KRL_2   KRG_1   KRG_2 SEALING
                          (KG/S)       (KG/S)       (KG/S)       (M/S)      (M/S)

 s-c 3  s22 1     1 -0.2000E-09  0.0000E+00 -0.2000E-09  0.000E+00 -0.557E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 3  s32 1     2 -0.4249E-10  0.0000E+00 -0.4249E-10  0.000E+00 -0.236E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 3  s42 1     3 -0.1681E-10  0.0000E+00 -0.1681E-10  0.000E+00 -0.281E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 2  s52 1     4 -0.1166E-09  0.0000E+00 -0.1166E-09  0.000E+00 -0.212E-11 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 2  s62 1     5 -0.8511E-10  0.0000E+00 -0.8511E-10  0.000E+00 -0.155E-11 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 1  s72 1     6 -0.4277E-08  0.0000E+00 -0.4277E-08  0.000E+00 -0.428E-10 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 1  s82 1     7 -0.1444E-08  0.0000E+00 -0.1444E-08  0.000E+00 -0.145E-10 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 1  s92 1     8  0.1389E-08  0.0000E+00  0.1389E-08  0.000E+00  0.139E-10 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 1  sA2 1     9  0.4222E-08  0.0000E+00  0.4222E-08  0.000E+00  0.423E-10 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 2  sB2 1    10  0.8123E-10  0.0000E+00  0.8123E-10  0.000E+00  0.148E-11 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 2  sC2 1    11  0.1124E-09  0.0000E+00  0.1124E-09  0.000E+00  0.205E-11 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 3  sD2 1    12  0.2312E-10  0.0000E+00  0.2312E-10  0.000E+00  0.386E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 3  sE2 1    13  0.4879E-10  0.0000E+00  0.4879E-10  0.000E+00  0.272E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-c 3  sF2 1    14  0.1794E-09  0.0000E+00  0.1794E-09  0.000E+00  0.499E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s-g11  s22 1    15  0.6287E-10  0.0000E+00  0.6287E-10  0.000E+00  0.131E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s22 1  s22 2    16  0.1653E-11  0.0000E+00  0.1653E-11  0.000E+00  0.287E-15 1.00000 1.00000 0.00000 0.00000 1.00000
 s22 1  s23 1    17 -0.7143E-10  0.0000E+00 -0.7143E-10  0.000E+00 -0.199E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s22 1  s32 1    18 -0.6734E-10  0.0000E+00 -0.6734E-10  0.000E+00 -0.141E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s32 1  s32 2    19  0.1642E-10  0.0000E+00  0.1642E-10  0.000E+00  0.571E-14 1.00000 1.00000 0.00000 0.00000 1.00000
 s32 1  s33 1    20 -0.1871E-10  0.0000E+00 -0.1871E-10  0.000E+00 -0.104E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s32 1  s42 1    21 -0.1075E-09  0.0000E+00 -0.1075E-09  0.000E+00 -0.224E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s42 1  s42 2    22  0.4838E-10  0.0000E+00  0.4838E-10  0.000E+00  0.505E-13 1.00000 1.00000 0.00000 0.00000 1.00000
 s42 1  s43 1    23 -0.1877E-11  0.0000E+00 -0.1877E-11  0.000E+00 -0.313E-13 1.00000 1.00000 0.00000 0.00000 1.00000
 s42 1  s52 1    24 -0.1709E-09  0.0000E+00 -0.1709E-09  0.000E+00 -0.357E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s52 1  s52 2    25  0.7751E-10  0.0000E+00  0.7751E-10  0.000E+00  0.882E-13 1.00000 1.00000 0.00000 0.00000 1.00000
 s52 1  s53 1    26  0.2080E-12  0.0000E+00  0.2080E-12  0.000E+00  0.208E-14 1.00000 1.00000 0.00000 0.00000 1.00000
 s52 1  s62 1    27 -0.3652E-09  0.0000E+00 -0.3652E-09  0.000E+00 -0.416E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s62 1  s62 2    28  0.5427E-10  0.0000E+00  0.5427E-10  0.000E+00  0.618E-13 1.00000 1.00000 0.00000 0.00000 1.00000
 s62 1  s63 1    29  0.3331E-12  0.0000E+00  0.3331E-12  0.000E+00  0.334E-14 1.00000 1.00000 0.00000 0.00000 1.00000
 s62 1  s72 1    30 -0.5049E-09  0.0000E+00 -0.5049E-09  0.000E+00 -0.575E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s72 1  s72 2    31  0.1687E-09  0.0000E+00  0.1687E-09  0.000E+00  0.106E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s72 1  s73 1    32  0.1215E-10  0.0000E+00  0.1215E-10  0.000E+00  0.122E-12 1.00000 1.00000 0.00000 0.00000 1.00000
 s72 1  s82 1    33 -0.4963E-08  0.0000E+00 -0.4963E-08  0.000E+00 -0.311E-11 1.00000 1.00000 0.00000 0.00000 1.00000
 s82 1  s82 2    34  0.4081E-10  0.0000E+00  0.4081E-10  0.000E+00  0.256E-13 1.00000 1.00000 0.00000 0.00000 1.00000
...
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

1         Gas release
```

```
                                                                                          KCYC =    17  -  ITER =    3  -  TIME = 0.00000E+00
 ELEMENT SOURCE INDEX      GENERATION RATE     ENTHALPY    FF(GAS)      FF(LIQ.)      P(WB)
                             (KG/S) OR (W)     (J/KG)                                 (PA)

  s85 1   SF 11    1           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
  s95 1   SF 12    2           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
  s86 1   SF 21    3           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
  s96 1   SF 22    4           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
  s87 1   SF 31    5           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
  s97 1   SF 32    6           0.00000E+00    0.00000E+00  0.00000E+00  0.00000E+00
...
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

1********** VOLUME- AND MASS-BALANCES ********************************************************************************************

 ********** [KCYC,ITER] = [  17,  3] *****                                  THE TIME IS  0.00000E+00 SECONDS, OR  0.00000E+00 YEARS


 PHASE VOLUMES IN PLACE
 GAS  0.00000E+00 M**3;   LIQUID  0.32884E+09 M**3

 MASS IN PLACE
 GAS  0.00000E+00 KG;     LIQUID  0.32833E+12 KG;    HYD  0.00000E+00 KG;    VAPOR  0.00000E+00 KG;   LIQUID WATER  0.32833E+12 KG

 *********************************************************************************************************************************
...
 ...ITERATING...  AT [   18, 1] --- DELTEX = 0.315576E+08   MAX. RES. = 0.516052E-02  AT ELEMENT LA7 6  EQUATION   2
 ...ITERATING...  AT [   18, 2] --- DELTEX = 0.315576E+08   MAX. RES. = 0.250732E-01  AT ELEMENT I52 7  EQUATION   2
 ...ITERATING...  AT [   18, 3] --- DELTEX = 0.315576E+08   MAX. RES. = 0.806883E+01  AT ELEMENT L68 6  EQUATION   1
 ...ITERATING...  AT [   18, 4] --- DELTEX = 0.315576E+08   MAX. RES. = 0.502717E+01  AT ELEMENT I42 6  EQUATION   1
 ...ITERATING...  AT [   18, 5] --- DELTEX = 0.315576E+08   MAX. RES. = 0.165418E+00  AT ELEMENT L68 6  EQUATION   1
 ...ITERATING...  AT [   18, 6] --- DELTEX = 0.315576E+08   MAX. RES. = 0.717273E-02  AT ELEMENT L68 6  EQUATION   1
 ...ITERATING...  AT [   18, 7] --- DELTEX = 0.315576E+08   MAX. RES. = 0.581024E-02  AT ELEMENT s85 1  EQUATION   1
 +++++++++ REDUCE TIME STEP AT (   18, 7) ++++++++++++++++   NEW DELT = 0.788940E+07
 ...ITERATING...  AT [   18, 1] --- DELTEX = 0.867834E+07   MAX. RES. = 0.141914E-02  AT ELEMENT LA6 6  EQUATION   2
 ...ITERATING...  AT [   18, 2] --- DELTEX = 0.867834E+07   MAX. RES. = 0.335762E-02  AT ELEMENT I52 7  EQUATION   2
 ...ITERATING...  AT [   18, 3] --- DELTEX = 0.867834E+07   MAX. RES. = 0.173394E+01  AT ELEMENT I42 6  EQUATION   1
 ...ITERATING...  AT [   18, 4] --- DELTEX = 0.867834E+07   MAX. RES. = 0.350461E+00  AT ELEMENT L66 6  EQUATION   1
 ...ITERATING...  AT [   18, 5] --- DELTEX = 0.867834E+07   MAX. RES. = 0.289302E-01  AT ELEMENT L66 6  EQUATION   1
 %%% IFC GEOCHEMICAL SEALING: STRONGEST SEALING (0.6694) AT CONNECTION NO.    73 (s63 1  s73 1)
 L64 6(   18,6) ST = 0.27500E+00 DT = 0.86783E+07 DX1= 0.46080E+04 DX2= 0.10001E+02 T =  30.000 P =  5930977. S = 0.94034E-03
 ...ITERATING...  AT [   19, 1] --- DELTEX = 0.867834E+07   MAX. RES. = 0.227726E+00  AT ELEMENT ToE 1  EQUATION   1
```

```
 ...ITERATING...  AT [   19, 2] --- DELTEX = 0.867834E+07   MAX. RES. = 0.477431E-01  AT ELEMENT I42 7  EQUATION   1
 %%% IFC : PRESSURE IN ELEMENT l-g45 IS  17.345 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  14.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT TcE 1 IS  43.980 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT ToE 1 IS  43.948 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT TlE 1 IS  44.224 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT TiE 1 IS  41.579 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT TSE 1 IS  40.071 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT o-o 2 IS  15.087 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  14.922 MPa. POROSITY REDUCTION STOPPED.
%%% IFC GEOCHEMICAL SEALING: STRONGEST SEALING (0.5906) AT CONNECTION NO.    73 (s63 1  s73 1)
 L64 6(   19,3) ST = 0.55000E+00 DT = 0.86783E+07 DX1= 0.80705E+07 DX2= -.81572E-04 T =  30.000 P = 14001440. S = 0.85877E-03
 ...ITERATING...  AT [   20, 1] --- DELTEX = 0.142009E+08   MAX. RES. = 0.851875E-01  AT ELEMENT TaE18  EQUATION   1
 ...ITERATING...  AT [   20, 2] --- DELTEX = 0.142009E+08   MAX. RES. = 0.172525E-01  AT ELEMENT L67 6  EQUATION   1
 %%% IFC : PRESSURE IN ELEMENT l-g45 IS  18.288 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  14.960 MPa. POROSITY REDUCTION STOPPED.
 %%% IFC : PRESSURE IN ELEMENT TcE 1 IS  42.551 MPa, HIGHER THAN LITHOSTATIC PRESSURE OF  39.960 MPa. POROSITY REDUCTION STOPPED.
%%% IFC GEOCHEMICAL SEALING: STRONGEST SEALING (0.5142) AT CONNECTION NO.    73 (s63 1  s73 1)
 L97 6(   20,3) ST = 0.10000E+01 DT = 0.14201E+08 DX1= -.69358E+06 DX2= 0.18642E-03 T =  30.000 P = 13329835. S = 0.54514E-03

 CPU-TIME SINCE LAST OUTPUT:     52.52 SEC;   TOTAL CPU-TIME:    350.12 SEC

 >>>>>>>>>>>>>> TIME = 0.315576E+08 DT = 0.142009E+08       KCYC =   20       ITER =    3

1********* VOLUME- AND MASS-BALANCES ********************************************************************************************

 ********** [KCYC,ITER] = [  20,  3] *****                                 THE TIME IS  0.31558E+08 SECONDS, OR  0.10000E+01 YEARS


 PHASE VOLUMES IN PLACE
 GAS  0.15010E-01 M**3;   LIQUID  0.32884E+09 M**3

 MASS IN PLACE
 GAS  0.12150E+00 KG;     LIQUID  0.32833E+12 KG;    HYD  0.53227E+02 KG;    VAPOR  0.45583E-03 KG;   LIQUID WATER  0.32833E+12 KG

 *******************************************************************************************************************************

...
```

Figure 28. Excerpt of iTOUGH2-IFC output file

8. Summary and Concluding Remarks

The developed iTOUGH2-IFC code and the related IFC model is intended to capture safety-relevant features and processes for simulating flow of liquid and gas in a SF/HLW/ILW repository in Opalinus Clay. The computational approach combines a site- and process-specific conceptual model with numerical simulation of two-phase, two-component flow, and is based on a module of the TOUGH simulator (Pruess et al., 1999) as implemented in iTOUGH2 (Finsterle, 2007abc). The implemented approach captures these features and processes explicitly in an appropriately simplified process model.

To achieve computational efficiency, the repository system and its elements as well as the geosphere are represented in a simplified manner. Specifically, advantage is taken from approximate symmetries encountered in the system, and from expected flow patterns. Following this approach, less only 2.5% of the emplacement tunnels of the SF/HLW facility need to be modeled. The remainder of the tunnel system, however, is represented in full.

While the main features and processes are simulated using the built-in modeling capabilities of TOUGH2, a limited number of FEPs (i.e., pathway dilation, mechanical and chemical alterations of backfill materials, the EDZ, and the host rock) are represented by abstraction models. According to Order 690.09 (p. 2, bullet 2), the basis and justification for these representations can be taken from previous Nagra reports, specifically Nagra (2002b, NTB 02-05; NTB 02-05, 2004); consequently, the details of these submodels or their abstraction are not discussed in this report. In their implementation within the IFC, these submodels can be provided either as parameterized functions or as look-up tables.

The correct implementation of new features built into the iTOUGH2 code has been tested (see Section 6). The mesh was generated using an automatic procedure that reduces the risk of introducing discretization errors (see Section 4.3), and property values were carefully selected (see Section 4.4). Nevertheless, the code and model should undergo additional testing for correctness, robustness, and efficiency. Specifically, the continuity of the tunnel system and its connection to the geosphere should be further inspected. The efficiency of the simulation may be improved by adjusting certain property values, computational parameters, program options, and mesh resolution. Property adjustments and mesh coarsening need to be justified through sensitivity analyses.

The iTOUGH2-IFC code and the numerical repository model have been designed and built such that they can be modified and enhanced to accommodate new insights, computation resources, and other needs of Nagra's probabilistic safety assessment of a repository for spent fuel, high-level waste, and long-lived intermediate-level wastes in Switzerland.

9. Comments and Recommendations

This section summarizes some observations and makes suggestions regarding alternative implementations, supporting studies, and future developments. Section 9.1 contains recommendations regarding investigations that could be performed to justify certain simplifying assumptions made in the IFC, and to analyze their impacts on model predictions. Section 9.2 lists iTOUGH2-IFC capabilities that are currently not used, but could be invoked to refine the IFC. Section 9.3 discusses miscellaneous issues.

9.1 Testing of Assumptions

9.1.1 Resaturation and Multi-Component Gas Generation

The IFC only considers a single gas component (hydrogen). However, some of the pore space may be initially filled with air (as a result of dry-out during the construction phase). Moreover, the gas generated by corrosion and waste degradation consists of multiple components (hydrogen being the dominant molecule). Representing the gas mixture as a single-component gas (hydrogen) is a simplifying assumption. It is recommended that the impact of this simplification on compressibility, solubility, and other performance-relevant processes and parameters be examined in a separate study using a multi-component module of the TOUGH suite of simulators.

9.1.2 Gas Migration within Waste Emplacement Tunnels

It is recommended that gas generation and gas flow within a backfilled emplacement tunnel segment of the length of a waste canister (including canister spacing) be studied in detail to confirm the appropriateness of the line-source assumption, and to justify the discretization and effective parameters used for simulating gas flow along the emplacement tunnel.

9.1.3 Appropriateness of Representative Emplacement Tunnel Approach

To significantly increase computational efficiency, the array of waste emplacement tunnels is not fully discretized, but replaced by a single representative tunnel, which is then replicated (see Sections 4.2.2 and 5.1). This approach is based on symmetry assumptions that are a simplification of the real system and its expected behavior. Specifically, the symmetry assumption is violated near the edges of the tunnel array. Moreover, the pressure and saturation conditions in the construction and operation tunnels, to which the waste emplacement tunnels are connected, are non-uniform, leading to non-symmetric flow conditions. Finally, the regional-scale hydrologic conditions and non-symmetry of the entire repository system have a non-symmetric impact on the near-field conditions. It is recommended that the simplification inherent in the representative emplacement tunnel approach be tested using a separate, comprehensive model of the facility.

9.1.4 Coupled Hydrologic-Mechanical Effects under Two-phase Conditions

Tunnel convergence is simulated by externally specifying a time-dependent porosity reduction (see Section 3.3.4). This approach does not consider coupled hydro-mechanical effects. For example, it is unlikely that materials consolidate under imposed stress changes at a rate that is independent of whether the pore space is gas filled or fully liquid saturated. Prescribing a porosity reduction in a fully water saturated, tight formation may lead to abrupt and excessive pressure increases due to the small water compressibility.

The consolidation behavior under two-phase conditions could be examined theoretically, analytically, and numerically, to gain confidence in the simplified representation of tunnel convergence in the IFC model, or to provide a basis for an alternative abstraction.

9.2 Simulation Capabilities not Invoked by Current Base-Case Model

9.2.1 Water Consumption

FEP 1.3.13, i.e., the consumption of water due to corrosion reactions, is not considered a relevant process and is thus not included in the base-case model. However, the iTOUGH2-IFC code is capable of handling a phase-specific water withdrawal rate, which could be made proportional to the time-dependent gas generation rate. Sensitivity analyses on the effects of water consumption could be performed.

9.2.2 Gas Production Limited by Water Availability

Corrosion and gas generation rates depend on the availability of water, which may be limited near the waste packages due to reduced liquid saturation combined with low permeability of the surrounding material. The coupled effect of gas generation, fluid displacement and water availability, which potentially limits further gas generation, could be examined using appropriate coupled process models that account for two-phase flow and reactive transport.

9.2.3 Consistency in Treatment of Property Changes

Certain coupled geomechanical and geochemical processes are accounted for in a simplified manner by externally imposing changes in hydrogeologic properties, i.e., porosity, permeability, and the capillary-strength parameter of the van Genuchten capillary pressure curve. All the processes described in Section 3.3 essentially lead to an increase or reduction in porosity. However, the inherent correlations among porosity, permeability, and capillary strength are not accounted for in a consistent manner. Specifically, pathway dilation is implemented as a change in permeability and capillary strength, while porosity remains unchanged; EDZ self-sealing processes are implemented as a change in permeability and porosity, while capillary strength remains unchanged; tunnel convergence is implemented as a change in porosity, while permeability and capillary strength remain unchanged; and finally, uplift and geochemical processes are implemented as a change in permeability, while porosity and capillary strength remain unchanged. The justification for this variable treatment of changes in potentially correlated parameters is not obvious. A consistent implementation of property changes would be straightforward.

9.2.4 Representation of Uplift

Several effects resulting from uplift are neglected in the simplified treatment discussed in Section 3.3.4, but could be implemented. Changes in two-phase flow parameters (e.g., reduction in capillary strength) could be implemented analogous to Section 3.3.3. Uplift and erosion changes the depth of the host rock and thus the depth-dependent pathway-dilation effects. Changes in vertical effective stress due to uplift could be implemented by specifying a time-dependent surface elevation in Eq. (1). Most important, the pressure at the top boundary of the model is also affected by uplift and erosion; the corresponding time-dependent Dirichlet boundary condition could be provided as a function of the erosion rate using standard iTOUGH2-IFC features.

9.2.5 Representation of Fractures

Fractures and discontinuities (FEPs 1.3.1 and 1.3.2) on a relatively small scale could be included using the double-porosity, dual-permeability, or multiple interacting continua (MINC) approaches (Pruess and Narasimhan, 1985), or using an effective continuum model for relative permeability and capillary pressure (Doughty, 1999); all these approaches are available in iTOUGH2-IFC. (Note that in Opalinus Clay, fractures appear to be hydraulically active only if the overburden is reduced to less than 200 m due to uplift or erosion (Nagra, 2007a, AN 07-115).)

9.2.6 Representation of Gas Channeling Effects

The displacement of water by (low-viscosity) gas in a heterogeneous porous medium may lead to flow channeling effects. In Nagra (2007a, AN 07-115), such effects are mentioned as potentially relevant for gas flow in transmissive discontinuities (R9; FEP 1.3.2) and the EDZ (R10; FEP 1.3.4). These small-scale features (compared to the size of a computational element) can be approximately accounted for in a continuum model by the Active Fracture Model (AFM; Liu et al., 1998), which is implemented in iTOUGH2-IFC (Finsterle, 2007b, Appendix A7). The AFM accounts for flow channeling effects within a fracture network and individual fractures. It is based on the van Genuchten model, requiring one additional parameter. The impact of this parameter on repository performance should be evaluated by sensitivity analyses.

9.3 Miscellaneous Comments

9.3.1 Initial Conditions

As discussed in Section 4.6, the system is initially (i.e., prior to gas generation) assumed to be at steady state, that is, in equilibrium with the imposed boundary pressures, which results in fully saturated conditions throughout the model domain. Perturbations induced by, for example, repository construction (affecting pressure and saturation distribution in the vicinity of waste emplacement tunnels), heat output during the early post-closure stage (affecting temperature, pressure, and saturation distribution), or other short- or long-term transient effects not explicitly represented in the model, will lead to a deviation from this idealized initial state.

A starting time for IFC simulations that evaluate the long-term performance of the repository system has to be selected. The choice of this starting time affects computational demands, specifically because the early-time perturbations lead to strong transients that are computationally expensive because time steps are relatively small. Moreover, it determines which effects (e.g., resaturation, thermal output) have to be included in the simulation model or, if omitted, which simplifications need to be justified. Finally, the starting time determines the initial conditions and the difficulty with which they are to be obtained. These three aspects regarding the choice of the starting time need to be balanced. In the current base-case model, the starting time was chosen to be the time gas generation is initiated. However, the initial conditions (while simple and efficient to calculate) do not properly reflect the perturbation induced by repository construction, which leads to a pressure drop, pre-closure dry-out effects, and unsaturated conditions in and near the tunnels, nor does it account for early-time post-closure effects, such as the release of decay heat. Most of the calculation time is spent to resolve the initial period with high gas generation rates in the intermediate-level waste facility. Justifying this particular choice of the starting time and initial conditions in the current base-case model is beyond the scope of this report on the development of the iTOUGH2-IFC code and IFC model.

There are essentially two ways to obtain initial conditions:

1. The initial distribution of pressure, saturation or hydrogen mass fraction (which are the primary variables solved by the numerical model) are calculated by iTOUGH2-IFC prior to or as part of the PSA simulation. Depending on the processes to be included in the initial condition field, this simulation may be a simple steady-state calculation (as described in Section 4.6), or a complex sequence of steady-state and transient simulations with time-dependent boundary conditions (e.g., to represent repository construction).
2. Initial conditions are pre-calculated externally using numerical simulations or simplified abstractions or scenarios, and provided to the iTOUGH2-IFC simulator at run time during a PSA analysis.

The first approach has the advantage that the initial conditions are automatically available in the required format, and that no residual transients have to be resolved at early time due to errors induced by mapping, non-equilibrium conditions, and other effects that are likely to be introduced at the interface between the externally provided information and the iTOUGH2-IFC initial condition file. A disadvantage of the first approach is that it may be computationally demanding.

A new set of initial conditions needs to be provided or calculated each time a parameter is adjusted during the PSA sampling, if this parameter affects the initial conditions. This could be accomplished in a more natural and more accurate way if the first approach is used.

9.3.2 Performance-Affecting Parameters and Options

The computational efficiency of the IFC depends on the sampled parameter set, which leads to potentially significantly different flow behavior, which in turn affects time-step size and convergence rates of the simulator. The iTOUGH2-IFC code and IFC model must be able to handle a large variety of parameter combinations in a robust manner. Computational efficiency is also affected by certain parameters that are not part of the parameter set to be varied within PSA (see Table 22). Moreover, adjustments of these parameters are not expected to significantly affect the simulated system behavior, i.e., they are not safety-relevant. Finally, the values of some of these parameters are unknown, unmeasured, or highly uncertain, i.e., no preference to a specific value can be reasonably justified. Provided that uncertainty in these parameters is not subject to evaluation in the probabilistic analysis, and that they have a significant impact on the numerical stability and performance of the simulation, a study could be performed to investigate which value should be picked to aid computational efficiency. The following is a list of potential candidate parameters for such an analysis, which includes (1) compiler options, (2) computational parameters, (3) hydrogeological parameters, and (4) changes in model conceptualization:

- Compiler options for code optimization, including parallelization
- Choice of linear equation solver (TOUGH2 variable `MOP(21)`)
- Choice of preconditioner (TOUGH2 variables `ZPROC` and `OPROC`)
- Linear equation solver parameters (TOUGH2 variables `RITMAX` and `CLOSUR`)

- Convergence criteria for Newton-Raphson iterations (TOUGH2 variables `RE1`, `RE2`, `MOP2(1)`, and `WNR`)
- Increment factor for numerically computing derivatives (TOUGH2 variable `DFAC`)
- Weighting scheme for mobility and permeability at interfaces (TOUGH2 variable `MOP(11)`)
- Parameters affecting automatic time step control (TOUGH2 variables `MOP(16)`, `NOITE`, `DELTMX`, and `REDLT`)
- Residual gas saturation (TOUGH2 variable `RP(2)`)
- Linearization of liquid relative permeability near saturation (TOUGH2 variable `RP(5)`)
- Linearization of capillary pressure near residual liquid saturation (TOUGH2 variable `CP(3)`)
- Different residual saturations for capillary pressure and relative permeability curves (TOUGH2 variable `CP(7)`)
- Initial gas saturation after phase change (variable `ZERO` in subroutine EOS)
- Vapor pressure reduction at low liquid saturations (TOUGH2 variable `MOP2(4)`)
- Gas diffusion (TOUGH2 variables `TORTX`, `DIFF0`, `TEXP`, and `BE`)

It is highly recommended to analyze model regions and processes (specifically phase appearances and disappearances) causing convergence difficulties and associated time-step reductions. Justifiable adjustment in those regions and in parameters controlling the problematic process should be investigated.

As demonstrated in Figure 27, the inclusion of geomechanical and geochemical FEPs significantly affects the efficiency of the simulation. It is recommended that the impact of each of these FEPs on the simulation results be evaluated and put in context with prediction uncertainties due to parameter variability, other conceptual simplifications, and computational errors. Insignificant processes may be omitted, enhancing computational efficiency.

10. Acknowledgment

I would like to thank Michael Ballmer (TK Consult AG) for his very careful checking of the IFC model mesh, Uli Kuhlmann (TK Consult AG) for support with the generation of Table 22, and Yingqi Zhang (LBNL) for the review of the draft report. This work was supported by a grant (Order No. 6425) from the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra), Wettingen, Switzerland. The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC02-05CH11231.

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A1. Code Modifications

iTOUGH2 V6.0 with equation-of-state module EOS5 (nonisothermal two-phase flow of water and hydrogen) was modified to implement the requirements of the IFC. Table A - 1 summarizes the modifications made.

Table A - 1. Code Modifications

Purpose	File	Description
Replicate state calculated in a parent element to one or more daughter elements. Daughter elements are dummy Dirichlet boundary elements. Allows connecting simplified submodel (e.g., single emplacement drift) to site model (e.g., geosphere)	maxsize.inc	Add new parameters `MAXCOPIED` and `MAXCOPY` for dimensioning new arrays
	elements.inc	Define new variables `MCOPY`, `NCOPY(MAXCOPIED)`, `ELEMCOPIED(MAXCOPIED)`, and `ELEMCOPY(MAXCOPIED,MAXCOPY)`
	t2fIFC.f	Read in new keyword `COPY` in subroutine `INPUT`; add new subroutine COPYELEM
	it2main.f	Call `COPYELEM` in subroutine `CALLTOUG` after convergence
Remove temperature dependency of fluid properties (Henry's coefficient, saturated vapor pressure, water density, water viscosity)	eosIFC.f	Call subroutines `SAT`, `VISW`, `COWAT`, and `HEN` only once to calculate related fluid properties as a function of reference temperature. Provide reference temperature as variable `POR` for special "material" `REFCO`. By default, the reference temperature is 30 °C. User-specified water density and viscosity can be provided as `PERM(1)` and `PERM(2)` for `REFCO`, respectively.
Store IFC-related parameters and variables	ifc.inc	Contains COMMON blocks with IFC-related parameters and variables
Read in parameters for incorporation special hydromechanical and hydro-geochemical FEPs	t2fIFC.f	Read in keyword "`IFC  `" in subroutine INPUT; call new subroutine IFC_INPUT
		Subroutine IFC_INPUT: read in model parameters for special FEPs
		Subroutine IFC_INIT: Initializes IFC parameters
		Subroutine IFC_INDATA: prints IFC parameters to output file
Read in information for interfacing with PICNIC	t2fIFC.f	Read in keyword "`PICNIC`" in subroutine INPUT; call new subroutine IFC_PICNIC_INPUT
		Subroutine IFC_PICNIC_INPUT: read PICNIC interface parameters
Write PICNIC interface files	t2fIFC.f	Subroutine OutPicnic: Writes select simulation results to PICNIC transfer files
Calculate geomechanical property changes	t2fIFC.f	Calculate time-dependent porosities and permeabilities in subroutine IFC_MechUpdate
Calculate geochemical property changes	t2fIFC.f	Calculate time-dependent permeabilities in subroutine IFC_ChemSealing
Update time-dependent properties	t2fIFC.f	Subroutine CONVER: Update porosities and permeabilities according to the implementation of FEPs 1.4.1, 1.4.3, and 1.4.7.

A2. Unix Script File for Meshgeneration

Generation of IFC (sub)meshes is controlled by Unix (Bourne shell, *sh*) script files that create input files for the iTOUGH2-IFC internal mesh generator, call supporting Fortran routines for mesh manipulation (see Appendix A3), and directly perform minor edits of the mesh file. The master Unix script file is shown in Figure A - 1; it calls the other script files that generate submeshes, and combines the resulting ELEME and CONNE blocks into a single file, before moving the local coordinates of the entire mesh to the reference coordinate system.

```
#! /bin/sh
#
# sh.IFC_mesh
# Unix shell script file to generate IFC mesh:
#
# S. Finsterle
# V1.1
#
echo
echo Start shell script sh.IFC_mesh
echo ================================
echo Date      : `date`
echo Directory : `pwd`
echo
#
# --- Generate emplacement tunnels (creates ET.mes and PILOT.mes)
#
sh.IFC_ET_mesh
#
# --- Generate LMA emplacement tunnels (creates LMA1.mes and LMA2.mes)
#
sh.IFC_LMA_mesh
#
# --- Generate operations tunnel (creates OT.mes)
#
sh.IFC_OT_mesh
#
# --- Generate construction tunnel (creates CT.mes)
#
sh.IFC_CT_mesh
#
# --- Generate Geosphere Module (creates G.mes)
#
sh.IFC_G_mesh
#
# --- Insert tunnels (access tunnel, part of operations and construction tunnel, shaft,
central area, detour tunnel, etc.)
#
sh.IFC_tunnel_mesh
#
# --- Generate Local Aquifer Module (creates A.mes)
#
sh.IFC_A_mesh
#
# --- Separate blocks ELEME and CONNE
#
cat ET.mes    | sed -n '1,/CONNE/p' | grep -v CONNE                        > eleme
cat ET.mes    | sed -n '/CONNE/,/+++/p'                                    > conne
#
cat PILOT.mes | sed -n '1,/CONNE/p'       | grep -v ELEME | grep -v CONNE >> eleme
cat PILOT.mes | sed -n '/CONNE/,/+++/p'   | grep -v CONNE                 >> conne
#
cat LMA1.mes  | sed -n '1,/CONNE/p'       | grep -v ELEME | grep -v CONNE >> eleme
cat LMA1.mes  | sed -n '/CONNE/,/+++/p'   | grep -v CONNE                 >> conne
#
cat LMA2.mes  | sed -n '1,/CONNE/p'       | grep -v ELEME | grep -v CONNE >> eleme
cat LMA2.mes  | sed -n '/CONNE/,/+++/p'   | grep -v CONNE                 >> conne
```

Figure A - 1. Master Unix script file for generation of IFC mesh

```
#
cat GT.mes    | sed -n '1,/CONNE/p'      | grep -v ELEME | grep -v CONNE >> eleme
cat GT.mes    | sed -n '/CONNE/,/+++/p'  | grep -v CONNE                 >> conne
#
cat A.mes     | sed -n '1,/CONNE/p'      | grep -v ELEME | grep -v CONNE >> eleme
cat A.mes     | sed -n '/CONNE/,/+++/p'  | grep -v CONNE                 >> conne
#
cat OT.mes    | sed -n '1,/CONNE/p'      | grep -v ELEME | grep -v CONNE >> eleme
cat OT.mes    | sed -n '/CONNE/,/+++/p'  | grep -v CONNE                 >> conne
#
cat CT.mes    | sed -n '1,/CONNE/p'      | grep -v ELEME | grep -v CONNE >> eleme
cat CT.mes    | sed -n '/CONNE/,/+++/p'  | grep -v CONNE                 >> conne
#
# --- Remove all "+++" and empty lines, and concatenate the ELEME and CONNE blocks
#
cat eleme     | sed '/^ *$/d'                                           > temp.in
cat conne     | sed '/^ *$/d' | sed '/CONNE/{x;p;x;}' | grep -v +++    >> temp.in
cat >> temp.in << EOF

EOF
#
# --- Move mesh to center elevation of repository (AN 08-173, Table 2)
#
./Codes/xMoveMesh << EOF
temp.in                                 # input mesh file
temp.out                                # output mesh file
   0.0                                  # dx
   0.0                                  # dy
-198.9                                  # dz
EOF
mv temp.out temp.in
#
# --- Run one time step
#
tough2 -m temp.in -mesh onestep 9
rm onestep.sav
mv onestep.mes IFC.mes
#
echo Script sh.IFC_mesh completed: `date`
echo ===========================
```

Figure A - 1 (cont.). Master Unix script file for generation of IFC mesh

A short excerpt from file *sh.IFC_ET_mesh* is shown in Figure A - 2. It generates the representative waste emplacement tunnel (RWET) for spent fuel and high-level wastes. The following main steps are performed:

(1) A Cartesian grid is created using the iTOUGH2-IFC mesh generator.

(2) Fortran program MoveMesh is called to translate the mesh to a convenient local coordinate system.

(3) All elements are renamed for easy identification and to avoid redundancies with other submeshes.

(4) Fortran program AssignMesh is called to assign material names to subdomains with properties for waste, backfill, EDZ, Opalinus Clay, seal, lock, etc.

(5) Fortran program CombineElements is called to create averaging planes at the submesh boundaries for later connection to the lower-resolution geosphere mesh and submeshes of the construction and operations tunnel.

(6) Minor adjustments are made (removal of redundant connections, adjustment of angles, etc.), and the final submesh is assembled.

```
#! /bin/sh
#
# sh.IFC_ET_mesh
# Unix shell script file to generate IFC mesh:
#
# - emplacement tunnel
# - abutments, seals, and lock
#
# S. Finsterle
# V1.1
#
echo
echo Start shell script sh.IFC_ET_mesh
echo ==================================
echo Date      : `date`
echo Directory : `pwd`
echo
#
# --- Generate Emplacement Tunnel Module and
#     Seal-and-Lock Module
#
cat > ETM.t2 << EOF
TOUGH2 input file for generating base mesh for Emplacement Tunnel Module
MESHMAKER ----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
-2.74809             4.8% slope
NX       1      0.50 Waste package
NX       1      0.50 Emplacement tunnel
NX       2      0.50 EDZ ET
NX       1      1.00 Opalinus clay/lock
NX       1      1.00 Opalinus clay/EDZ lock
NX       1      2.00 Opalinus clay
NX       1      4.00 Opalinus clay
NX       1     10.00 Opalinus clay
NY       1      1.00 Averaging element, concrete wall, connects to CTM
NY       1      8.00 Abutment (note: 20 m starting tunnel in CTM)
NY       1     12.00 Seal
NY       1      4.50 ET, no WPs
NY       3    115.00 ET south
NY       1      1.00 fault
NY       3    115.00 ET north
NY       1      4.50 ET, no WPs
NY       1     12.00 Seal
NY       1      7.00 Abutment
NY       1      1.00 Abutment transition zone and radial EDZ around lock
NY       1     20.00 Lock (Note: 15 m bend included in OTM)
NY       1      1.00 Averaging element, concrete wall, connects to OTM
NZ       1      1.00 Averaging element, connects top to Geosphere module
NZ       1      6.00 Opalinus clay
NZ       1      3.00 Opalinus clay
NZ       1      1.00 Opalinus clay/EDZ lock
NZ       2      0.50 EDZ upper/lock
NZ       4      0.50 ET/abutment/seal/lock
NZ       2      0.50 EDZ lower
NZ       1      1.00 Opalinus clay
NZ       1      3.00 Opalinus clay
NZ       1      6.00 Opalinus clay
NZ       1      1.00 Averaging element, connects bottom to Geosphere module


ENDFI ---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
EOF
#
# --- Run TOUGH2 to generate base mesh for ETM
#
tough2 -mesh ETM.t2 9
rm ETM.sav
```

Figure A - 2. Excerpt from Unix script file *sh.IFC_ET_mesh* for generating the mesh for the representative waste emplacement tunnel

```
#
# --- Move mesh to center point: SW corner @ (0/0/0)
#
./Codes/xMoveMesh << EOF
ETM.mes                                 # input mesh file
temp.out                                # output mesh file
 510.0                                  # dx
  21.5                                  # dy
  13.0                                  # dz
EOF
#
# --- Start all element names of the ET for spent fuels with the letter "s"
#
mv temp.out temp.in
cat temp.in | sed 's/^A/s/'             > temp.out
mv temp.out temp.in
cat temp.in | sed 's/^s\(....\)A/s/\1s/' > temp.out
mv temp.out temp.in
...
#
# --- Assign EDZ around ET and sealing structures
#
./Codes/xAssignRock << EOF
temp.in                                 # input mesh file
temp.out                                # output mesh file
EDZsf                                   # material type
2                                       # cylindrical region
 510.0                                  # xstart
 510.0                                  # xend
  22.5                                  # ystart
 762.5                                  # yend
   0.0                                  # zstart
   0.0                                  # zend
   2.25                                 # radius
EOF
mv temp.out temp.in
#
(...)
#
# --- Create averaging planes
#     ======================
#
# -- Averaging plane from emplacement tunnel to construction tunnel module
#    ... from abutment to CTM
#
./Codes/xCombineElements << EOF
temp.in                                 # input mesh file
temp.out                                # output mesh file
s-c 1                                   # element name
START                                   # material type
   0.0                                  # element volume
   0.50                                 # nodal distance to element
2                                       # cylindrical region
 510.0                                  # xstart
 510.0                                  # xend
  12.5                                  # ystart
  22.5                                  # yend
   0.0                                  # zstart
   0.0                                  # zend
   1.25                                 # radius
   1                                    # number of repetitions in X direction
   1                                    # number of repetitions in Y direction
   1                                    # number of repetitions in Z direction
EOF
mv temp.out temp.in
#
(...)
#
```

Figure A - 2 (cont.). Excerpt from Unix script file *sh.IFC_ET_mesh* for generating the mesh for the representative waste emplacement tunnel

```
#
# --- Remove connections between averaging elements
#
grep -v "s-...s-" temp.in > temp.out
mv temp.out temp.in
#
# --- Remove vertical angle (only consider slope along ET)
#
cat temp.in | sed 's/0.9988E+00/0.1000E+01/' > temp.out
mv temp.out temp.in
#
# --- Make tunnel horizontal in sealing sections
#
cat temp.in  | sed 's/^\(..\)\([2,3,D-G]\)\(.*\)-.4794E-01/\1\2\30.0000E+00/' | \
               sed 's/x\(.*\)-.4794E-01/x\10.0000E+00/' > temp.out
#
(...)
#
# --- Run one time step
#
tough2 -m temp.in -mesh onestep 9
rm onestep.sav
grep -v "s-" onestep.mes > MESH
cat onestep.out | sed 's/-0\./ -./g' > temp.out
mv temp.out onestep.out
xExt -xyz onestep.out
cat onestep.out.1 | sed 's/Zone.*$/Zone i=14 j=15 k=9/' > ET.tec
#
(...)
echo Script sh.IFC_ET_mesh completed: `date`
echo ===============================
```

Figure A - 2 (cont.). Excerpt from Unix script file *sh.IFC_ET_mesh* for generating the mesh for the representative waste emplacement tunnel

A3. Supporting Fortran Mesh Manipulation Programs

The following contains a short description of the utility Fortran programs written to manipulate basic iTOUGH2-IFC meshes. The input parameters needed to run these programs are also listed. These programs are called by the Unix script files described in Section A2.

Program MoveMesh simply adds constants to the X-, Y-, and Z-coordinates of the TOUGH2 mesh file. Input parameters are listed in Table A - 2.

Table A - 2. Input parameters for MoveMesh

Parameter	**Description**
filein	Name of original TOUGH2 mesh file
fileout	Name of TOUGH2 mesh file with shifted coordinates
dx	Shift in X coordinate
dy	Shift in Y coordinate
dz	Shift in Z coordinate

Program AssignRock assigns a material name to all elements with center coordinates within a user-specified region The region can be a box or a cylinder. Input parameters are listed in Table A - 3.

Table A - 3. Input parameters for AssignRock

Parameter	**Description**
filein	Name of original TOUGH2 mesh file
fileout	Name of TOUGH2 mesh file with material name assigned
cbmat	Material name (consistent with name in block `ROCKS`)
ishape	Defines shape of region (1 = box; 2 = cylinder)
xmin	Minimum X-coordinate (of box or cylinder axis)
xmax	Maximum X-coordinate (of box or cylinder axis)
ymin	Minimum Y-coordinate (of box or cylinder axis)
ymax	Maximum Y-coordinate (of box or cylinder axis)
zmin	Minimum Z-coordinate (of box or cylinder axis)
zmax	Maximum Z-coordinate (of box or cylinder axis)
radius	Radius of cylinder (only if *ishape* = 2)

Program DeleteElements deletes all elements (and associated connections) with center coordinates within a user-specified region. The region can be a box or a cylinder, or can be defined by a material name. Input parameters are listed in Table A - 4.

Table A - 4. Input parameters for DeleteElements

Parameter	**Description**
filein	Name of original TOUGH2 mesh file
fileout	Name of TOUGH2 mesh file with certain elements deleted
ishape	Defines shape of region (1 = box; 2 = cylinder, 3 = material name)
cbmat	Material name (only if *ishape* = 3)
xmin	Minimum X-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
xmax	Maximum X-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
ymin	Minimum Y-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
ymax	Maximum Y-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
zmin	Minimum Z-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
zmax	Maximum Z-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
radius	Radius of cylinder (only if *ishape* = 2)

Program AddTunnel inserts cylindrical tunnel elements and an associate, concentric, cylintrical EDZ zone into an existing mesh file. The tunnel axis is defined by a polygon. Input parameters are listed in Table A - 5.

Table A - 5. Input parameters for AddTunnel

Parameter	**Description**
filein	Name of original TOUGH2 mesh file
fileout	Name of TOUGH2 mesh file with tunnel inserted
elemtun	Name of tunnel element (formal AAAII)
elemedz	Name of EDZ element (formal AAAII)
mattun	Material name of tunnel element
mattun	Material name of tunnel element
matedz	Material name of EDZ element
nseg	Number of segments defining tunnel axis
x, y, z, r, redz	X-, Y-, and Z-coordinate, tunnel radius, and EDZ radius of (*nseg* + 1) points defining the polygon of the tunnel axis

Program CombineElements combines all elements with center coordinates within a user-specified region into a single element. The region can be a box or a cylinder. Multiple, uniformly spaced regions with identical shape can be defined. All elements in all regions can either be combined into one single element, or into separate elements, one for each region. The original elements are removed, and the respective connections are replaced with multiple connections to the new element(s). Input parameters are listed in Table A - 6.

Table A - 6. Input parameters for CombineElements

Parameter	Description
filein	Name of original TOUGH2 mesh file
fileout	Name of TOUGH2 mesh file with certain elements combined
cbound	Name of new element (format AAAII)
cbmat	Material name assigned to new element
cvolume	Volume of new element; if zero, the volume is the sum of all volumes of the original elements within the region
distance	Nodal distance of new element to interface with existing elements
ishape	Defines shape of region (1 = box; 2 = cylinder)
xmin	Minimum X-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
xmax	Maximum X-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
ymin	Minimum Y-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
ymax	Maximum Y-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
zmin	Minimum Z-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
zmax	Maximum Z-coordinate (of box or cylinder axis, only if *ishape* ≠ 3)
radius	Radius of cylinder (only if *ishape* = 2)
irx	Number of repetitions of region in X direction. If negative, all elements in all regions will be combined in a single new element; if positive, all elements in each region will be combined into separate new elements, one for each region.
dx	Move domain in X direction (only if *irx* ≠ 0)
iry	Number of repetitions of region in Y direction. If negative, all elements in all regions will be combined in a single new element; if positive, all elements in each region will be combined into separate new elements, one for each region.
dy	Move domain in Y direction (only if *iry* ≠ 0)
ira	Number of repetitions of region in Z direction. If negative, all elements in all regions will be combined in a single new element; if positive, all elements in each region will be combined into separate new elements, one for each region.
dz	Move domain in Z direction (only if *irz* ≠ 0)

A4. Template iTOUGH2-IFC Input File

The following is a generic iTOUGH2-IFC input file for simulating hydrogen gas generation in a repository for spent fuel, high- and intermediate-level wastes. The numerical mesh and initial conditions are provided in separate files.

- Block `ROCKS` and `RPCAP` implement the base-case material properties described in Section 4.4.
- Block COPY contains the list of parent and daughter grid blocks to replicate the calculated system state from the elements at the interface between the representative waste emplacement tunnel and pilot facility and the operations and construction tunnels as well as the geosphere; these conditions are copied to the appropriate internal Dirichlet boundary elements. See Section 5.1 for details.
- Block `GENER` contains the gas generation rates (see Table 20 and Table 21, adjusted to the individual volumes of the grid blocks representing waste).
- Block `IFS` defines all parameters needed to describe the special FEPs. See Section 5.2 for details.
- Block `PICNIC` defines the cross sections for the extraction of calculated flow rates, saturations, and porosities for subsequent input into the PICNIC-TD code. See Section 5.3for details.

The standard TOUGH2 manual (*Pruess et al*., 1999) should be consulted for details.

```
Gas release
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
OPALI    2     2650.      .1200 1.000E-20 1.000E-20 2.000E-21              1000.   Opalinus Clay
 8.055E-09
   11          0.50     0.003                          0.00
   11          1.67  18.0E+06    1.0E30
Fopal    2     2650.      .1200 1.000E-20 1.000E-20 2.000E-21              1000.   Potential fault in Opalinus Clay
 8.055E-09
   11          0.50     0.003                          0.00
   11          1.67  18.0E+06    1.0E30
bOPAL    2     2650.      .1200 1.000E-20 1.000E-20 2.000E-21             -1000.   Opalinus Clay boundary
 8.055E-09
   11          0.50     0.003                          0.00
   11          1.67  18.0E+06    1.0E30
FAULT    2     2650.      .1000 1.000E-17 1.000E-17 1.000E-17              1000.   generic fault, not used
 1.000e-08
   11          0.20      0.01                          0.00
   11          2.00   0.1E+06    1.0E30
bFAUL    2     2650.      .1000 1.000E-17 1.000E-17 1.000E-17             -1000.   fault boundary
 1.000e-08
   11          0.20      0.01                          0.00
   11          2.00   0.1E+05    1.0E30
bMALM    2     2650.      .2000 1.000E-16 1.000E-16 1.000E-16             -1000.   Malm boundary
 1.000e-08
   11          0.20      0.01                          0.00
   11          2.00    0.1+06    1.0E30
DOGGE    2     2650.      .2000 1.000E-19 1.000E-19 1.000E-19              1000.   Dogger
 1.000e-08
   11          0.20      0.01                          0.00
   11          2.00   10.0+06    1.0E30
Fdogg    2     2650.      .2000 1.000E-19 1.000E-19 1.000E-19              1000.   Potential fault in Dogger
 1.000e-08
   11          0.20      0.01                          0.00
   11          2.00   10.0+06    1.0E30
WEDEL    2     2650.      .1000 5.000E-17 5.000E-17 5.000E-17              1000.   Wedelsandstein
 1.000e-08
   11          0.90      0.01                          0.00
```

```
   11          2.00    0.2+06    1.0E30
Fwede    2    2650.     .1000 5.000E-17 5.000E-17 5.000E-17               1000.   Potential fault in Wedelsandstein
 1.000e-08
   11          0.90     0.01                        0.00
   11          2.00    0.2+06    1.0E30
bWEDE    2    2650.     .1000 5.000E-17 5.000E-17 5.000E-17              -1000.   Wedelsandstein boundary
 1.000e-08
   11          0.90     0.01                        0.00
   11          2.00    0.2+06    1.0E30
LIAS     2    2650.     .1000 5.000E-21 5.000E-21 5.000E-21               1000.   Lias + Upper Keuper
 2.618e-09
   11          0.25     0.01                        0.00
   11          2.00    1.0+06    1.0E30
Flias    2    2650.     .1000 5.000E-21 5.000E-21 5.000E-21               1000.   Potential fault in Lias + Keuper
 2.618e-09
   11          0.25     0.01                        0.00
   11          2.00    1.0+06    1.0E30
SANDS    2    2650.     .0500 2.000E-15 2.000E-15 2.000E-15               1000.   Sandsteinkeuper
 1.000E-08
   11          0.90     0.01                        0.00
   11          2.00    0.1+06    1.0E30
Fsand    2    2650.     .0500 2.000E-15 2.000E-15 2.000E-15               1000.   Potential fault Sandsteinkeuper
 1.000E-08
   11          0.90     0.01                        0.00
   11          2.00    0.1+06    1.0E30
bSAND    2    2650.     .0500 2.000E-15 2.000E-15 2.000E-15              -1000.   Sandsteinkeuper boundary
 1.000E-08
   11          0.90     0.01                        0.00
   11          2.00    0.1+06    1.0E30
KEUPE    2    2650.     .1000 5.000E-21 5.000E-21 5.000E-21               1000.   Lower Keuper
 1.000e-09
   11          0.25     0.01                        0.00
   11          2.00    1.0+06    1.0E30
Fkeup    2    2650.     .1000 5.000E-21 5.000E-21 5.000E-21               1000.   Potential fault in Lower Keuper
 1.000e-09
   11          0.25     0.01                        0.00
   11          2.00    1.0+06    1.0E30
```

```
bMUSC    2     2650.      .1000 1.000E-18 1.000E-18 1.000E-18              -1000.   Muschelkalk boundary
 1.000e-08
   11           0.20      0.00                           0.00
   11           2.00    1.0+06    1.0E30
EDZsf    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ emplacement tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZpi    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ pilot facility
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZco    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ construction tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZop    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ operations tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZac    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ access tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZvt    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ connection tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZce    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ central area
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZkt    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ control tunnel
 2.335E-11
   11            0.0       0.0                           0.00
   11           1.67   3.0E+06    1.0E30
EDZdt    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19               1000.   EDZ detour tunnel
```

```
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
EDZsh    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19              1000.   EDZ shaft
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
EDZl1    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19              1000.   EDZ in LMA1
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
EDZl2    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19              1000.   EDZ in LMA2
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
EDZse    2     2650.      .4000 5.000E-20 5.000E-20 5.000E-20              1000.   EDZ seal
 5.000E-09
   11          0.20      0.00                            0.00
   11          2.00  10.0E+06    1.0E30
bEDZs    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19             -1000.   EDZ emplacement tunnel boundary
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
bEDZp    2     2650.      .2200 1.000E-19 1.000E-19 1.000E-19             -1000.   EDZ pilot facility boundary
 2.335E-11
   11           0.0       0.0                            0.00
   11          1.67   3.0E+06    1.0E30
WAsf     2     2650.      .0010 1.000E-20 1.000E-20 1.000E-20              1000.   spent fuel and high level waste
 2.140E-09
   11          0.01      0.00                            0.00
   11          2.00   0.1E+06    1.0E30
WApil    2     2650.      .0010 1.000E-20 1.000E-20 1.000E-20              1000.   pilot waste
 2.140E-09
   11          0.01      0.00                            0.00
   11          2.00   0.1E+06    1.0E30
WAlm1    2     2650.      .0010 1.000E-15 1.000E-15 1.000E-15              1000.   intermediate-level waste 1
 0.0
```

```
   11           0.25     0.00                         0.00
   11           2.00   4.0E+03    1.0E30
WAlm2    2     2650.      .0010 1.000E-15 1.000E-15 1.000E-15              1000.   intermediate-level waste 2
 0.0
   11           0.25     0.00                         0.00
   11           2.00   4.0E+03    1.0E30
SEAL     2     2650.      .3000 1.000E-18 1.000E-18 1.000E-18              1000.   seal emplacement tunnels)
      0.0                                                                          (S/B-80/20 highly compacted)
   11           0.20     0.01                         0.00
   11           2.00   1.0E+06    1.0E30
SEALa    2     2650.      .3000 1.000E-19 1.000E-19 1.000E-19              1000.   seal access tunnels (S/B-70/30)
      0.0
   11           0.20     0.01                         0.00
   11           2.00   3.0E+06    1.0E30
SEALs    2     2650.      .4000 1.000E-19 1.000E-19 1.000E-10              1000.   seal shaft
      0.0                                                                          (compacted bentonite and gravel)
   11           0.25     0.00                         0.00
   11           2.00  18.0E+06    1.0E30
ABUTM    2     2650.      .3000 1.000E-16 1.000E-16 1.000E-16              1000.   abutment (gravel)
 3.580E-09
   11           0.10     0.01                         0.00
   11           3.00   0.1E+06    1.0E30
ETsf     2     2650.      .4000 1.000E-19 1.000E-19 1.000E-19              1000.   backfilled emplacement tunnel
      0.0                                                                          (compacted bentonite)
   11           0.25     0.00                         0.00
   11           2.00  18.0E+06    1.0E30
ETpil    2     2650.      .4000 1.000E-19 1.000E-19 1.000E-19              1000.   backfilled pilot facility
      0.0                                                                          (compacted bentonite)
   11           0.25     0.00                         0.00
   11           2.00  18.0E+06    1.0E30
ETlm1    2     2650.      .2500 1.000E-15 1.000E-15 1.000E-15              1000.   backfilled LMA1 (mortar)
      0.0
   11           0.25     0.00                         0.00
   11           2.00   4.0E+03    1.0E30
ETlm2    2     2650.      .2500 1.000E-15 1.000E-15 1.000E-15              1000.   backfilled LMA2 (mortar)
      0.0
   11           0.25     0.00                         0.00
```

```
   11           2.00   4.0E+03    1.0E30
Tshaf    2     2650.     .3000 1.000E-12 1.000E-12 1.000E-12               1000.   Shaft (above OPA; gravel)
       0.0
   11           0.25      0.01                          0.00
   11           2.00   1.0E+03    1.0E30
TacCO    2     2650.     .2200 1.000E-12 1.000E-12 1.000E-12               1000.   Access tunnel
       0.0                                                                         crushed Opalinus Clay backfill
   11           0.25      0.00                          0.00
   11           2.00   1.0E+03    1.0E30
TURNO    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   turn-out SF/HLW/Pilot facility
bTURN    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18              -1000.   turn-out SF/HLW/Pilot facility
START    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   starter tunnel SF/HLW/Pilot
bSTAR    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18              -1000.   starter tunnel SF/HLW/Pilot
LOCK     0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   backfilled lock (S/B 70/30)
Tacce    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Access tunnel (S/B 70/30)
Tconn    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Connection tunnel (S/B 70/30)
Tcons    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Construction tunnel (S/B 70/30)
Tcont    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Control tunnel (S/B 70/30)
Tdeto    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Detour tunnel (S/B 70/30)
Toper    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Operations tunnel (S/B 70/30)
Tcent    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Central area (S/B 70/30)
Tlma1    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Connection to LMA1 (S/B 70/30)
Tlma2    0     2650.     .3000 1.000E-18 1.000E-18 1.000E-18               1000.   Connection to LMA2 (S/B 70/30)

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8   For all tunnels backfilled with
   11           0.25      0.00                          0.00                       S/B 70/30
   11           2.00   1.0E+06    1.0E30
PARAM----1----*-123456789012345678901234----*----5----*----6----*----7----*----8
 6-29999    9998100000100021000400003000
-1.000E+14             1.0E09                           9.81
    1.0E-3
        86.1E+05                  0.0                  30.0
MOMOP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    2    6
```

```
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
3  Z3   O1     0.025   1.0E-06
TIMES*---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   11   203.15576E133.15576E12
             0.0
     3.15576E+09
     6.31152E+09
    1.577880E+10
     3.15576E+10
     6.31152E+10
    1.577880E+11
     3.15576E+11
     6.31152E+11
    1.577880E+12
     3.15576E+12

COPY ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1     s-o 1
S-o 1
    1     s-o 2
S-o 2
    1     s-o 3
S-o 3
    1     s-c 1
S-c 1
    1     s-c 2
S-c 2
    1     s-c 3
S-c 3
    1     s-g10
S-g10
    1     s-g11
S-g11
    1     s-g20
S-g20
    1     s-g21
S-g21
```

```
    1     s-g30
S-g30
    1     s-g31
S-g31
    1     s-g40
S-g40
    1     s-g41
S-g41
    1     s-g50
S-g50
    1     s-g51
S-g51
    1     s-g60
S-g60
    1     s-g61
S-g61
    1     s-g70
S-g70
    1     s-g71
S-g71
    1     s-g80
S-g80
    1     s-g81
S-g81
    1     s-g90
S-g90
    1     s-g91
S-g91
    1     p-o 1
P-o 1
    1     p-o 2
P-o 2
    1     p-o 3
P-o 3
    1     p-g70
P-g70
    1     p-g71
```

```
P-g71
    1     p-g80
P-g80
    1     p-g81
P-g81
    1     p-g90
P-g90
    1     p-g91
P-g91

GENER T--1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
s85 1SF 11                   6     COM2                                           SF/HLW/Pilot: 4.88E-11 kg/s/m
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
s95 1SF 12                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
s86 1SF 21                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
s96 1SF 22                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
```

```
   6.31153E+12             0.0
       1.0E+50             0.0
s87 1SF 31                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
s97 1SF 32                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
s88 1SF 41                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.2200E-11
   6.31152E+12      1.2200E-11
   6.31153E+12             0.0
       1.0E+50             0.0
s98 1SF 42                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.2200E-11
   6.31152E+12      1.2200E-11
   6.31153E+12             0.0
       1.0E+50             0.0
s89 1SF 51                   6     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0      1.4030E-09
   6.31152E+12      1.4030E-09
   6.31153E+12             0.0
       1.0E+50             0.0
```

```
s99 1SF 52                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
s8A 1SF 61                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
s9A 1SF 62                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
s8B 1SF 71                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
s9B 1SF 72                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
p8A 1PIL61                  6     COM2
      -1.0E+50            0.0
```

```
          0.0             0.0
          1.0      1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
p9A 1PIL62                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
p8B 1PIL71                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
p9B 1PIL72                  6     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0     1.4030E-09
   6.31152E+12     1.4030E-09
   6.31153E+12            0.0
       1.0E+50            0.0
L64 6LMA 1                 16     COM2                                             LMA1
      -1.0E+50            0.0
           0.0            0.0
           1.0     5.5599E-08
    31557600.0     5.5599E-08
    94672800.0    5.39874E-08
   315576000.0    8.86361E-09
   946728000.0    8.86361E-09
  3155760000.0    7.89667E-09
  9467280000.0    6.36568E-09
 31557600000.0    3.62602E-09
```

```
 94672800000.0     1.61157E-09
   3.15576E+11     8.05783E-10
   9.46728E+11     4.02891E-10
   3.15576E+12     1.61157E-10
   5.36479E+12             0.0
      1.00E+50             0.0
L74 6LMA 2                  16     COM2                                              LMA1
     -1.0E+50              0.0
          0.0              0.0
          1.0      5.5599E-08
   31557600.0      5.5599E-08
   94672800.0     5.39874E-08
  315576000.0     8.86361E-09
  946728000.0     8.86361E-09
 3155760000.0     7.89667E-09
 9467280000.0     6.36568E-09
31557600000.0     3.62602E-09
94672800000.0     1.61157E-09
  3.15576E+11     8.05783E-10
  9.46728E+11     4.02891E-10
  3.15576E+12     1.61157E-10
  5.36479E+12             0.0
     1.00E+50             0.0
L84 6LMA 3                  16     COM2                                              LMA1
     -1.0E+50              0.0
          0.0              0.0
          1.0      5.5599E-08
   31557600.0      5.5599E-08
   94672800.0     5.39874E-08
  315576000.0     8.86361E-09
  946728000.0     8.86361E-09
 3155760000.0     7.89667E-09
 9467280000.0     6.36568E-09
31557600000.0     3.62602E-09
94672800000.0     1.61157E-09
  3.15576E+11     8.05783E-10
  9.46728E+11     4.02891E-10
```

```
   3.15576E+12     1.61157E-10
   5.36479E+12             0.0
      1.00E+50             0.0
L94 6LMA 4                  16      COM2                                              LMA1
      -1.0E+50             0.0
           0.0             0.0
           1.0      5.5599E-08
    31557600.0      5.5599E-08
    94672800.0     5.39874E-08
   315576000.0     8.86361E-09
   946728000.0     8.86361E-09
  3155760000.0     7.89667E-09
  9467280000.0     6.36568E-09
 31557600000.0     3.62602E-09
 94672800000.0     1.61157E-09
   3.15576E+11     8.05783E-10
   9.46728E+11     4.02891E-10
   3.15576E+12     1.61157E-10
   5.36479E+12             0.0
      1.00E+50             0.0
L65 6LMA 5                  16      COM2                                              LMA1
      -1.0E+50             0.0
           0.0             0.0
           1.0      5.5599E-08
    31557600.0      5.5599E-08
    94672800.0     5.39874E-08
   315576000.0     8.86361E-09
   946728000.0     8.86361E-09
  3155760000.0     7.89667E-09
  9467280000.0     6.36568E-09
 31557600000.0     3.62602E-09
 94672800000.0     1.61157E-09
   3.15576E+11     8.05783E-10
   9.46728E+11     4.02891E-10
   3.15576E+12     1.61157E-10
   5.36479E+12             0.0
      1.00E+50             0.0
```

```
L75 6LMA 6                      16     COM2                                              LMA1
      -1.0E+50                 0.0
           0.0                 0.0
           1.0         5.5599E-08
    31557600.0         5.5599E-08
    94672800.0        5.39874E-08
   315576000.0        8.86361E-09
   946728000.0        8.86361E-09
  3155760000.0        7.89667E-09
  9467280000.0        6.36568E-09
 31557600000.0        3.62602E-09
 94672800000.0        1.61157E-09
   3.15576E+11        8.05783E-10
   9.46728E+11        4.02891E-10
   3.15576E+12        1.61157E-10
   5.36479E+12                0.0
      1.00E+50                0.0
L85 6LMA 7                      16     COM2                                              LMA1
      -1.0E+50                 0.0
           0.0                 0.0
           1.0         5.5599E-08
    31557600.0         5.5599E-08
    94672800.0        5.39874E-08
   315576000.0        8.86361E-09
   946728000.0        8.86361E-09
  3155760000.0        7.89667E-09
  9467280000.0        6.36568E-09
 31557600000.0        3.62602E-09
 94672800000.0        1.61157E-09
   3.15576E+11        8.05783E-10
   9.46728E+11        4.02891E-10
   3.15576E+12        1.61157E-10
   5.36479E+12                0.0
      1.00E+50                0.0
L95 6LMA 8                      16     COM2                                              LMA1
      -1.0E+50                 0.0
           0.0                 0.0
```

```
          1.0      5.5599E-08
   31557600.0      5.5599E-08
   94672800.0     5.39874E-08
  315576000.0     8.86361E-09
  946728000.0     8.86361E-09
 3155760000.0     7.89667E-09
 9467280000.0     6.36568E-09
31557600000.0     3.62602E-09
94672800000.0     1.61157E-09
  3.15576E+11     8.05783E-10
  9.46728E+11     4.02891E-10
  3.15576E+12     1.61157E-10
  5.36479E+12             0.0
     1.00E+50             0.0
LA4 6LMA 9                 16     COM2
     -1.0E+50             0.0
          0.0             0.0
          1.0     2.77995E-07
   31557600.0     2.77995E-07
   94672800.0     2.69937E-07
  315576000.0     4.43181E-08
  946728000.0     4.43181E-08
 3155760000.0     3.94834E-08
 9467280000.0     3.18284E-08
31557600000.0     1.81301E-08
94672800000.0     8.05783E-09
  3.15576E+11     4.02891E-09
  9.46728E+11     2.01446E-09
  3.15576E+12     8.05783E-10
  5.36479E+12             0.0
     1.00E+50             0.0
LA5 6LMA10                 16     COM2
     -1.0E+50             0.0
          0.0             0.0
          1.0     2.77995E-07
   31557600.0     2.77995E-07
   94672800.0     2.69937E-07
```

```
   315576000.0     4.43181E-08
   946728000.0     4.43181E-08
  3155760000.0     3.94834E-08
  9467280000.0     3.18284E-08
 31557600000.0     1.81301E-08
 94672800000.0     8.05783E-09
   3.15576E+11     4.02891E-09
   9.46728E+11     2.01446E-09
   3.15576E+12     8.05783E-10
   5.36479E+12             0.0
      1.00E+50             0.0
L66 6LMA11                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.43406E-08
    31557600.0     3.43406E-08
    94672800.0     3.33452E-08
   315576000.0     5.47458E-09
   946728000.0     5.47458E-09
  3155760000.0     4.87736E-09
  9467280000.0     3.93175E-09
 31557600000.0      2.2396E-09
 94672800000.0     9.95379E-10
   3.15576E+11     4.97689E-10
   9.46728E+11     2.48845E-10
   3.15576E+12     9.95379E-11
   5.36479E+12            0.0
      1.00E+50            0.0
L76 6LMA12                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.43406E-08
    31557600.0     3.43406E-08
    94672800.0     3.33452E-08
   315576000.0     5.47458E-09
   946728000.0     5.47458E-09
  3155760000.0     4.87736E-09
```

```
  9467280000.0     3.93175E-09
 31557600000.0      2.2396E-09
 94672800000.0     9.95379E-10
   3.15576E+11     4.97689E-10
   9.46728E+11     2.48845E-10
   3.15576E+12     9.95379E-11
   5.36479E+12           0.0
      1.00E+50           0.0
L86 6LMA13                  16     COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0     3.43406E-08
    31557600.0     3.43406E-08
    94672800.0     3.33452E-08
   315576000.0     5.47458E-09
   946728000.0     5.47458E-09
  3155760000.0     4.87736E-09
  9467280000.0     3.93175E-09
 31557600000.0      2.2396E-09
 94672800000.0     9.95379E-10
   3.15576E+11     4.97689E-10
   9.46728E+11     2.48845E-10
   3.15576E+12     9.95379E-11
   5.36479E+12           0.0
      1.00E+50           0.0
L96 6LMA14                  16     COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0     3.43406E-08
    31557600.0     3.43406E-08
    94672800.0     3.33452E-08
   315576000.0     5.47458E-09
   946728000.0     5.47458E-09
  3155760000.0     4.87736E-09
  9467280000.0     3.93175E-09
 31557600000.0      2.2396E-09
 94672800000.0     9.95379E-10
```

```
   3.15576E+11     4.97689E-10
   9.46728E+11     2.48845E-10
   3.15576E+12     9.95379E-11
   5.36479E+12           0.0
      1.00E+50           0.0
LA6 6LMA15                 16      COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0     1.71703E-07
    31557600.0     1.71703E-07
    94672800.0     1.66726E-07
   315576000.0     2.73729E-08
   946728000.0     2.73729E-08
  3155760000.0     2.43868E-08
  9467280000.0     1.96587E-08
 31557600000.0      1.1198E-08
 94672800000.0     4.97689E-09
   3.15576E+11     2.48845E-09
   9.46728E+11     1.24422E-09
   3.15576E+12     4.97689E-10
   5.36479E+12           0.0
      1.00E+50           0.0
L67 6LMA16                 16      COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0     3.27053E-08
    31557600.0     3.27053E-08
    94672800.0     3.17573E-08
   315576000.0     5.21389E-09
   946728000.0     5.21389E-09
  3155760000.0      4.6451E-09
  9467280000.0     3.74452E-09
 31557600000.0     2.13295E-09
 94672800000.0      9.4798E-10
   3.15576E+11      4.7399E-10
   9.46728E+11     2.36995E-10
   3.15576E+12      9.4798E-11
```

```
   5.36479E+12             0.0
      1.00E+50             0.0
L77 6LMA17                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.27053E-08
    31557600.0     3.27053E-08
    94672800.0     3.17573E-08
   315576000.0     5.21389E-09
   946728000.0     5.21389E-09
  3155760000.0      4.6451E-09
  9467280000.0     3.74452E-09
 31557600000.0     2.13295E-09
 94672800000.0      9.4798E-10
   3.15576E+11      4.7399E-10
   9.46728E+11     2.36995E-10
   3.15576E+12      9.4798E-11
   5.36479E+12             0.0
      1.00E+50             0.0
L87 6LMA18                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.27053E-08
    31557600.0     3.27053E-08
    94672800.0     3.17573E-08
   315576000.0     5.21389E-09
   946728000.0     5.21389E-09
  3155760000.0      4.6451E-09
  9467280000.0     3.74452E-09
 31557600000.0     2.13295E-09
 94672800000.0      9.4798E-10
   3.15576E+11      4.7399E-10
   9.46728E+11     2.36995E-10
   3.15576E+12      9.4798E-11
   5.36479E+12             0.0
      1.00E+50             0.0
L97 6LMA19                  16     COM2
```

```
      -1.0E+50            0.0
           0.0            0.0
           1.0    3.27053E-08
    31557600.0    3.27053E-08
    94672800.0    3.17573E-08
   315576000.0    5.21389E-09
   946728000.0    5.21389E-09
  3155760000.0     4.6451E-09
  9467280000.0    3.74452E-09
 31557600000.0    2.13295E-09
 94672800000.0     9.4798E-10
   3.15576E+11     4.7399E-10
   9.46728E+11    2.36995E-10
   3.15576E+12     9.4798E-11
   5.36479E+12            0.0
      1.00E+50            0.0
LA7 6LMA20                 16     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0    0.63527E-07
    31557600.0    1.63527E-07
    94672800.0    1.58787E-07
   315576000.0    2.60694E-08
   946728000.0    2.60694E-08
  3155760000.0    2.32255E-08
  9467280000.0    1.87226E-08
 31557600000.0    1.06648E-08
 94672800000.0     4.7399E-09
   3.15576E+11    2.36995E-09
   9.46728E+11    1.18497E-09
   3.15576E+12     4.7399E-10
   5.36479E+12            0.0
      1.00E+50            0.0
L68 6LMA21                 16     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0    0.63527E-09
```

```
    31557600.0     1.63527E-09
    94672800.0     1.58787E-09
   315576000.0     2.60694E-10
   946728000.0     2.60694E-10
  3155760000.0     2.32255E-10
  9467280000.0     1.87226E-10
 31557600000.0     1.06648E-10
 94672800000.0      4.7399E-11
   3.15576E+11     2.36995E-11
   9.46728E+11     1.18497E-11
   3.15576E+12      4.7399E-12
   5.36479E+12             0.0
      1.00E+50             0.0
L78 6LMA22                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     0.63527E-09
    31557600.0     1.63527E-09
    94672800.0     1.58787E-09
   315576000.0     2.60694E-10
   946728000.0     2.60694E-10
  3155760000.0     2.32255E-10
  9467280000.0     1.87226E-10
 31557600000.0     1.06648E-10
 94672800000.0      4.7399E-11
   3.15576E+11     2.36995E-11
   9.46728E+11     1.18497E-11
   3.15576E+12      4.7399E-12
   5.36479E+12             0.0
      1.00E+50             0.0
L88 6LMA23                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     0.63527E-09
    31557600.0     1.63527E-09
    94672800.0     1.58787E-09
   315576000.0     2.60694E-10
```

```
   946728000.0     2.60694E-10
  3155760000.0     2.32255E-10
  9467280000.0     1.87226E-10
 31557600000.0     1.06648E-10
 94672800000.0      4.7399E-11
   3.15576E+11     2.36995E-11
   9.46728E+11     1.18497E-11
   3.15576E+12      4.7399E-12
   5.36479E+12             0.0
      1.00E+50             0.0
L98 6LMA24                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     0.63527E-09
    31557600.0     1.63527E-09
    94672800.0     1.58787E-09
   315576000.0     2.60694E-10
   946728000.0     2.60694E-10
  3155760000.0     2.32255E-10
  9467280000.0     1.87226E-10
 31557600000.0     1.06648E-10
 94672800000.0      4.7399E-11
   3.15576E+11     2.36995E-11
   9.46728E+11     1.18497E-11
   3.15576E+12      4.7399E-12
   5.36479E+12             0.0
      1.00E+50             0.0
LA8 6LMA25                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     8.17633E-09
    31557600.0     8.17633E-09
    94672800.0     7.93933E-09
   315576000.0     1.30347E-09
   946728000.0     1.30347E-09
  3155760000.0     1.16128E-09
  9467280000.0      9.3613E-10
```

```
 31557600000.0     5.33239E-10
 94672800000.0     2.36995E-10
   3.15576E+11     1.18497E-10
   9.46728E+11     5.92487E-11
   3.15576E+12     2.36995E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I42 5LMA26                  16     COM2                                        LMA2
     -1.0E+50              0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I43 5LMA27                  16     COM2
     -1.0E+50              0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
```

```
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I44 5LMA28                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I45 5LMA29                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
```

```
      1.00E+50            0.0
I46 5LMA30                 16     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0    1.30821E-08
    31557600.0    1.30821E-08
    94672800.0    1.27029E-08
   315576000.0    2.08556E-09
   946728000.0    2.08556E-09
  3155760000.0    1.85804E-09
  9467280000.0    1.49781E-09
 31557600000.0    8.53182E-10
 94672800000.0    3.79192E-10
   3.15576E+11    1.89596E-10
   9.46728E+11     9.4798E-11
   3.15576E+12    3.79192E-11
   5.36479E+12            0.0
      1.00E+50            0.0
I47 5LMA31                 16     COM2
      -1.0E+50            0.0
           0.0            0.0
           1.0    1.30821E-08
    31557600.0    1.30821E-08
    94672800.0    1.27029E-08
   315576000.0    2.08556E-09
   946728000.0    2.08556E-09
  3155760000.0    1.85804E-09
  9467280000.0    1.49781E-09
 31557600000.0    8.53182E-10
 94672800000.0    3.79192E-10
   3.15576E+11    1.89596E-10
   9.46728E+11     9.4798E-11
   3.15576E+12    3.79192E-11
   5.36479E+12            0.0
      1.00E+50            0.0
I42 7LMA32                 16     COM2
      -1.0E+50            0.0
```

```
           0.0           0.0
           1.0   1.30821E-08
    31557600.0   1.30821E-08
    94672800.0   1.27029E-08
   315576000.0   2.08556E-09
   946728000.0   2.08556E-09
  3155760000.0   1.85804E-09
  9467280000.0   1.49781E-09
 31557600000.0   8.53182E-10
 94672800000.0   3.79192E-10
   3.15576E+11   1.89596E-10
   9.46728E+11    9.4798E-11
   3.15576E+12   3.79192E-11
   5.36479E+12           0.0
      1.00E+50           0.0
I43 7LMA33                16     COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0   1.30821E-08
    31557600.0   1.30821E-08
    94672800.0   1.27029E-08
   315576000.0   2.08556E-09
   946728000.0   2.08556E-09
  3155760000.0   1.85804E-09
  9467280000.0   1.49781E-09
 31557600000.0   8.53182E-10
 94672800000.0   3.79192E-10
   3.15576E+11   1.89596E-10
   9.46728E+11    9.4798E-11
   3.15576E+12   3.79192E-11
   5.36479E+12           0.0
      1.00E+50           0.0
I44 7LMA34                16     COM2
      -1.0E+50           0.0
           0.0           0.0
           1.0   1.30821E-08
    31557600.0   1.30821E-08
```

```
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I45 7LMA35                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I46 7LMA36                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
```

```
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I47 7LMA37                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     1.30821E-08
    31557600.0     1.30821E-08
    94672800.0     1.27029E-08
   315576000.0     2.08556E-09
   946728000.0     2.08556E-09
  3155760000.0     1.85804E-09
  9467280000.0     1.49781E-09
 31557600000.0     8.53182E-10
 94672800000.0     3.79192E-10
   3.15576E+11     1.89596E-10
   9.46728E+11      9.4798E-11
   3.15576E+12     3.79192E-11
   5.36479E+12             0.0
      1.00E+50             0.0
I42 6LMA38                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
```

```
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
I43 6LMA39                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
I44 6LMA40                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
```

```
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
I45 6LMA41                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
I46 6LMA42                  16     COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
```

```
I47 6LMA43                  16      COM2
      -1.0E+50             0.0
           0.0             0.0
           1.0     3.92464E-08
    31557600.0     3.92464E-08
    94672800.0     3.81088E-08
   315576000.0     6.25667E-09
   946728000.0     6.25667E-09
  3155760000.0     5.57412E-09
  9467280000.0     4.49342E-09
 31557600000.0     2.55955E-09
 94672800000.0     1.13758E-09
   3.15576E+11     5.68788E-10
   9.46728E+11     2.84394E-10
   3.15576E+12     1.13758E-10
   5.36479E+12             0.0
      1.00E+50             0.0
```

```
IFC  ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    A         B         C         D         E         F          FEP 1.3.19
       3.0   1.0E-21      0.25     2.5E4     2.0E6     399.5
    1                        EDZ self-sealing                           FEP  1.4.1
    2                        Number of EDZ types
    2                        Number of materials in EDZ type 1, LMA
EDZl1
EDZl2
this                         File name containing permeability modifier look-up table
    2                        Number of data points in permeability modifier look-up table
       0.0       1.0
   1.57788E11   0.01
this                         File name containing porosity modifier look-up table
    2                        Number of data points in porosity modifier look-up table
       0.0       1.0
   1.57788E11   0.10
   13                        Number of materials in EDZ type 2, all other tunnel EDZs
EDZsf
EDZpi
EDZco
EDZop
EDZac
EDZvt
EDZce
EDZkt
EDZdt
EDZsh
EDZse
bEDZs
bEDZp
this                         File name containing permeability modifier look-up table
    2                        Number of data points in permeability modifier look-up table
       0.0       1.0
   1.57788E10   0.01
this                         File name containing porosity modifier look-up table
    2                        Number of data points in porosity modifier look-up table
```

```
      0.0       1.0
   1.57788E10   0.10
    1                          LMA tunnel convergence                  FEP  1.4.3
    4                          Number of materials defining LMA backfill material
ETlm1
ETlm2
WAlm1
WAlm2
this                           File name containing porosity modifier look-up table
    2                          Number of data points in permeability modifier look-up table
      0.0       1.0
   1.57788E10   0.80
    1                          Uplift                                  FEP  1.4.7
this                           File name containing permeability modifier look-up table
    2                          Number of data points in permeability modifier look-up table
      0.0       1.0
   3.15576E13  100.0
    1                          Geochemical sealing       FEPs 1.5.2, 1.5.4, 1.5.11
    2                          Number of geochemical interface types
   19                          Number of material pairs for 1st interface type
ETsf      EDZsf                Materials defining interface with geochemical sealing
ABUTM     EDZsf
LOCK      EDZsf
ETpil     EDZpi
ABUTM     EDZpi
LOCK      EDZpi
SEAL      EDZse
SEALa     EDZse
ETlm1     EDZl1
ETlm2     EDZl2
Tconn     EDZvt
Tcons     EDZco
Toper     EDZop
Tcent     EDZce
Tacce     EDZac
TacCO     EDZac
Tcont     EDZkt
```

```
Tdeto     EDZdt
Tshaf     EDZsh
 3.15576E09                  Clogging time
 1.0                         Parameter l
 0.4                         Parameter m
 0.01                        Parameter kappa
 0.001                       Sealing layer thickness
    2                        Number of material pairs for 2nd interface type
ETlm1     SEAL               Materials defining interface with geochemical sealing
ETlm2     SEAL
 6.31152E09                  Clogging time
 1.0                         Parameter l
 0.45                        Parameter m
 0.01                        Parameter kappa
 0.001                       Sealing layer thickness

PICNIC --1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1                              Assign total flow to cross section
this                               Read cross sectional information from this file
Repository footprint above         Name used to identify 1. cross section/PICNIC leg
    130.00      0.00   -100.00     X, Y, and Z coordinate of 1. point of quadrilateral
    130.00    800.00   -100.00     X, Y, and Z coordinate of 2. point of quadrilateral
    930.00    800.00   -100.00     X, Y, and Z coordinate of 3. point of quadrilateral
    930.00      0.00   -100.00     X, Y, and Z coordinate of 4. point of quadrilateral
Emplacement tunnel @ CT
    509.00     22.50   -199.90
    509.00     22.50   -197.90
    511.00     22.50   -197.90
    511.00     22.50   -199.90

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure A - 3. Template iTOUGH2-IFC input file

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