TRANSPORT OF RADIONUCLIDES FROM DEEP GEOLOGICAL REPOSITORY / TESTING OF CONCEPTUAL AND NUMERIC MODELS – FINAL REPORT

Authors:
Libor Gvoždík, Petr Kabele, Jakub Říha,
Ondřej Švagera, Dagmar Trpkošová, Aleš Vetešník
et al.

PROGEO, s. r. o.
Roztoky, March 2020
Project name: Research support for the safety assessment of the deep geological repository

Subproject name: Transport of radionuclides from deep geological repository/Testing of conceptual and numeric models

Partial report name: Transport of radionuclides from deep geological repository/Testing of conceptual and numeric models – Final report

Final report

Registration number of the client: SÚRAO TZ 463/2020/ENG

Registration number of the supplier: PB-2020-ZZ-S2222-041-Transport8_EMG

Investigating institutions:
ÚJV Řež, a. s.¹, PROGEO, s. r. o.², Česká geologická služba³, FJFI ČVUT⁴, FSV ČVUT⁵, Technická univerzita v Liberci⁶

Authors: Libor Gvoždík², Petr Kabele⁵, Jakub Říha⁶, Ondřej Švagera³, Dagmar Trpkošová¹, Aleš Vetešník⁴

Team of authors: Zita Bukovská³, Marie Grecká¹, Jakub Jankovec², Jiřina Královcová⁶, Jakub Kryl³, Jiří Maryška⁶, Martin Milický², Jan Uhlík², Patrik Urban⁴, Tereza Zelinková³
# Contents

1 Introduction .................................................................................................................. 14

2 Project methodology and solution procedure .......................................................... 16

3 Measurement of fracture networks and their processing ........................................ 18
   3.1 Sources and methodology of obtaining structural data ........................................ 18
   3.2 Identification of populations and other parameters of the fracture network ..... 20
   3.3 Description of input data for GeoDFN model ...................................................... 23

4 GeoDFN models – DFraM .......................................................................................... 28
   4.1 The concept of modelling rock mass by the DFN method ..................................... 28
   4.2 Content and format of structural-geological data ................................................ 28
   4.3 Assumptions and methods adopted for identification and generation of GeoDFN models in the DFraM v.2 program ................................................................. 30
      4.3.1 Methods of DFN parameter identification based on SG data ....................... 31
      4.3.2 Methods of DFN model generation ............................................................... 32
   4.4 Construction of GeoDFN models ......................................................................... 32
      4.4.1 Model version v0 .......................................................................................... 32
      4.4.2 Model version v1 .......................................................................................... 34
      4.4.3 Model version v2 .......................................................................................... 35

5 HydroDFN – hydraulic and transport models ......................................................... 39
   5.1 Detailed concept of HydroDFN models, boundary conditions ......................... 40
   5.2 Calculation methodology for HydroDFN models in individual software packages ... 42
      5.2.1 ADFNE/GoldSim ....................................................................................... 42
      5.2.2 Flow123d .................................................................................................. 45
      5.2.3 NAPSAC ................................................................................................... 46
   5.3 Uniform fracture network preparation for HydroDFN models ............................ 48
      5.3.1 Version v0 .................................................................................................. 50
      5.3.2 Version v1 .................................................................................................. 54
      5.3.3 Version v2 .................................................................................................. 55
   5.4 Results and comparison – flow and transport simulation .................................... 58
      5.4.1 Version v0 .................................................................................................. 58
      5.4.2 Version v1 .................................................................................................. 62
      5.4.3 Version v2 .................................................................................................. 64
   5.5 Export of results from NAPSAC to GoldSim ...................................................... 69
   5.6 DFN model upscaling into CPM .......................................................................... 71
      5.6.1 Upscaling methodology in NAPSAC software ............................................ 71
6 GoldSim ................................................................................................................................. 76
6.1 GoldSim input parameters, transfer of data from HydroDFN models and data processi
6.2 Selection of transport path (particle trajectory) ................................................................. 78
6.3 Parameters and description of transport path ................................................................. 81
6.4 Model calibration .............................................................................................................. 83
6.5 Transport computations - results of model versions v0 and v1 with use of four tracers
6.6 Sensitivity ......................................................................................................................... 89
7 Assessment, experience, problems with tasks processing and project resolution
7.1 Structural data measurement and processing ................................................................. 93
7.2 Construction of GeoDFN, DFraM .................................................................................... 93
7.2.1 Recommendations regarding the mapping of fracture networks and processing of the data ......................................................... 94
7.2.2 Recommendations for the primary analysis of recorded trace lengths ............ 94
7.2.3 Preliminary proposal of refined methodology for parameter optimization with DFraM v.2 program .............................................. 96
7.3 Processing of HydroDFN models ..................................................................................... 97
7.4 ADFNE/GoldSim ............................................................................................................. 97
7.5 ConnectFlow (NAPSAC, NAMMU) ................................................................................ 98
7.6 Flow123d ......................................................................................................................... 100
7.7 GoldSim .......................................................................................................................... 100
8 Conclusion and proposed next steps ................................................................................. 101
9 Literature ............................................................................................................................. 105
List of figures:

Fig. 1 Localization of documented sections in the area of URF Bukov.................................19

Fig. 2 An example of proceeding of 3D model making of documented section with a description of individual data ..........................................................................................................................20

Fig. 3 (a) Schmidt network; (b) an example of the projection of the surface and the pole of the surface onto the Schmidt network, adapted according to McClay (1987)...............21

Fig. 4 Stereographic projection of poles of measured fractures divided into individual populations and highlighted fractures according to their transmissivity index (TI) with indication of directions of main stresses $\sigma_1$ a $\sigma_3$ ......................................................................................................................22

Fig. 5 Geometry of model version v0 – plan view (left), vertical section (right). The disposal borehole is shown in red, the near-field domain is marked by grey colour. Dimensions are in metres..........................................................33

Fig. 6 Complementary cumulative distribution function of recorded trace lengths. Two anomaly traces with very short length < 0,2 m are marked by a red ellipse .......................35

Fig. 7 Average trace lengths and areal densities of the fracture system traces evaluated for individual populations based on the mapping data and the models .........................37

Fig. 8 Complementary cumulative distribution functions of the fracture system trace lengths evaluated based on the mapping data and on the model.................................38

Fig. 9 Methods for generation of pipes (red lines) in 3D fractures. Left image: central method; right image: triangulation method (adopted from Alghalandis a Xu 2018)...............44

Fig. 10 HydroDFN connective fracture network version v0 generated in NAPSAC – whole network (left), detail near the deposition borehole (right) ........................................51

Fig. 11 Vertical cross-section through GeoDFN and HydroDFN version v0 fracture network (NAPSAC) – connective HydroDFN fractures in yellow, isolated fractures removed from GeoDFN in black.........................................................................................52

Fig. 12 Testing of fracture shape influence on flow and transport – HydroDFN network with octagonal fractures (upper right); relation between octagonal, square and rectangular fracture shape (lower right); comparison of particles trajectories (left) .........................................................53

Fig. 13 GeoDFN (left) a HydroDFN (right) fracture network for model v1 ..............................55

Fig. 14 HydroDFN fracture network for model v2 – original version with low connectivity .......56

Fig. 15 Vertical cross-section of the HydroDFN network through the disposal holes line – original version with low connectivity ...........................................................................56

Fig. 16 Resulting v2 HydroDFN model – vertical cross-section through the disposal holes line ...............................................................................................................................57

Fig. 17 Resulting v2-EDZ HydroDFN model with inclusion of fracture representing the disturbed zone in the tunnel floor - vertical cross-section through the disposal holes line.....58

Fig. 18 Breakthrough curves of advective transport – common assignment of model v0 ......59

Fig. 19 Model v0 – computational network in Flow123d on the left, results of flow simulation in NAPSAC on the right (values of hydraulic height in fractures) .................................60

Fig. 20 Evaluation of the overall flow through the model for 100 various realizations of the fracture network – NAPSAC ........................................................................................................61
Fig. 21 Evaluation of the lengths of trajectories for 100 different fracture network versions – NAPSAC – the graph shows results for 42 disposal boreholes which were interconnected with the fracture network.................................................................61

Fig. 22 Evaluation of the delay times for 100 different fracture network versions – NAPSAC – the graph shows results for 42 disposal boreholes which were interconnected with the fracture network .................................................................62

Fig. 23 Breakthrough curves of advective transport – common assignment of model v1 ......63

Fig. 24 Model v1 – computational network in Flow123d on the left, results of flow simulation in NAPSAC on the right (values of hydraulic height in fractures) .................................................................64

Fig. 25 Model v1 – velocity field plotted for the source fracture intersecting the disposal borehole........................................................................................................................................64

Fig. 26 Model v2 – results of flow simulation in Flow123d, gradient in the direction of axis x on the left, gradient in the direction of axis y on the right .................................................................65

Fig. 27 Model v2 – NAPSAC – delay times (breakthrough curves) for advective transport from individual disposal boreholes – gradient X (left) and gradient Y (right) .................................................................67

Fig. 28 Comparison of summary breakthrough curves for the model variants executed in NAPSAC ........................................................................................................................................67

Fig. 29 Model v2 – particle tracking simulation in NAPSAC – gradient in the direction of axis x – version without tunnel on the left, version with EDZ on the right .................................................................68

Fig. 30 Model v2 – particle tracking simulation in NAPSAC – gradient in the direction of axis y – version without tunnel on the left, version with EDZ on the right .................................................................68

Fig. 31 Hydraulic conductivity of CPM model obtained by DFN model upscaling in NAPSAC – model version v0, model size 100x100x100 m, regular grid of CPM model with cell size 5x5x5 m........................................................................................................................................73

Fig. 32 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v0 calculated in NAPSAC and NAMMU, regular grid of CPM model with the cell size of 5x5x5 m........................................................................................................................................74

Fig. 33 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v0 calculated in NAPSAC and NAMMU, regular grid of CPM model with the cell size of 2x2x2 m........................................................................................................................................74

Fig. 34 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v1 calculated in NAPSAC (DFN) and MT3D (CPM), regular grid of CPM model with the cell size of 2x2x2 m ........................................................................................................................................74

Fig. 35 Visualisation of 100 transport paths (with one starting point) exported from HydroDFN model. Sections of macrofractures are distinguished in colour according to the value of transport aperture........................................................................................................................................75

Fig. 36 Radiological criterion R₁, order of particles is based on ascending F-quotient ........80

Fig. 37 Radiological criterion R₂, order of particles is based on ascending F-quotient ........80

Fig. 38 Particles sorted by ascending value of total F-quotient ........................................81

Fig. 39 Selection of transport paths and macrofractures intersected by certain particles .....82

Fig. 40 Parameters of the transport path segment ................................................................82
Fig. 41 Particles sorted by ascending F-quotient, data from hydrogeological model (interim version v0) were available for red coloured particles ..........................................................84

Fig. 42 Conformity of total balance from MODFLOW and GoldSim simulations ..................84

Fig. 43 Comparison of mass flow rate from MODFLOW and GoldSim simulations for two selected particles 46 and 54 ..........................................................85

Fig. 44 Comparison of mass flow rate from MODFLOW and GoldSim simulations for two selected particles 91 a 94 ..........................................................86

Fig. 45 Comparison of mass flow rate from MODFLOW simulation for four particles with very similar F-quotient ..........................................................86

Fig. 46 Transport model version v0 – comparison of results. Red lines - ÚJV, blue lines – FJFI with use of ADFNE flow results, green lines – FJFI with use of NAPSAC flow results .......88

Fig. 47 Transport model version v1 – comparison of results. Red lines - ÚJV, blue lines – FJFI with use of ADFNE flow results, green lines – FJFI with use of NAPSAC flow results .......88

Fig. 48 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer A, model v0 ..........................................................89

Fig. 49 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer B, model v0 ..........................................................89

Fig. 50 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer C, model v0 ..........................................................90

Fig. 51 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer D, model v0 ..........................................................90

Fig. 52 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer A, model v1 ..........................................................90

Fig. 53 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer B, model v1 ..........................................................91

Fig. 54 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer C, model v1 ..........................................................91

Fig. 55 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer D, model v1 ..........................................................91

Fig. 56 Comparison of unit mass flow rate of tracer A in case of different fracture width, model v0 ...........................................................................................................91

Fig. 57 Comparison of unit mass flow rate of tracer B in case of different fracture width, model v0 ...........................................................................................................92

Fig. 58 Comparison of unit mass flow rate of tracer C in case of different fracture width, model v0 ...........................................................................................................92
Fig. 59 Complementary cumulative frequency of trace length obtained from the survey and from the model. Colour dashed lines correspond to power-law distribution.

List of tables:

Tab. 1 Localization and marking of measured sections at URF Bukov ..................................................19
Tab. 2 Percentage of transmissivity indexes (TI) for individual populations .................................23
Tab. 3 Example of field SG documentation.........................................................................................24
Tab. 4 List of individual terms, which contains field SG documentation with their explanation ........................................................................................................................................25
Tab. 5 Example of input *.xlsx file with SG data to DFraM program....................................................27
Tab. 6 List of individual terms contained in SG documentation modified for DFraM with their explanation ........................................................................................................................................27
Tab. 7 Input parameters for generation of GeoDFN model version v0 in program DFraM v.2. Parameter xmin applies to the distribution of the circumscribed ellipses’ semi-major axis length ........................................................................................................................................33
Tab. 8 Parameters of the GeoDFN model version v1 identified on the basis of SG data from site 296 URF Bukov. Parameter xmin applies to the distribution of the circumscribed circles’ radii ........................................................................................................................................34
Tab. 9 Initial values used for the optimization of GeoDFN model version v2. Parameter xmin applies to the distribution of the circumscribed circles’ radii........................................................................................................................................36
Tab. 10 Parameters of the GeoDFN model version v2 identified on the basis of SG data from site 296 URF Bukov. Parameter xmin applies to the distribution of the circumscribed circles’ radii ........................................................................................................................................36
Tab. 11 Characteristics of the fracture system traces evaluated from the mapping data and from the models ........................................................................................................................................37
Tab. 12 Overview of basic fracture parameters in a vtk file created for hydrogeological models in NAPSAC ........................................................................................................................................50
Tab. 13 Fracture population parameters used for model v0 GeoDFN generation in NAPSAC ........................................................................................................................................51
Tab. 14 Characterization and discretisation of computational mesh in individual SW .........................52
Tab. 15 Basic summary of GeoDFN a HydroDFN model characteristics .................................54
Tab. 16 Overview of flow and transport simulation results – common assignment, model v0 ........................................................................................................................................59
Tab. 17 Overview of flow and transport simulation results – common assignment, model v1 ........................................................................................................................................63
Tab. 18 Model v2 – NAPSAC – the values of specific flows at source points of the intersections of the disposal boreholes and the fracture network ........................................................................................................................................66
Tab. 19 Structure of *.sum output file .....................................................................................................69
Tab. 20 Structure of *.list output file .....................................................................................................70
Tab. 21 Structure of *.MACROFRACTURES_Q.list output file ..............................................70
Tab. 22 Parameters $G_N$ and $H_N$ for calculation of criteria $R_1$ and $R_2$ (Posiva 2014) ........79
Tab. 23 Example of transport parameters. Parameters with label PipeX are parameters corresponding to certain transport path segment for one certain particle, parameters with label pathX apply to all parts of the transport path of one particle.................................................................83
Tab. 24 Length (in metres) of selected transport path segments of particles 1 – 5 (each transport path is consisted of total 20 segments).................................................................83
Tab. 25 Transport parameters of four fictional tracers used in comparative computation......87
List of abbreviations:

1D one-dimensional
2D two-dimensional
3D three-dimensional
CPM continuous porous medium
CGS Czech Geological Survey
CTU Czech Technical University in Prague
DFN discrete fracture network
ECPM equivalent continuous porous medium
EDZ excavation disturbed zone
FJFI Faculty of Nuclear Sciences and Physical Engineering at CTU
FSV Faculty of Civil Engineering at CTU
GS GoldSim
HG hydrogeological
RM rock massif
DGR deep geological repository for radioactive waste
MLMC Multi Level Monte Carlo
PFL Posiva flow-log – an equipment developed by Posiva Oy for measurement of conductive fractures
URF underground research facility (Bukov in this case)
RW radioactive waste
SG structural geology, structural-geological
SW software
SKB the Swedish Nuclear Fuel and Waste Management Company
SÚRAO Radioactive Waste Repository Authority
TI transmissivity index
TUL Technical University of Liberec
ÚJV ÚJV Řež, a. s.
WDP waste disposal package
Abstract
The main purpose of the current report is to review and document the existing approaches, tools and input data regarding the radionuclides transport from deep geological repository. The part of the rock mass between disposal holes and major hydraulically conductive features is the subject of interest. The main content of the project was:

- characterization of fracture systems in selected part of URF Bukov and processing of the input measured data for geological models,
- optimization of fracture population parameters based on measured data and preparation of detailed geological GeoDFN models in DFraM software,
- processing and evaluation of hydrogeological HydroDFN models of the groundwater flow and the advective transport in NAPSAC, Flow123d and ADFNE software,
- interaction and transfer of the modelling results from HydroDFN models to GoldSim
- an important part was the development and testing of procedures and methodologies both in individual phases of the project and in the mutual interconnection of results and data between investigators and software.

Keywords
deep geological repository, groundwater flow, radionuclide transport, conductive fractures, discrete fracture network modelling

Abstrakt
Hlavním cílem řešeného úkolu T8 bylo dokumentovat a analyzovat (případně doplnit nebo modifikovat do vlastních postupů) existující přístupy a vybraná vstupní data pro popis transportu radionuklidů z prostoru hlubinného úložiště v blízkém okolí UOS. Základní náplní projektu byla:

- charakterizace puklinových systémů ve vybrané části PVP Bukov a zpracování vstupních měřených dat pro geologické modely,
- optimalizace parametrů puklinových populací na základě měřených dat a příprava detailních geologických GeoDFN modelů v programu DFraM,
- zpracování a vyhodnocení hydrogeologických HydroDFN modelů proudění podzemní vody a advektivního transportu v programech NAPSAC, Flow123d a ADFNE,
- interakce a převod výsledků hydraulických a transportních modelů do modelu GoldSim,
- důležitou součástí byl vývoj a testování postupů a metodik jak v dílčích samostatných fáziích projektu, tak při vzájemném propojení výsledků a dat mezi jednotlivými řešiteli a softwary.

Klíčová slova
hlubinné úložiště, proudění podzemní vody, advektivní transport, charakteristiky puklin, model diskrétní puklinové sítě
1 Introduction

This report was compiled as part of the SÚRAO-commissioned “Research Support for the Safety Assessment of a Deep Geological Repository” project which forms part of the development programme for the construction of the future Czech deep geological repository for radioactive waste (hereinafter referred to as DGR). The objective of the project is to collect the data, models, arguments and other information required so as to be able to construct the models necessary for the evaluation of potential sites for the construction of the DGR from the point of view of long-term safety. Following the conclusion of a public procurement procedure, a four-year contract was signed in July 2014 with ÚJV Řež, a.s. and its various subcontractors: the Czech Geological Survey; the Czech Technical University in Prague; the Technical University of Liberec; the Institute of Geonics of the Czech Academy of Sciences; and the Arcadis CZ a.s., PROGEO s.r.o.; Chemcomex Praha, a.s. and Research Centre Řež s.r.o. corporations on the provision of research support for the assessment of long-term safety in the following areas:

i. The behaviour of spent nuclear fuel (SNF) and those forms of radioactive waste (RAW) that are not suitable for disposal in surface repositories in a deep geological repository environment.

ii. The behaviour of SNF and RAW waste disposal packages (WDP) in a deep geological repository environment.

iii. The behaviour of buffer backfill and other construction materials in a deep geological repository environment.

iv. Disposal chamber boring techniques and their influence on the properties of the surrounding rock environment.

v. The behaviour of the rock environment.

vi. The transport of radionuclides from the DGR.

vii. Other characteristics of the candidate sites which may potentially affect overall DGR safety.

The main objective of this partial project “Transport of Radionuclides from Deep Geological Repository / Testing of Conceptual and Numeric Models” (Transport 8; T8) was to use suitable software tools for testing the flow and transport of radionuclides in fracture systems of the isolating part of the rock massif between the wall of the disposal borehole and the area connected to regional conductive structures. This final paper documents the performed works and results obtained during project execution. The final chapter summarizes the recommendations and ideas for the follow-up works.

Scope of the Transport 8 project:

- Posiva and SKB literature search with focus on description of the fracture environment and DFN modelling – dealt with in a separate report by Milický et al. (2019),
- Characterization of fracture systems in selected part of URF Bukov – field measurement, processing of input data for geological models – performed by the staff of the Czech Geological Survey (CGS),
- Preparation of detailed geological models (GeoDFN) in DFraM software – determination (calibration) of parameters of fracture populations on the groundwork of measured data, GeoDFN models generation – performed by the staff of the Faculty of Civil Engineering of the Czech Technical University in Prague (FSV),
• Processing of hydrogeological models (HydroDFN) of groundwater flow and transport of radionuclides based on the DFN method – simulated in NAPSAC, Flow123d, and ADFNE programs and performed by the staff of PROGEO, Technical University of Liberec (TUL) and Faculty of Nuclear Sciences and Physical Engineering of the Czech Technical University in Prague (FJFI),

• Interaction and transfer of the results from hydraulic and transport models into GoldSim model enabling interconnection of processes in the field of close and remote interactions – performed by the staff of ÚJV Řež (ÚJV) and FJFI,

• Analysis of results of the processed models and evaluation of the importance of fractures and their mutual connectivity for the transport of radionuclides in the isolating part of the massif,

• Important part was the development and testing of procedures and methodologies in both individual partial project phases and during mutual interconnection of the results and data among individual solvers (output data from one project phase became the input data in the follow-up phase).
2 Project methodology and solution procedure

The project resolution procedure was based on its assignment, defined goals, and proposed schedule of the works. Isolating part of the rock massif within the Transport 8 project represents a hypothetical block of the rock massif around the DGR, respectively in the vicinity of the disposal borehole. Border of this block is delimited by the nearest envisaged permeable fault zones or major open fractures in the distance of 50 meters from the disposal borehole. The block of the isolating part of the massif is not completely impermeable - it is disturbed by a mutually interconnected network of less important fractures.

In the first phase of the project, we performed a foreign literature search dealing with the issue of fracture systems in depths corresponding to that of the DGR. At the same time, we performed structural measurement of fractures in URF Bukov in order to provide real input data for geological models processing as early as possible. At the same time, we started working on generation of a stochastic GeoDFN fracture model version v0, which was based on the data obtained from the literature search. A methodology for detailed HydroDFN models was also discussed and approved in the initial phase of the project.

GeoDFN models covering the block of interest within the rock massif were prepared on the groundwork of the processed structural data from URF Bukov during the next phase of the project. At the same time, HydroDFN model version v0 was created and the flow and advective transport were calculated in order to allow for commencement with work on the transport models in GoldSim software.

HydroDFN model versions v1 and v2 were prepared and flows and advective transport in the fracture network were calculated on the groundwork of generated GeoDFN models in the last phase of the project. Parallel simulations were carried out in three software packages and the achieved results were continuously compared and presented. Upscaling of the DFN fracture network into CPM model was performed in model versions v0 and v1 and results obtained in both conceptual approaches were compared. Influence of tunnel’s EDZ on tracer transport was simulated in model version v2. At the same time, detailed flow and advective transport results were exported from NAPSAC software for all model versions and these were then used as the groundwork for transport simulations processing in GoldSim software for 4 fictive tracers with various parameters of diffusion and sorption in the rock matrix.

Detailed methodologies and procedures used while working on individual parts of the project are described in relevant chapters:

- Measurement of fractures and collection of structural data in Chapter 3,
- Identification and creation of GeoDFN models in Chapter 4,
- Preparation of HydroDFN models and advective transport calculation in Chapter 5,
- Realization of transport models in GoldSim software in Chapter 6.

Due to a relatively short project duration (approximately 1 year) and broad scope of the preformed works, some key areas of the project received more attention to the detriment of others, less important for the overall project result. Works, which had to be preferred, were based on the unique character of the Transport 8 project – this was the first project organized by SÚRAO which also included HydroDFN modelling (GeoDFN models were already included in the project documented by Kabele et al. 2018). In many cases, it was therefore necessary to adapt the original procedures or develop new procedures for data processing and exchange. Many situations revealed that the specialized software tools for DFN modelling had their limits.
or that their declared functions were not suitable for given task type and it was necessary to seek for alternative solutions. The experience collected during the project is summarized in Chapter 7 by individual solvers. Chapter 8 provides a conclusion from the works and also a proposal regarding the next steps.
3 Measurement of fracture networks and their processing

Structural measurements, in this case a set of information about brittle fractures such as joints or faults, are the source data for creating valid mathematical models of the fracture network (DFN, de facto GeoDFN and HydroDFN). The files contain essential information about the orientation and strike of these structures, as well as their spatial links (terminations), characteristics of mineral fillings, water conduction, or indications about the presence of water on these structures in the past (e.g. limonitization). By preparing this data using a unified methodology and using a modern workflow on models in 3D, it is possible to achieve extensive datasets providing all available information that enters the processes of mathematical modelling of DFN.

3.1 Sources and methodology of obtaining structural data

Two data sources were used as the input structural geological data for this project. The first was an archive data file obtained from the URF Bukov in the framework of the project Characterization of the URF Bukov (Bukovská et al. 2017), which was also conceptually used for the creation of a DFN model of the URF area in the project Mathematical modelling of rock massif by the DFN method (Kabele et al. 2018). This dataset was based on a combination of structural mapping and its plotting on a 3D model of URF corridors (access corridor BZ–XIIJ and corridor B–XII), created by laserscanning. The aim was to cover domains with the occurrence of water saturated fractures, where it was at least generally possible to express the potential of surrounding fractures for water conduction, i.e. transmissivity, hereinafter referred to as TI or transmissivity index. After analysing the available data from the archive materials, it was found that the amount and the resulting quality of the data did not fully meet the purposes of this project. The methodology for the creation of geological DFN models (GeoDFN) is a systematic activity, which requires a methodological procedure during the actual collection of this data. The basic principles of this methodology are described in Kabele et al. (2018) and with other related projects this methodology is being constantly extended and improved.

The second source of data was new structural data obtained from the accessible area of URF Bukov where localized tributaries of groundwater and related water saturated fractures occurred. Based on reconnaissance of the PVP area, 5 documented localities were determined (Fig. 1). These are places with tributaries shown in Tab. 1.
Tab. 1 Localization and marking of measured sections at URF Bukov

<table>
<thead>
<tr>
<th>The original name of the inflow</th>
<th>URF corridor</th>
<th>Marking the documentation point</th>
<th>The length of the section in the corridor</th>
</tr>
</thead>
<tbody>
<tr>
<td>BK06</td>
<td>B–XIIJ</td>
<td>2960001</td>
<td>165–184 m</td>
</tr>
<tr>
<td>BK15</td>
<td>B–XIIJ</td>
<td>2960002</td>
<td>200–214 m</td>
</tr>
<tr>
<td>BK31</td>
<td>BZ₁–XII</td>
<td>2960003</td>
<td>10–26 m</td>
</tr>
<tr>
<td>BK32</td>
<td>BZ₁–XII</td>
<td>2960004</td>
<td>25–37 m</td>
</tr>
<tr>
<td>BK35</td>
<td>BZ₁–XII</td>
<td>2960005</td>
<td>57–69 m</td>
</tr>
</tbody>
</table>

In order to obtain a representative dataset from the above mentioned sections, photogrammetric models were created on the basis of photographic documentation in Agisoft Metashape (Fig. 2), which were subsequently referenced in MOVE using the ground plan of corridors obtained from DIAMO s.p. and clearly defined areas measured in-situ by geological compass. In addition, the structural measurements were also plotted into the five models in MOVE, which are localized by an in-situ graphic drawing of structures on the photograph, which is taken together with the structural measurements (Fig. 2). In this way, it is possible to link the acquired structural record to the 3D model of the documented section, hereinafter referred to as the so-called “observation window”, with the corresponding model surface.
3.2 Identification of populations and other parameters of the fracture network

Among the key methods for successful creation of the GeoDFN model is the distribution of structural geological (SG) data into individual populations based on their spatial characteristics. The individual populations are delineated from the projection of the area defined by the direction of inclination (azimuth) and the inclination (dip) on the lower hemisphere in the Schmidt equal-area projection. In this projection, the structures are represented as great circles (curves following the meridian of inclination, whose top points towards the azimuth). For the projection of large amounts of data and their separation into populations, the poles of these planes are projected, which are a point representation of the top of a great circle projected through the center of the hemisphere by 90° (Fig. 3). These projections create a cloud of points from which individual populations can be determined. If the point projections of poles of the planes form visible clusters, they can be included in one of the populations. The steep structures whose poles occur at the edge of the projection can be grouped into the same populations, although their azimuth is exactly the opposite, since the mechanism of their formation or reactivation was probably the same and originated in a similar stress regime.
In this project, a total of 9 populations covering all measured data and their directions were extracted from the obtained SG data (400 measurements). From these populations, the GeoDFN parameters are estimated, which are described in the following chapters. Theoretically, even more populations can be found, but it should be taken into account that the data is subsequently processed statistically and too small datasets cannot be properly evaluated. Therefore, it is necessary to take an individual approach to each dataset. Also with each population, there is a need for this population to determine the parameters of the statistical distributions of the DFN model (see chapter 4), a process with high computational time requirements.

Another parameter determined for individual fractures and subsequently for individual populations is the so-called transmissivity index, which represents the potential of individual fractures to conduct water and with it potentially leaked radionuclides into the surrounding rock mass (RM). This information is important to create a connective HydroDFN network, but its identification is not easy. For the basic characterization of conductive and non-conductive structures, field mapping in the area of the URF Bukov was used, where 5 long-term active fractures were identified. These correspond to the locations of selected documented sections (BK06, BK15, BK31, BK32 and BK35). In their surroundings, structures associated with these fractures or using local saturation of RM by water penetrating through were identified. These also showed signs of active (wet surface of the structure or dripping or flowing water) or already extinct (limonitization, sinters, precipitated mineral film etc.) aquifers. These structures were considered to be actively conductive for the purpose of the project.

The aim of investigating and documenting conductivity characteristics is not to determine precisely which structures in the documented rock mass are permeable, as this task would require using of RM characteristics in a much wider area, including detailed studies from drilling works made underground and especially on the surface by deep boreholes, where it would be possible to monitor changes in the activity of individual fractures and failures across the vertical depth profile. For the characterization of RM in terms of conductivity, the project used knowledge from the projects Posiva (Mattila and Tammisto 2012) or TRUE, where the large datasets and a number of deep boreholes identified properties of RM fractures and their relations to individual stress components measured at different depths of HM. These projects are described in more detail in the research Milicky et al. (2019). The approach to identifying potentially conductive fractures within the project reflected these studies.
In particular, knowledge about the influence of stress tensor on the opening or reactivation of fractures was applied. Due to the limited amount of information about the stress state of RM in the URF Bukov, the findings of the project Characterization of the URF and the resulting measurements of the stress state determined by the Institute of Geonics AS CR were applied. The maximum compressional stress \( \sigma_1 \) in the case of the best performing tests on boreholes KS3 and KS4 is sub-horizontal in the direction of 41° de facto. 221° and the smallest compressional stress \( \sigma_3 \) determining the potential opening direction of the structures was also determined to be sub-horizontal and perpendicular to \( \sigma_1 \) (Souček et al. 2017). Potentially conductive structures were considered to be subvertical (inclination of approx. 80 – 90°), having the same strike with \( \sigma_1 \) in the range up to 5° and had thus undergone the maximum dilatation in the \( \sigma_3 \) direction. These structures were identified as potentially conductive and were assigned a transmissivity index (TI) of 2. Structures on which the presence of water was documented within the URF were identified as conductive and assigned TI 1. Other structures were designated TI 0 and were considered as non-conductive.

![Fig. 4 Stereographic projection of poles of measured fractures divided into individual populations and highlighted fractures according to their transmissivity index (TI) with indication of directions of main stresses \( \sigma_1 \) and \( \sigma_3 \)](image)

The resulting data were recalculated to the percentage of TI in individual populations (Tab. 2) and a table was created, which was used for the follow-up modelling. The aim was to achieve a percentage of permeable fractures in individual populations, such as those obtained in the Posiva projects, where the maximum permeable fractures in the datasets ranged to about 5% for RMM depths from 300 to 600 m (Mattila and Tammisto 2012). As can be seen from the plotted TI of Fig. 4, the conductive fractures do not fully correspond to the potentially conductive fractures. Indeed, a higher percentage of potentially conductive fractures relates only to the hypothetical possibility that these fractures could become conductive, based on the above-described stress state of RM. Further study of the stress state of RM, e.g. by overcoring methods at deep borehole intervals, could better define the boundary conditions for these potentially conductive fractures and thus refine the input model parameters.
3.3 Description of input data for GeoDFN model

The input data for the GeoDFN model, as mentioned in the previous chapter, must have a uniform structure. As an example Tab. 3 and

<table>
<thead>
<tr>
<th>Population</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>Sum [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>43.48</td>
<td>2.17</td>
<td>54.35</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>78.57</td>
<td>2.38</td>
<td>19.05</td>
<td>100</td>
</tr>
<tr>
<td>3</td>
<td>16.67</td>
<td>0.00</td>
<td>83.33</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>93.33</td>
<td>3.33</td>
<td>3.33</td>
<td>100</td>
</tr>
<tr>
<td>5</td>
<td>98.25</td>
<td>0.00</td>
<td>1.75</td>
<td>100</td>
</tr>
<tr>
<td>6</td>
<td>95.00</td>
<td>3.33</td>
<td>1.67</td>
<td>100</td>
</tr>
<tr>
<td>7</td>
<td>96.97</td>
<td>3.03</td>
<td>0.00</td>
<td>100</td>
</tr>
<tr>
<td>8</td>
<td>95.83</td>
<td>2.78</td>
<td>1.39</td>
<td>100</td>
</tr>
<tr>
<td>9</td>
<td>92.59</td>
<td>5.56</td>
<td>1.85</td>
<td>100</td>
</tr>
</tbody>
</table>
Tab. 4 provides a record and explanation of field documentation, which is commonly used in structural mapping and is extended by several terms that are critical to DFN modelling. It is mainly a record of ending of individual fractures and unique identifier (ID) of structures.

**Tab. 3 Example of field SG documentation**

<table>
<thead>
<tr>
<th>DFN</th>
<th>Position (m)</th>
<th>B typ</th>
<th>A, B, Z, Z, D, FA</th>
<th>Dip</th>
<th>Endin g_on</th>
<th>Lenght (m)</th>
<th>N- of fractures</th>
<th>N- of fractures</th>
<th>Thickness (mm)</th>
<th>Water</th>
<th>Str_east dip</th>
<th>Str_dip</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>45</td>
<td>174.6</td>
<td>P</td>
<td>290</td>
<td>85</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>175.3</td>
<td>E</td>
<td>297</td>
<td>54</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>47</td>
<td>176.0</td>
<td>P</td>
<td>119</td>
<td>65</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>48</td>
<td>176.2</td>
<td>P</td>
<td>190</td>
<td>59</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>176.9</td>
<td>P</td>
<td>38</td>
<td>73</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>176.8</td>
<td>P</td>
<td>109</td>
<td>73</td>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: DFN = Decision Field Network; SG = Section Group; B typ = B type; A, B, Z, Z, D, FA = Additional terms critical to DFN modelling.
Tab. 4 List of individual terms, which contains field SG documentation with their explanation

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFN</td>
<td>Recording of unique number of measured structure in a given section</td>
</tr>
<tr>
<td>Position</td>
<td>Measurement position in relation to the corridor length</td>
</tr>
<tr>
<td>S type</td>
<td>Type of measured structure (S - foliation; P - fracture; PZ - fracture zone; Z - fault ...)</td>
</tr>
<tr>
<td>Dip azimuth</td>
<td>Direction of inclination of measured structure</td>
</tr>
<tr>
<td>Dip</td>
<td>Inclination of the measured structure</td>
</tr>
<tr>
<td>Ending on</td>
<td>Number of the structure on which the measured structure ends</td>
</tr>
<tr>
<td>Length</td>
<td>Estimated structure length - an additional information when it is possible that this structure will be less visible in the 3D model</td>
</tr>
<tr>
<td>N of fractures</td>
<td>Number of structures of similar orientation in the vicinity - additional information for understanding the spatial relationships of structures</td>
</tr>
<tr>
<td>N of fractures/length unit</td>
<td>The number of structures of the same orientation per unit of length - is given especially for fracture zones</td>
</tr>
<tr>
<td>Infill</td>
<td>Mineral infill of the structure</td>
</tr>
<tr>
<td>Thickness</td>
<td>Mineral infill thickness of structure in mm; if the filler is less than 1 mm, the value is given as the so-called „hair filler“</td>
</tr>
<tr>
<td>Water</td>
<td>The fracture is aquiferous, or there are signs of water on its surface or surroundings</td>
</tr>
<tr>
<td>Str azimuth</td>
<td>Direction of inclination of linear kinematic indicators, so-called striations, from which it is possible to estimate the sense of motion on a given surface</td>
</tr>
<tr>
<td>Str dip</td>
<td>Inclination of linear kinematic indicators</td>
</tr>
<tr>
<td>Sense</td>
<td>Sense of movement on the surface (D - dextral; S - sinistral; N – normal fault; T – thrust fault)</td>
</tr>
<tr>
<td>Comment</td>
<td>Additional comments related to the structure</td>
</tr>
</tbody>
</table>
Tab. 5 and Tab. 6 shows an example of the same data, but already in a format that is readable in DFraM, and also contains information about distribution of fractures into populations, extent of fracture IDs, and determination of lines start points and lines end points that represent traces of fractures in documented sections, de facto observation windows. Measurement positions, fracture trace lengths and transmissivity indexes for each fracture are also included in the table as additional information.
Tab. 5 Example of input *.xlsx file with SG data to DFraM program

<table>
<thead>
<tr>
<th>Name</th>
<th>Unique fracture ID consisting of number of locality, number of outcrop, number of wall of outcrop and number of fracture</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dip</td>
<td>Inclination of fracture after possible modification in MOVE, which enters the GeoDFN calculation</td>
</tr>
<tr>
<td>Azimuth</td>
<td>Direction of inclination of fracture after possible modification in MOVE</td>
</tr>
<tr>
<td>Strike</td>
<td>Direction of the fracture strike, which is based on the measurement of the direction of inclination, and which enters the GeoDFN calculation</td>
</tr>
<tr>
<td>Population</td>
<td>Number of population into which the fracture belongs</td>
</tr>
<tr>
<td>Ending on population</td>
<td>ID of the fracture on which the documented fracture ends</td>
</tr>
<tr>
<td>Ending on population</td>
<td>Fracture populations where the documented fractures ends</td>
</tr>
<tr>
<td>X,Y,Z measurement</td>
<td>X, Y and Z coordinates of the measurement position on the documented section (3D model) in the S-JTSK coordinate system</td>
</tr>
<tr>
<td>X,Y,Z start point</td>
<td>X, Y and Z coordinates of the beginning of the fracture trace on the documented section (3D model) in the S-JTSK coordinate system</td>
</tr>
<tr>
<td>X,Y,Z end point</td>
<td>X, Y and Z coordinate of the end of the fracture trace on the documented section (3D model) in the S-JTSK coordinate system</td>
</tr>
<tr>
<td>Length</td>
<td>Fracture trace length</td>
</tr>
<tr>
<td>Transmissivity</td>
<td>The transmissivity index, which takes values from 0 to 2</td>
</tr>
</tbody>
</table>

Tab. 6 List of individual terms contained in SG documentation modified for DFraM with their explanation

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unique fracture ID</td>
<td>Consists of the number of locality, number of outcrop, number of wall of outcrop and number of fracture.</td>
</tr>
<tr>
<td>Dip</td>
<td>Inclination of fracture after possible modification in MOVE.</td>
</tr>
<tr>
<td>Azimuth</td>
<td>Direction of inclination of fracture after possible modification in MOVE.</td>
</tr>
<tr>
<td>Strike</td>
<td>Direction of the fracture strike, which is based on the measurement of the direction of inclination, and which enters the GeoDFN calculation.</td>
</tr>
<tr>
<td>Population</td>
<td>Number of population into which the fracture belongs.</td>
</tr>
<tr>
<td>Ending on ID</td>
<td>ID of the fracture on which the documented fracture ends.</td>
</tr>
<tr>
<td>Ending on population</td>
<td>Fracture populations where the documented fractures ends.</td>
</tr>
<tr>
<td>X,Y,Z measurement</td>
<td>X, Y and Z coordinates of the measurement position on the documented section (3D model) in the S-JTSK coordinate system.</td>
</tr>
<tr>
<td>X,Y,Z start point</td>
<td>X, Y and Z coordinates of the beginning of the fracture trace on the documented section (3D model) in the S-JTSK coordinate system.</td>
</tr>
<tr>
<td>X,Y,Z end point</td>
<td>X, Y and Z coordinate of the end of the fracture trace on the documented section (3D model) in the S-JTSK coordinate system.</td>
</tr>
<tr>
<td>Length</td>
<td>Fracture trace length.</td>
</tr>
<tr>
<td>Transmissivity</td>
<td>The transmissivity index, which takes values from 0 to 2.</td>
</tr>
</tbody>
</table>
4 GeoDFN models – DFraM

Identification of parameters and generation of GeoDFN models in the present task T8 is based on the methodology and computer program DFraM v.1, which were developed in the course of realization of the previous project “PB-2016-ZL-U1351-030-DFN Mathematical modelling of brittle fractures in rock mass by means of the DFN method” and which are described in detail in the project final report (Kabele et al. 2018). The original methodology has been further elaborated and the DFraM code has been refined and developed (DFraM v. 2) based on new findings and experience.

4.1 The concept of modelling rock mass by the DFN method

Hydrogeological (HG) transport and retention properties of rock mass are dominantly affected by the presence of brittle structures – faults and fractures. Brittle structures occur in different sizes. For HG simulations on block-scale models, it is necessary, in particular, to take into account small fractures (with sizes on the order of $10^{-1}$–$10^{-1}$ m) as well as large structures with lengths reaching the order of $10^1$ – $10^2$ m. As we have described in the previous chapter, geological information on orientation, size, and abundance of these structures is obtained mainly by mapping their traces on areal exposures of the rock mass (outcrops, tunnel walls) or from borehole logs. The larger structures are less frequent and their position and geometry can be usually described in a deterministic way. On the contrary, smaller fractures occur, even in a compact rock mass, in enormous quantities ($10^{-1}$ – $10^1$ per 1 m$^3$). Discrete Fracture Network (DFN) is one of the possible approaches to modelling of these fractures for the purpose of HG computations. Individual fractures are represented as spatially distributed planar entities (usually polygons). Considering the fractures’ large quantity, DFN models are formulated in a statistical sense, that is, location, orientation, and size of the fractures are described by means of appropriate statistical distributions. As structural-geological (SG) mapping methods provide only very limited insight into the rock-mass volume, parameters of these distributions are determined by inverse analysis so as to achieve the best possible correspondence between the recorded SG data and the model. Once the statistical models’ parameters are identified, it is possible to generate an arbitrary number of random realizations of fracture networks, so-called GeoDFN models. GeoDFN models of block size consist of hundreds of thousands to millions of fractures. However, many of these fractures are not connective or conductive, thus, they may be ignored in HG simulations. Such reduced models are then called HydroDFN. The subject of the present chapter is the construction of GeoDFN models, while their reduction to HydroDFN will be dealt with in the subsequent chapter.

4.2 Content and format of structural-geological data

Version 2 of DFraM program makes it possible to identify parameters of DFN models based on data acquired by mapping and pre-processing (see Chapter 3) of fracture traces on areal exposures of the rock mass, such as outcrops or tunnel walls. Data must be supplied in the form of xlsx files, which must strictly comply with the following format:

Individual observation areas (e.g. outcrops) are labeled by strings with structure xxxxxxxy, where:

- $xxx$ ... are 3 digits indicating the site (following the SÚRAO system),
• yyyy ... are 4 digits indicating the location of observation (e.g. outcrop location),
• a ... is a letter a, b, c, etc. indicating the specific observation surface (window), e.g.,
  when an outcrop is split to several planar sub-regions (see Kabele et al. 2018). If the
  observation location consists of only one surface, then the letter a is used.

Individual fracture traces recorded on surface xxxyyyyya are labeled by strings with structure
xxxyyyyyazzzz, where zzzz are 4 digits identifying, in a unique way, each fracture.

A dataset with the following structure must be supplied for each analysed site xxx. Names,
format, and content of individual files must comply with the specifications described hereafter.

1) One file named xxx_relevance.xlsx, which contains 2 or 3 columns without header:
   column A: identifier of the observation surface (window),
   column B: observation relevance parameter (value from 1-10, see Kabele et al. 2018),
   column C: optional, rock type (numerical value according to agreed-upon key).

2) One file named xxx_transmisivity.xlsx, containing 5 columns with the header:

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>Sum</td>
</tr>
</tbody>
</table>

   Column A contains numerical identifiers (IDs) of fracture populations (fracture sets) in
   ascending order starting from 1, columns B-D contain, for the corresponding population,
   the percentual proportion of fractures with transmissivity index 0, 1, or 2, respectively
   (see Chapter 3) and column E contains the checksum, which must be equal to 100.

3) One file named xxx_termination.xlsx, which serves for the description of termination of
   fractures among populations. This functionality has not been fully implemented yet.
   Therefore, for the time being, a file must be used which contains population IDs in
   ascending order starting from 1 in the first row at positions starting from column B and
   the same in column A starting from row 2. All cells in the area with nonzero values in
   the first row and in the first column must contain the value of 0.

4) For each observation surface one file named xxxyyyyya_BB.xlsx, which contains 4
   columns with the header:

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>X(East)</td>
<td>Y(North)</td>
<td>0</td>
<td>Z</td>
</tr>
</tbody>
</table>

   Columns A-C contain the S-JTSK coordinates of the vertices of a convex polygon which
   delimits the observation surface. Column D contains the numerical IDs of the vertices.
   The vertices are numbered counter-clockwise in the ascending order starting from 1.

5) For each area of observation one file named xxxyyyyya.xlsx, which contains 18 columns
   with the header:
4.3 Assumptions and methods adopted for identification and generation of GeoDFN models in the DFraM v.2 program

The computer program DFraM v.2 offers two main functionalities: (1) identification of DFN parameters based on SG data and (2) generation of random realizations of DFN models with given parameters. The program uses the following fundamental assumptions:

1) Individual fractures are idealized as planar polygons inscribed in ellipses. The ratio of semi-major to semi-minor axes, \(a/b\), can be either fixed to a chosen value or it can be randomly generated within a given range. Polygons may be regular or irregular; the number of vertices can be fixed to a given value or it can be a randomly generated value in a given range.

2) The centroids of the circumscribed ellipses are generated within the space of the modelled rock mass domain by Poisson process.

3) The fractures’ orientations are defined by their respective normal vectors \(\mathbf{n}\); the directions of these vectors follow Fisher distribution with probability density function:

\[
f(\mathbf{n}) = \frac{\kappa}{4\pi \sinh(\kappa)} e^{\kappa \mathbf{\mu} \cdot \mathbf{n}},
\]

where \(\kappa\) is the concentration parameter and \(\mathbf{\mu}\) is the mean vector.

4) The sizes of individual fractures depend on the length of the semi-major axis \(a\). These lengths follow the power-law distribution with probability density function:

\[
f(a) = \frac{\alpha - 1}{x_{\min}^{\alpha - 1}} \left( \frac{a}{x_{\min}} \right)^{-\alpha} \quad \text{for } a \geq x_{\min} \text{ and } \alpha > 1,
\]

where we call \(x_{\min}\) the location parameter and \(\alpha\) the shape parameter or the distribution exponent.

5) The number of fractures generated in the model is given by the product of parameter \(P_{30}\) (the number of the master ellipse centroids per unit volume) and the volume of the modelled domain.
6) The fracture system may be sub-divided into populations (sets), while each population may be described by different values of all parameters.

In addition to the earlier-mentioned length of the semi-major axis of the circumscribed ellipse $a$, to describe the fracture size we define the equivalent radius $r_{eq}$ as the radius of a circle with the same area as the generated fracture. Note that, if the fractures are generated as regular polygons with a constant number of vertices and the semi-axes ratio $a/b$ is constant, then the relation between $r_{eq}$ and $a$ is linear and the distribution of $r_{eq}$ also follows the power law. Otherwise, the distribution of $r_{eq}$ may deviate from the ideal power-law distribution.

### 4.3.1 Methods of DFN parameter identification based on SG data

Feasible methods of SG survey (Chapter 3) offer only very limited insight into the fracture system of the rock mass body. In the case of model site 296 URF Bukov, which is the subject of the present project T8, the “observation windows” are only 2D surfaces on tunnel walls. Fracture traces, that is, the intersections of the fractures with the observation windows, are then the only observable attributes of the spatial fracture network. For each recorded trace, the endpoints’ coordinates, dip, and strike were determined using the methods described in Chapter 3.

The values of parameters $\kappa$ and $\mu$ of Fisher distribution (4.1) are determined for each fracture population based on dips and strikes measured for individual traces using the generally known relations for the maximum likelihood estimates (MLE; Fisher et al. 1993; Kabele et al. 2018). The calculation takes into account the effect of orientational bias (Terzaghi 1965) as well as the measurement relevance by means of weighting factors applied to the fractures’ normal vectors (Kabele et al. 2018).

An optimization procedure based on minimization of objective functions is applied for the calculation of parameters $x_{min}$ and $\alpha$ of the power-law distribution of the fracture size (4.2) as well as for calculation of parameter $P_{30}$. The objective functions, defined in terms of observable variables, quantify the difference between the measurements and model while taking into account the relevance of individual measurements. We use the average trace length $l_0$ and traces’ areal density $P_{20}$ (number of traces per unit area) evaluated on the observation windows as the observable variables.

In this regard, let us note one property of the power-law distribution. Assuming that a random variable $a$ follows the distribution according to Eq. (4.2) and the number of fractures with $a \geq x_{min}$ per unit volume in the population is $P_{30}[x_{min}, \infty]$. If we remove all members of the population with size $x_{min} \leq a < x_1$, then the frequency (per unit volume) of the remaining members can be expressed using the probability density function as:

$$P_{30}[x_1, \infty] = P_{30}[x_{min}, \infty] \int_{a=x_1}^{\infty} f(a) da = P_{30}[x_{min}, \infty] \cdot x_1^{(1-\alpha)} \cdot x_{min}^{(\alpha-1)}.$$  

(4.3)

We utilize this property in such a way that, for a suitably chosen value of the parameter $x_{min}$, we can achieve a sufficient correspondence between the observation and the model by optimizing only the remaining two parameters, that is $\alpha$ and $P_{30}$. 
4.3.2 Methods of DFN model generation

If the fracture density $P_30$ and the values of the parameters of the distributions (4.1) and (4.2) are known, then the DFraM v.2 software can be used to generate an arbitrary number of stochastic realizations of DFN in a domain delimited by constant values of coordinates of the reference system (usually S-JTSK). Furthermore, each fracture is randomly assigned a value of transmissivity index (TI), respecting the values' percentual proportion given in the xxx_transmissivity.xlsx file (see Sect. 4.2). It is possible to specify the random seed of the pseudo-random generator for each DFN realization, which makes it possible to reproduce calculations.

The resulting DFN model is saved in the text vtk format as POLYDATA dataset. Individual fractures are POLYGON-type cells and they are assigned the following scalar attributes: population ID, transmissivity index (TI), size of the fracture area, length of the semi-major and semi-minor axes of the circumscribed ellipse, and coordinates of the circumscribed ellipse centroid. Files in the vtk format can be visualized, for example, by the Paraview software (https://www.paraview.org/). They are also suitable for import to other software used in the T8 project for HG simulations.

4.4 Construction of GeoDFN models

In the scope of the T8 project, we have constructed several GeoDFN models, on which we tested the methods of DFN parameter identification and DFN generation, as well as subsequent conversion to HydroDFN models suitable for HG calculations. As, in the course of the project realization, the methods and software were a subject of continued development, parameters of individual model versions may differ, even though they were identified based on the same input data.

4.4.1 Model version v0

Model version v0 encompassed a domain with dimensions 100 m x 100 m x 100 m surrounding an imaginary disposal borehole (Fig. 5). A near-field domain was modelled in the proximity of the borehole. Fractures with $r_{eq} \geq 0.25$ m were represented in this domain, while only fractures with $r_{eq} \geq 1$ m were considered in the remaining volume.
Fig. 5 Geometry of model version v0 – plan view (left), vertical section (right). The disposal borehole is shown in red, the near-field domain is marked by grey colour. Dimensions are in metres.

Model parameters of fracture network version v0 were based on the parameters’ values presented in report SKB R-09-20 (Joyce et al. 2010). Therefore, we did not perform the identification of parameters from the SG data for this model. Individual fractures were generated as regular octagons inscribed to ellipses with constant semi-axes ratio $b/a = 0.8$. In this case, the relation between the semi-major axis length and the fracture equivalent radius was $a = 1.1783 r_{eq}$. The maximum size of the generated fractures was set to $a = 10\,000\,m$ in order to minimize the effect of the upper truncation of the power-law distribution. The values of the input parameters for DFraM v.2 program, which correspond to the parameters of the generated DFN, are listed in Tab. 7.

Tab. 7 Input parameters for generation of GeoDFN model version v0 in program DFraM v.2. Parameter $x_{\text{min}}$ applies to the distribution of the circumscribed ellipses’ semi-major axis length

<table>
<thead>
<tr>
<th>Population</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fisher distribution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu$ dip [deg]</td>
<td>89</td>
<td>88</td>
<td>84</td>
<td>88</td>
<td>4</td>
</tr>
<tr>
<td>$\mu$ strike [deg]</td>
<td>202</td>
<td>236</td>
<td>330</td>
<td>285</td>
<td>275</td>
</tr>
<tr>
<td>$\kappa$ [-]</td>
<td>17.8</td>
<td>14.3</td>
<td>12.9</td>
<td>14</td>
<td>15.2</td>
</tr>
<tr>
<td>Power law distribution – near field</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$x_{\text{min}}$ [m]</td>
<td>0.295</td>
<td>0.295</td>
<td>0.295</td>
<td>0.295</td>
<td>0.295</td>
</tr>
<tr>
<td>$\alpha$ [-]</td>
<td>3.5</td>
<td>3.7</td>
<td>4.1</td>
<td>4.1</td>
<td>3.38</td>
</tr>
<tr>
<td>$P_{30}$ [1/m$^3$]</td>
<td>0.04384</td>
<td>0.16920</td>
<td>0.03652</td>
<td>0.03003</td>
<td>0.33236</td>
</tr>
<tr>
<td>Power law distribution – far field</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$x_{\text{min}}$ [m]</td>
<td>1.178</td>
<td>1.178</td>
<td>1.178</td>
<td>1.178</td>
<td>1.178</td>
</tr>
<tr>
<td>$\alpha$ [-]</td>
<td>3.5</td>
<td>3.7</td>
<td>4.1</td>
<td>4.1</td>
<td>3.38</td>
</tr>
<tr>
<td>$P_{30}$ [1/m$^3$]</td>
<td>0.00137</td>
<td>0.00401</td>
<td>0.0005</td>
<td>0.00041</td>
<td>0.01227</td>
</tr>
</tbody>
</table>

To construct the final model, firstly, two networks were generated:

(A) with the near-field parameters in domain $(-10\,m, 10\,m)^3$,
(B) with the far-field parameters in domain $(-50\,m, 50\,m)^3$. 

33
Secondly, all fractures with centroids located in the domain \((-10 \text{ m}, 10 \text{ m})^3\) were removed from the network (B) and this network was merged with the network (A). One realization of the model was generated, which consisted of 23 308 fractures.

### 4.4.2 Model version v1

To construct the model version v1 we used data from the structural-geological survey on the site 296 URF Bukov, which had been supplied by CGS. The dataset encompassed traces of 400 fractures subdivided into 9 populations, which had been recorded on five almost planar and vertical quadrilateral surfaces on tunnel walls (Fig. 1 in Chapter 3).

The values of Fisher distribution parameters were determined as maximum likelihood estimates based on the orientations of the mapped fractures. The calculation involved the reorientation of normal vectors according to the principal direction and Terzaghi’s correction.

To identify the parameters of the power-law distribution of fracture size and density \(P_{30}\), DFN networks in domains with the minimum distance of 50 m or 20 m from the mapped tunnel walls (160.2 m x 163.8 m x 100 m) or (80 m x 80 m x 25 m), respectively, were generated. All fractures were squares inscribed in circles with radius \(a\). In this case, the relation between the radius of the circumscribed circle and the equivalent radius takes the form of \(a = \sqrt{\frac{\pi}{2}} r_{eq}\). As only fractures with an equivalent radius larger than about 0.25 m were deemed significant for the subsequent HG calculations, we set the value of \(x_{\min} = 0.3 \text{ m}\) for all populations. The maximum size of the generated fractures was set to \(a = 1000 \text{ m}\) in order to minimize the effect of the upper truncation of the power-law distribution. The values of parameter \(\alpha\) and fracture density \(P_{30}\) were identified individually for each population by minimizing the objective functions, while only those generated fractures were taken into account, which were longer than the shortest recorded trace of the respective population \(l_{r,\min}\). The obtained values of the parameters are listed in Tab. 8.

<table>
<thead>
<tr>
<th>Population</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fisher distribution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\mu) dip [deg]</td>
<td>85.365</td>
<td>36.871</td>
<td>3.36</td>
<td>87.507</td>
<td>62.308</td>
<td>88.629</td>
<td>78.236</td>
<td>88.629</td>
<td>83.253</td>
</tr>
<tr>
<td>(\mu) strike [deg]</td>
<td>222.949</td>
<td>49.597</td>
<td>313.665</td>
<td>316.78</td>
<td>133.438</td>
<td>346.277</td>
<td>1.04</td>
<td>269.482</td>
<td>85.957</td>
</tr>
<tr>
<td>(\kappa) [-]</td>
<td>35.056</td>
<td>2.704</td>
<td>28.633</td>
<td>25.351</td>
<td>2.913</td>
<td>18.73</td>
<td>3.815</td>
<td>17.3</td>
<td>3.962</td>
</tr>
<tr>
<td>Power law distribution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(x_{\min}) [m]</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>(P_{30}) [1/m^3]</td>
<td>0.288</td>
<td>0.188</td>
<td>0.086</td>
<td>0.248</td>
<td>0.278</td>
<td>0.273</td>
<td>0.131</td>
<td>0.611</td>
<td>0.332</td>
</tr>
</tbody>
</table>

Parameters listed in Tab. 8 were used to generate GeoDFN model version v1 in the domain \((-50 \text{ m}, 50 \text{ m})^3\). Values of transmissivity index were randomly assigned to the fractures in accordance with Tab. 2 in Chapter 3, which was based on observations made by CGS. The resulting model consisted of 2 435 000 fractures.

Unfortunately, it was found through subsequent verification that during the parameter identification phase, there was an error in the processing of input data by the DFraM program,
which caused that incorrect reference trace lengths were used. This error adversely affected the calculated values of $\alpha$ and $P_{30}$. Nevertheless, in the light of the fact that the difference from the rectified values of the parameters was not significant for the tested methodology of conversion to HydroDFN model, the network with parameters from Tab. 8 was used for the ensuing HG calculations.

4.4.3 Model version v2

To determine parameters and subsequently construct the model version v2 we used the same data from structural-geological survey as we did for the model version v1. However, the data reading error in DFraM program had been eliminated and a refined configuration of the optimization process was used.

The values of Fisher distribution parameters were determined in the same way as for model version v1. They are listed in Tab. 8.

To identify the parameters of the power-law distribution of fracture size and density $P_{30}$, DFN networks in domains with the minimum distance of 50 m from the surveyed tunnel walls (160.2 m x 163.8 m x 100 m) were generated. All fractures were squares inscribed in circles with radius $a$, thus $a = \sqrt{\frac{\pi}{2}} r_{eq}$. As in the case of the model version v1 we set the value of $x_{min} = 0.3$ m for all populations and the maximum size of the generated fractures was set to $a = 1 000$ m. The values of parameter $\alpha$ and fracture density $P_{30}$ were identified individually for each population by minimizing the objective functions. In order to accelerate the calculation convergence, we used the parameters’ values obtained in the course of the optimization of the previous versions of the model as the initial values for the present minimization process. We also performed a refined pre-analysis of the measured trace lengths, which revealed two anomalies – very short traces, which likely had been recorded by a mistake (Fig. 6). These traces were consequently ignored. While evaluating the objective functions, only those generated fractures were taken into account, which were longer than the shortest recorded trace of the given population $l_{r,min}$. Initial values of parameters, which served as the input for the minimization procedure, are listed in Tab. 9. The optimized values are listed in Tab. 10.

---

*Fig. 6 Complementary cumulative distribution function of recorded trace lengths. Two anomaly traces with very short length < 0.2 m are marked by a red ellipse*
Tab. 9 Initial values used for the optimization of GeoDFN model version v2. Parameter $x_{\text{min}}$ applies to the distribution of the circumscribed circles’ radii

<table>
<thead>
<tr>
<th>Population</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_{\text{min}}$ [m]</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$\alpha_0$ [-]</td>
<td>3.141</td>
<td>2.943</td>
<td>3.408</td>
<td>3.154</td>
<td>3.031</td>
<td>2.716</td>
<td>3.5</td>
<td>3.103</td>
<td></td>
</tr>
<tr>
<td>$\alpha_1$ [-]</td>
<td>3.5</td>
<td>3.3</td>
<td>3.8</td>
<td>3.9</td>
<td>3.5</td>
<td>3.4</td>
<td>3.0</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>$P_{30}$ [1/m³]</td>
<td>0.17</td>
<td>0.15</td>
<td>0.034</td>
<td>0.246</td>
<td>0.285</td>
<td>0.232</td>
<td>0.069</td>
<td>0.581</td>
<td>0.282</td>
</tr>
<tr>
<td>$l_{r,\text{min}}$ [m]</td>
<td>0.27</td>
<td>0.27</td>
<td>0.46</td>
<td>0.21</td>
<td>0.27</td>
<td>0.2</td>
<td>0.22</td>
<td>0.21</td>
<td>0.2</td>
</tr>
</tbody>
</table>

To verify the optimized values of the parameters of the fracture size power-law distribution and fracture density $P_{30}$, 10 realizations of DFN were generated. Virtual observation windows with the same shape, size, and orientation as the surveyed tunnel walls were placed in these models. The number of traces $N_t$, the average trace length $l_\phi$, the traces’ areal density $P_{20}$ and intensity $P_{21}$, and the complementary cumulative distribution function were evaluated both on real and virtual windows. Observation data and model results can be compared in Tab. 11, Fig. 7 and Fig. 8. To assess the quality of the parameter optimization, one should primarily focus on the comparison of $N_t$ or $P_{20}$ and $l_\phi$ (Tab. 11, Fig. 7), as these were the observable variables whose objective functions were minimized. The trends of the complementary cumulative distribution functions should be also examined (Fig. 8). The values of intensity $P_{21}$ in Tab. 11 provide additional insight. However, it is necessary to consider that this characteristic is related both to the abundance and the length distribution of traces. Therefore, any discrepancy in $N_t$ or $P_{20}$ and $l_\phi$ is projected to $P_{21}$ as well. In addition, the values of $P_{21}$ may be affected by the presence of a few very long traces, which may not occur in the realizations of the stochastic model.

By examining Tab. 11 it is obvious that a good agreement between observation and model (within 6%) was achieved for $N_t$ and $P_{20}$ for most populations, which indicates that the volume density of fractures $P_{30}$ was optimized correctly. The exceptions are populations 3, 4, 6, and 8. The recorded sample of population 3 contained only 6 traces, while the models reproduced 5.2 traces. Thus, even though the relative error is 13%, in absolute terms it corresponds to less than 1 trace. Populations 4, 6, and 8 are a different case: the relative differences between observation and model are above 25%. By comparing the initial (Tab. 9) and optimized (Tab. 10) values of the volume fracture density $P_{30}$, it is obvious that these are the only populations for which the optimization converged to the initial values. This indicates that the initial values may have not been chosen appropriately and the optimization process identified an incorrect local minimum of the objective function. We assume that this problem can be alleviated by adopting the refined methodology for setting up the initial values, which is described in Section 7.2.3.
In terms of the fracture size distribution, Fig. 8 shows that, in general, the trends of the complementary cumulative distribution functions were captured well by the model for all populations. This indicates that optimum values of the shape parameter $\alpha$ was found and the model also reproduced the effects of traces’ truncation and censoring. Quantitatively, an acceptable relative difference of the average trace length of up to about 10% (which corresponds to the absolute difference of about 0.1 m) is seen for most populations. Larger differences may be associated with a small observation sample (population 3) or an inaccurate estimate of the fractures volume density (population 8). We anticipate that the results can be further improved if the range of traces lengths, over which the optimization is executed, is determined by the updated approach described in Section 7.2.3.

### Tab. 11 Characteristics of the fracture system traces evaluated from the mapping data and from the models

<table>
<thead>
<tr>
<th>Pop.</th>
<th>$N_i [-]$</th>
<th>$l_0 [m]$</th>
<th>$P_{20} [1/m^2]$</th>
<th>$P_{21} [m/m^2]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>46</td>
<td>45.6</td>
<td>-1%</td>
<td>1.02</td>
</tr>
<tr>
<td>2</td>
<td>42</td>
<td>43.9</td>
<td>5%</td>
<td>1.45</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>5.2</td>
<td>-13%</td>
<td>0.81</td>
</tr>
<tr>
<td>4</td>
<td>30</td>
<td>20.2</td>
<td>-33%</td>
<td>0.72</td>
</tr>
<tr>
<td>5</td>
<td>57</td>
<td>53.5</td>
<td>-6%</td>
<td>1.04</td>
</tr>
<tr>
<td>6</td>
<td>60</td>
<td>45</td>
<td>-25%</td>
<td>1.10</td>
</tr>
<tr>
<td>7</td>
<td>33</td>
<td>32.6</td>
<td>-1%</td>
<td>1.55</td>
</tr>
<tr>
<td>8</td>
<td>71</td>
<td>50.8</td>
<td>-28%</td>
<td>0.90</td>
</tr>
<tr>
<td>9</td>
<td>53</td>
<td>52.1</td>
<td>-2%</td>
<td>1.18</td>
</tr>
<tr>
<td>All</td>
<td>398</td>
<td>348.9</td>
<td>-12%</td>
<td>1.097</td>
</tr>
</tbody>
</table>

**Fig. 7** Average trace lengths and areal densities of the fracture system traces evaluated for individual populations based on the mapping data and the models.
Fig. 8 Complementary cumulative distribution functions of the fracture system trace lengths evaluated based on the mapping data and on the model

The parameters of Fisher distribution listed in Tab. 8 and those of the power-law distribution listed in Tab. 10 were used to generate the GeoDFN model version v2 in a domain 100 m x 200 m x 100 m. Values of transmissivity index were randomly assigned to the fractures in accordance with Tab. 2 in Chapter 3. The resulting model consisted of 5 124 000 fractures.
A general methodology for hydrogeological and transport models executed within the framework of T8 project is based on important input assumptions:

- The analysed environment is close to the hydrogeological conditions existing at real DGR sites – groundwater flow and transport of radionuclides are, however, dealt-with for a hypothetical site and not for any particular site.
- The transport process is primarily simulated for a conservative tracer transported through the fracture network by groundwater flow; the GoldSim software also considers the influence of diffusion and sorption processes in the rock matrix.
- The assessed safety scenario considers failure of only one WDP (models v0 and v1), respectively of multiple WDP at the same time (model v2).
- Volume (thickness) of the isolating part of the rock massif depends on the pressure conditions of groundwater flow from the DGR area into the drainage area. Isolating part of the rock massif excludes category 1 – 3 fault zones (according to SKB classification) and the subsurface weathered zone.
- Credibility of the modelling works is supported by an adjustment and partial simplification of information available from the regional model for Kraví Hora site.
- Groundwater flow modelling results are greatly influenced by selection of boundary conditions. These conditions have to be chosen in such way that their impact upon any change (amendment/modification) of computational network geometry remains realistic. A generally valid rule is to situate the boundary conditions “in sufficient distance” from the area of priority interest of the simulation.
- From the perspective of scale, the modelling works have oriented on the description of processes in fractured rock environment. Processes involving flow and transport through engineering barriers are not considered in the modelling works with DFN and transport model.
- The fracture network has been specified with variable aperture (transmissivity) of fractures, however, without any further complicated heterogeneities, i.e., without any decrease in permeability and in the number of fractures and their opening towards greater depths, without preferential paths at the level of fractures (channeling), etc.

Flow and transport process simulations were performed for the isolating part of the rock massif in the source area near WDP:

- Basic impulse for spreading of radionuclides (in case of engineering barrier failure) consists in an intersection of WDP geometry and fracture connected to a system of connected fractures with groundwater flow. This concept was defined and analysed in the prepared flow and transport models.
- Advection (transport by groundwater flow through fracture network) is considered to be primary mechanism for radionuclides spreading in simulations. Description of the groundwater flow velocity field is crucial for follow-up assessment of transport processes. The model was used to analyse the impact of fracture network’s character in close vicinity of WDP area (fractures intersecting the WDP), influence of fracture network’s composition along the entire transport route, and the influence of local increase in rock massif’s permeability and interconnection of fractures by the EDZ on both the flow conditions and transport process,
• DFN approach was the primary concept used in the modelling as it is closer to the real fracture network (approximation by planar surfaces) – the flow can only take place through the fractures. Simulations based on the CPM concept, which is based on the fracture network’s geometry while neglecting or simplifying its complexity (“upsampling”), were performed at the same time. Rock massif’s permeability is input into the CPM model using the hydraulic conductivity tensor. Both concepts were compared by calculation of “identical” task using both DFN and CPM models.

5.1 Detailed concept of HydroDFN models, boundary conditions

Model results of the flow and follow-up transport must be independent on boundary conditions in any model. Boundary condition cannot be clearly defined in advance for the isolating part of the massif near the DGR, i.e., for the local model of the delimited rock block, and it is therefore necessary to issue from a larger-scale model solution, i.e., from the regional model. Boundary conditions for the delimited block of the isolating part of the massif can be generally taken over from the results applicable to the pressure flow field in the regional model. However, the definition of the pressure boundary condition at the border of the local model necessarily requires compliance with the balance criterion, i.e., equality between the overflow across the local model’s borders and the overflows across the same balance areas within the regional model. The local model loses a significant portion of its credibility without the compliance with this balance criterion.

The regional model from Kraví Hora, which had been obtained as a part of the HGModely project sheet (ZL 011), was used for the determination of boundary conditions for the local model. This regional model is highly complex – it simulates mine works, a large number of faults, changes to parameters with depth and with rock type, etc. For use in local HydroDFN model executed as a part of the T8 project, the original model was partly simplified with the aim of obtaining a suitable and corresponding boundary condition at the border of model domain of the local model for the delimited rock block:

• Pressure gradient calculated in the regional model has values between 0.01 and 0.1 m.m⁻¹ in the DGR depth (i.e., the groundwater level difference between 1 and 10 m over the distance of 100 m) – average hydraulic gradient of 0.05 m.m⁻¹ is specified in the direction of axis x (from left to right) in the analysed HydroDFN models.
• The boundary condition is defined as constant level of 405 m on the western (left) border of the model, constant level of 400 m on the eastern (right) border of the model, and as zero flow (impermeable border) on the remaining “surfaces” of the model (northern, southern, top, bottom).
• Flow rate calculated for the model cell 100x100x100 m (in regional model) has values between $1.8 \times 10^{-6}$ až $1.0 \times 10^{-4}$ m³.s⁻¹ in the DGR depth, with average value of $5.6 \times 10^{-5}$ m³.s⁻¹. However, these values, calculated in the regional model, represent the average flow rate in a given rock lithotype, including significant conductive open fractures (excludes category 1 – 3 fault zones according to the SKB classification) and do not take into account significant heterogeneity of the fractured rock. In the local HydroDFN model, in which less conductive fractures of smaller dimensions are specified, we assume lower flow rates.

Detailed concept of HydroDFN models for the isolating part of the massif was further specified in discussions during the inspection days:
HydroDFN model has been created on the groundwork of GeoDFN model generated in NAPSAC (version v0 only) and DFraM (all model versions) programs – minimal generated equivalent average of fracture size in the model was 0.5 m (roughly corresponding to the minimal length of fractures mapped by the CGS), maximal equivalent average of fracture size 100 m is proportional to the size of model domain in the local model.

Isolated fractures or fracture clusters, which did not form part of interconnected fracture network at the level of the model domain and did not actively participate in flow and transport were removed from the original GeoDFN model during HydroDFN model preparation. This considerably reduces the total number of fractures in the DFN model necessary for an efficient numeric calculation. Input hydraulic and transport parameters necessary for the calculation (aperture, transmissivity, porosity, etc.) are assigned to such connectivity fractures at the same time. Transfer from GeoDFN to HydroDFN took place in NAPSAC software which provides appropriate tools for this purpose.

Simulation of flow and advective transport in HydroDFN model was performed in NAPSAC, Flow123d, and ADFNE programs (flow was only analysed in the last one) – input geometry and parameters of the stochastic fracture network are uniform for all programs used and have been provided in the vtk file format.

Link to the regional model is established in the local DFN model through the defined pressure boundary conditions and balance criterion at the model border.

Basic size of the model is 100x100x100 m with disposal borehole located in the middle of the model domain (the model domain is larger (100x200x100 m) in version v2 due to inclusion of a higher number of disposal boreholes into the model).

Transport of the tracer through the fracture system of the isolating part of the massif is dealt-with in the area between the disposal borehole’s wall and the model border representing the failure zone or fracture with significant permeability – it thus covers the scenario of radionuclide escape through the wall of the disposal borehole into the fracture system and simulation of transport only through the fracture system within the rock massif, i.e., we do not assume inclusion of engineering barriers and fills of the disposal borehole into the model.

Dealing with one safety scenario but in various model versions differing by the fracture network, hydraulic and transport parameters, enabled achieving one of the basic project goals: specification and evaluation of the fracture system importance for transport of radionuclides within the isolating part of the rock massif.

It is not possible to determine the critical transport route in advance due to the stochastically generated fracture network; it always depends on specific intersections of the fracture network and the disposal borehole and on the intersections of the fracture network and the model borders.

Simulation of full transport (development of concentrations in time) was performed for the selected variant within the framework of CPM model processing in MODFLOW/MT3DMS software and it was compared with the results obtained from the “particle tracking" method.

From the perspective of geometry and parameters of the fracture network, the HydroDFN models were solved in three versions:

0. Model version v0 created by generation of fracture network with the fracture parameters evaluated for the Forsmark site (Joyce et al. 2010) – the main objective was to commence with the modelling works already in the phase when the outputs from
URF Bukov were not yet available. Another objective was to analyse the possibilities of the software for description and generation of the fracture network’s geometry.

1. Model version v1 – geometric parameters of the fracture network (i.e., the number of fractures, their direction and size) were obtained during measurements performed at URF Bukov, hydraulic parameters of conductive fractures (i.e., the relationship between the transmissivity of fractures and their size) were again taken over from the SKB materials; data obtained at URF Bukov provided an outline about the proposed number of potentially transmissive fractures within the framework of individual fracture populations (according to the transmissivity index assigned to individual generated fractures).

2. Model version v2 – size of the model domain was double compared to the previous two variants, however, the concept of the fracture network more or less corresponds to model version v1 – optimized parameters of fracture populations from the measurement performed at URF Bukov were further refined in GeoDFN and the total number of connective fractures in the model was increased in HydroDFN, i.e., the transmissivity index value was updated.

5.2 Calculation methodology for HydroDFN models in individual software packages

Simulation of flow and advective transport within the Transport 8 project was dealt-with simultaneously in three software packages – ADFNE (flow) together with GoldSim (transport) at FJFI, Flow123d at TUL and ConnectFlow/NAPSAC at PROGEO. This chapter documents the procedures how individual software packages deal with the problem of DFN modelling.

5.2.1 ADFNE/GoldSim

GoldSim models a transport through a DFN by means of the transfer function, \( N(t) \), which is obtained by composing the transfer functions of individual fractures, \( N_i(t) \) (GoldSim 2014). The transfer function of a general linear system is defined as the system response to a unit pulse at zero initial conditions. The system response to any input, in our case the input concentration \( C_{IN}(t) \) or inflow \( J_{IN}(t) \), is then calculated as the convolution of the transfer function \( N(t) \) with the input:

\[
C_{OUT}(r,t) = \int_{-\infty}^{+\infty} N(\tau)C_{IN}(0,t-\tau) d\tau.
\] (5.1)

The basic element of DFN in GoldSim is the Pipe object, which represents one or a part of a fracture (GoldSim 2014). This object uses the Laplace transform to find the transfer function of a wide variety of transport tasks associated with 1D advective-dispersive transport accompanied by perpendicular diffusion into immobile zones, such as a rock matrix or a stagnant water zone. The geometry of the Pipe object is defined by the length, the cross-sectional area where the flow occurs, and the wetted area where it diffuses into the rock matrix. Modeled contaminants enter at one end of the Pipe object (or along part of the fracture), are carried along the fracture by the advection, due to the dispersion, the shape of the input concentration is spread and at the same time diffusion or sorption into the matrix occurs. The simulation results in an evolution of the concentration or outflow at the other end of the Pipe object.
GoldSim, specifically the Contaminant Transport module, includes a *Network Pathway* object that allows the building of a transfer function for DFN that could consist of up to several tens of thousands of *Pipe* objects (GoldSim 2014). Since the solution to the transport task is obtained by convolution with the transfer function (5.1), the computational requirements for large DFN are the same as in the case of a single fracture, the only redundant computational requirement for the DFN model is the time needed to create the transfer function for DFN at the start of the simulation.

The GoldSim software environment supports uncertainty and sensitivity analysis. For DFN radionuclide transport simulation, a set of different fracture networks can be included in a *Network Pathway* object, and GoldSim selects a particular network during the simulation according to the *Random* parameter setting of the *Network Pathway* object. For example, if we define three networks and define the *Random* parameter as a uniform distribution between 0 and 3, each network has the same probability of occurrence. Conversely, if a user wants to run a simulation in which a particular network will be used, the Random parameter is replaced by the number of that network, and is thus constant.

The values of *Network Pathway* parameters are defined using an input file. This file is a text file that has the *.ltx file extension (GoldSim 2014). The file consists of several sections, which in turn define the individual DFN parameters. Each section begins with a BEGIN command and ends with an END command. Anything outside these sections is considered a commentary and is thus ignored. The first section defines the properties of each *Pipe* object. These include the length [m], the volume flow [m$^3$/ year], the flow area [m$^2$], the wetted surface [m$^2$], and the Fracture Set ID, which defines the material parameters of the *Pipe set* in the model. The second section defines the source term of the DFN. It starts with the BEGIN source_groups command. It might contain any number of source member sets. Each set starts with its ID, the number of *Pipe* objects in the set, and then the Pipe sequence number. The source member ID must correspond to the source member that was created in the GoldSim model. The section ends with an END statement. The third section defines the object into which the DFN flows. It starts with the BEGIN sink_groups command. As in the previous section, it can contain any number of object sets. Each set starts with its ID, the number of Pipe objects in the set, and then the Pipe sequence number. The ID must correspond to the object that was created in the GoldSim model for this purpose. The section ends with an END statement. The fourth section defines the connection of objects in the upstream direction in the fractures, i.e. from the sink to the source member. The section begins with the BEGIN upstream_connections command. Each subsequent line is dedicated to one *Pipe* object, the record begins with a Pipe sequence number, followed by the sequence numbers of all Pipe objects that are attached to it upstream. The section ends with an END statement. The fifth section defines the connection of objects downstream of the fractures, that is, from the source to the sink. The section begins with the BEGIN command downstream_connections. As in the previous case, each subsequent line is dedicated to one *Pipe* object. The entry begins with the Pipe sequence number and follows the sequence numbers of all Pipe objects that are attached to it in the flow direction. The section ends with an END statement.

To generate the input file for the *Network Pathway* object, it was necessary to create an external program that we programmed in the MATLAB programming environment. Our choice was motivated both by our experience in working in this programming environment and by the fact that in MATLAB a library of functions (ADFNE) for generation and work with DFN (Alghalandis 2017) has already been created. ADFNE is an open source function library written in a standard programming language that includes over 300 functions.
Fig. 9 Methods for generation of pipes (red lines) in 3D fractures. Left image: central method; right image: triangulation method (adopted from Alghalandis et al. 2018).

Generating and exporting DFN parameters for GoldSim in ADFNE can be divided into several steps. In the first step, the coordinates of the individual fractures are generated. If the DFN model is 2D, the fractures are modeled using lines, in the case of the 3D model, the fractures are convex polygons. Position, orientation, and fracture lengths are generated using appropriate distribution functions. Furthermore, the individual fractures are divided according to the intersections into the "pipes".

In Fig. 9, two methods are illustrated. The central method (left image) generates a “pipe” (red line) as the junction of the center of the intersection and the center of the fracture, the triangulation method (right image) uses Delaunay triangulation to create a “pipe” network in the part of the fracture delimited by intersections with other fractures. “Pipes” are further viewed as a graph from which a set of skeletons connecting the marginal lines is selected in the next step. Thus, those "pipes" that do not allow the flow of fluid are omitted. Furthermore, “pipes” are enriched with a graph structure. A data object is created containing the start and end points of pipes (grh.Node) and a data object for edges of “pipes” (grh.Edges). Additional attributes are introduced into these data structures, such as Pressure (start or end point pressure, part grh.Node), Flow (volume flow in “pipes”, part grh.Edges), which are obtained after solving the flow problem with specified boundary pressure conditions. The solution to the flow problem is based on the relationship between the volumetric flows in each “pipe” \( Q_{(i,j)} \) and the pressures at the start and end points of the “pipes” \( H_i, H_j \); a pair of indexes \((i,j)\) denotes vertices in a graphically understood fracture network.

Darcy’s law for flow in fracture can be written in the form (Alghalandis et al. 2013):

\[
Q_{(i,j)} = - \frac{k_{(i,j)} A_{(i,j)}}{\mu_{(i,j)}} (H_i - H_j),
\]

where \( A_{(i,j)} \) and \( l_{(i,j)} \) are, respectively, the cross section and length of the fracture leading from point \( i \) to \( j \), \( \mu \) [Pa·s] is the viscosity of the fluid filling the fractures and \( k_{(i,j)} \) is the permeability of the fractures. For the calculation of the \( H \) pressures at individual network points, it is then possible to use the equation:
where the network of joints between fractures is denoted as a graph $G$, $<i,j>$ denotes its edges. Summations thus run across all edges containing a given vertex. By inputting the pressure at the inlet, outlet and eventually at other points of the fracture network, a system of equations is created for the pressure values at other vertices $G$. Coefficients $C_{ij}$ are transmittance of fractures, which could be modeled using a cubic law, cf. (Priest 1993):

$$C_{ij} = \frac{g a_{i,j} b_{i,j}}{12 \theta l_{i,j}},$$

where $g$ is gravitational acceleration, $a_{i,j}$ aperture, $b_{i,j}$ width of fracture a $l_{i,j}$ length of fracture between points $i$ and $j \in G$ a $\theta$ kinematic viscosity; it holds $A_{i,j} = a_{i,j} b_{i,j}$.

A function to export the result from ADFNE to the DFN input file in GoldSim was created in Matlab. Part of this function is a procedure that cleans exported DFNs from pipes not involved in transport (zero or very small $Q_{i,j}$ values). Another part of the function is the procedure for determining connectivity, its output is in the “upstream” and “downstream” formats, as required by GoldSim.

### 5.2.2 Flow123d

This chapter deals with the methodology for modelling using the Flow123d simulation tool, version 3.0.2 (TUL 2019). For each fracture configuration the workflow was as follows:

1. Preparation of geometry and computational mesh based on set input created and distributed by PROGEO.
2. Assignment of hydraulic parameters to individual fractures based on set specification.
3. Simulation of flow.
4. Determination and evaluation of transport paths.
5. Advective transport simulation, evaluation of mass fluxes.

Geometry and computational mesh were realized using the Python API (Application Programming Interface) of GMSH SW (Geuzaine et al. 2009). Within its framework the individual fractures were input cut by a cube (cuboid in case of model v2) representing a model domain. Then, the fracture intersections were computed and physical groups were assigned (one for each fracture so that each fracture may have its hydraulic properties prescribed). The aforementioned operations are based on the OCC (OpenCascade) library whose implementation is not the most effective hence the preparation of computational mesh for Flow123d is quite time demanding. It can be overall pinpointed as a weak link of the procedure mentioned above. We were unable to create a hundred percent correct computational mesh (with currently available SW tools) for model v2 in which there is an order of magnitude more fractures than in models v0 av1. More about this can be found in the chapter that deals with conclusions and further work.

The groundwater flow simulation parameters assigned to each fracture are the hydraulic aperture and hydraulic conductivity. The hydraulic aperture of each fracture is given by the set input. The hydraulic conductivity is computed based on hydraulic aperture using the cubic law. The groundwater flow simulation boundary conditions were prescribed based on the set input.
The methodology for determination and description of transport paths is based on construction of weighted directed graph:

- From the set source element a graph is gradually constructed: the directed edges are added from element (vertex) currently marked as source towards each of its neighbors to which there is a positive flux.
- Individual directed edges are assigned a weight equal to an approximate transport time between element barycenters (computed based on knowledge of edge length and flow simulation results – velocities and fluxes).
- The graph ends on model domain boundary.

Then, we identify all elements that are on the model domain boundary and that are part of the constructed graph. For each of those we then find the shortest path through the graph using the Dijkstra algorithm. Finally, for each path, we compute its length as a sum of path edges lengths and delay time based on the computed length and known velocity values. The methodology for determination and description of transport paths was implemented in Python (version 3.7).

The advective transport simulations were done for a hypothetical conservative tracer (not accounting for hydrodynamic dispersion, molecular diffusion or sorption). In Flow123d the transport aperture is equal to the hydraulic one (which is different from what was used in other simulation SW). Fracture porosities were assumed to be unitary. The transport simulation results are evaluated using the time evolution of relative mass flux (normalized by source magnitude) over the outflow boundary.

5.2.3 NAPSAC

NAPSAC for mathematical modelling of flow and transport through discrete fracture network (the DFN concept) forms part of the software package named ConnectFlow (Wood 2018). ConnectFlow comprises two modelling programs – NAMMU and NAPSAC. NAMMU represents an application working on the groundwork of equivalent continuous porous medium concept (ECPM) while NAPSAC operates with the discrete fracture network (DFN) concept. ConnectFlow also enables combining of simulations performed in NAMMU and NAPSAC programs, thus offering a highly flexible application enabling connection of modelling in fracture and porous environments at various scales. Modelling is based on solving the mathematical formulation of a problem using the finite elements numeric method. NAPSAC program was used for mathematical modelling within the framework of the assigned task to generate the micro-fracture DFN networks while NAMMU was then used for their upscaling and conversion into continuous environment of the rock matrix in CPM.

NAPSAC/NAMMU programs have been developed in recent 30 years (formerly by AEA Technology, Serco Assurance, AMEC and currently by WOOD) and they have been verified at the international level (e.g., SKB, STRIPA mine, TRUE site, etc.). They also comply with international quality standards ISO 9001 and TickiT.

The modelling process in NAPSAC software is usually divided into several isolated but mutually following steps. The same situation occurred in the T8 project. Each step has its own input data file (in text format) in which relevant part of the simulation is defined in form of gradually layered commands (commands, subcommands, keywords):
1.a. Geometric model creation – MODEL.A output file (internal binary format) – the first step, which forms part of all simulations, is to define the model domain, fracture systems including geometric, hydraulic, and transport parameters (for T8, the fractures were imported from the uniform assignment but they can be also input manually or generated stochastically), refining of the fractures is defined (division of fracture areas into sub-fractures which are important for accuracy of calculation) and the boundary conditions are determined,

1.b. Geometric model adaptation – MODEL.B output file (internal binary format) – this step does not necessarily have to be part of every simulation, however, it was included in T8; MODEL.A was read in this step and connectivity analysis was performed (isolated and “dead-end” fractures were removed),

2. Flow calculation – SOLVE output file (internal binary format) – this step forms part of all simulations in which calculation of pressure and velocity field or transport is required; relevant model is read in the first place (MODEL.A or MODEL.B) and the flow calculation is then numerically solved according to defined parameters of the solver.

3. Transport calculation using the particle tracking method – PATH output file (internal binary format) – input for transport calculation comes from resolved groundwater flow (SOLVE); the input data file then defines the number of particles and source coordinates.

4. Extended export of results – additional data or detailed results can be exported within the framework of each step 1a, 1b, 2, 3 in addition to the basic output binary files (MODEL, SOLVE, PATH) and basic output text files (OUT – they document the performed simulation step, contain log data of the simulation tool, and provide statistical summary or overview of model results). The following exports were produced in connection with project T8 resolution:

- in step 1.b: DFN and IFZ files with detailed geometry of fractures and their intersection points – these files were further converted into vtk files with fracture network for uniform models assignment.
- in step 2:
  - DAT files with detailed values of pressures in the computational network nodes, which were used by FJFI in ADFNE calculations.
  - DAT files with detailed flow values in the intersection points of fractures at the model domain border for comparison with the results from CPM models.
  - PIPE files with detailed flow values in all fractures and at all intersection points of the fractures from the results of “pipe model” (NAPSAC calculates the pipe model for mutual connections of intersection points in fractures and it serves as the input for particle tracking calculation) – the outputs from PIPE file were converted into text files and used by ÚJV for GoldSim calculations.
- In step 3: PTV file with detailed particle tracking results – data was converted into text format and handed over to ÚJV as the groundwork for GoldSim calculations; at the same time, the data was processed into vtk file for visualization of trajectories in ParaView.
5. Upscaling of DFN model into CPM – MODEL.B from step 1 was used as the input for CPM model creation; output of the upscaling model were the files with hydraulic and transport parameters for import into the programs based on the CPM concept - for more details, see Chapter 5.6.

Uniform input fracture network was refined (tessellated) for more accurate flow and transport calculation – the input fractures (i.e., those generated in DFraM) are designated in NAPSAC as MACROFRACTURES. They were divided into smaller regular SUBFRACTURES after import into NAPSAC:

- macrofractures intersecting the disposal boreholes were divided into subfractures 0.2 x 0.2 m,
- other macrofractures were divided into subfractures 2 x 2 m (i.e., macrofractures smaller than 2 x 2 m were not divided).

The “approximate particle tracking” method was used in the NAPSAC software to solve the advective transport in DFN fracture network. This method is very fast from the perspective of calculation efficiency and provides sufficient accuracy (transport calculation based on a more accurate flow balance in fractures is available with the „direct particle tracking“ method, which is, however, much more demanding as regards the required time and is rather used for final model versions). Transport of 100 particles was simulated for delivery of detailed data for GoldSim; transport of 1000 particles (a higher number provides smoother curves) was simulated for statistic processing of the travel time and length of trajectories.

Particles were input for all intersection points of fractures and disposal borehole within the framework of advective transport simulation by the “particle tracking” method. Input of the particles also considered the calculated flows (velocities) in all intersection points and a higher number of particles was thus proportionally input at places with higher flow values.

ConnectFlow software was used for model results visualization – the user interface contains a tool for direct visualization of the model, input/output data, and their 3D processing (model fragments, 2D sections). Exported vtk files were visualized and processed in ParaView software.

5.3 Uniform fracture network preparation for HydroDFN models

The hydrogeological models (HydroDFN) fracture network ideally contains only the subset of geological model (GeoDFN) fractures that are interconnected to each other and to model boundary conditions. Within this so called “connectivity analysis” the isolated fractures and fracture clusters are deleted from the generated GeoDFN which leads to reduction of fracture count in a HydroDFN model (low fracture count or, respectively, low fracture intersection count leads to low element count and thus to effective numerical computation). The connectivity analysis for all model versions was performed in NAPSAC which has a relatively robust and fast tool for removal of isolated and dead-end fractures and fracture clusters.

The connectivity analysis is run in NAPSAC only after the model boundary conditions were defined – this is important mainly for definition of inner boundary conditions (typically engineered objects, i.e. boreholes or tunnels) which can significantly influence the connectivity of a mesh as a whole. Any change of boundary conditions (e.g. a solution of different repository situation, definition of new monitoring boreholes, change of model domain extent, etc.) triggers
a new connectivity analysis. The output of NAPSAC connectivity analysis is a new fracture network which is then converted to vtk format.

Into thevtkfile, which primarily contains only the geometrical characteristics of the fractures (from input GeoDFN the following is acquired: sizes of half-axes, area, population ID, transmissivity index), the hydraulic and transport parameters of fractures (needed for simulations) were further added.

The fracture hydraulic properties in theDFNmodel can be defined in three different ways using these parameters:

- transmissivity $T \text{[m}^2\text{·s}^{-1}]$,
- hydraulic aperture $a_h \text{[m]}$,
- hydraulic conductivity $K \text{[m} \cdot \text{s}^{-1}]$ of fracture zone and its thickness $b_h \text{[m]}$.

The mutual relation between these hydraulic parameters is based on cubic, respectively Darcy law:

$$ T = \frac{\rho g a_h^3}{12 \mu} = K b_h. \quad (5.1) $$

A velocity of advective movement of a conservative tracer in a fracture is influenced by given transport properties:

- fracture transport aperture $a_t \text{[m]}$,
- fracture porosity $\phi_a [-]$,
- fracture zone porosity $\phi_b [-]$.

The mutual relation of these parameters is given by:

$$ a_t = a_h \phi_a = b_h \phi_b. \quad (5.2) $$

The values of transmissivity $T$ and transport aperture $a_t$ of individual fractures are in all model versions computed according to equations used in SKB computations. The power law with direct correlation between $T$ and fracture size $r$ is used for transmissivity computation (Rhén et al. 2008):

$$ T = a r^b. \quad (5.3) $$

Equation for square fractures generated in NAPSAC:

$$ T = a \pi^{-0.50} L^b. \quad (5.4) $$

Values of individual fracture transport aperture are computed based on transmissivity again using the power law:

$$ a_t = c T^{0.5}. \quad (5.5) $$

Values for parameters a, b, c are adapted from Crawford (2008):

- $a = 1.8 \cdot 10^{-10}$,
- $b = 1.0$,
- $c = 0.5$.

For hydraulic simulations in NAPSAC the following values of physical parameters were used:

- $g = 9.81 \text{ m} \cdot \text{s}^{-2}$,
• $\rho = 1000.0 \text{ kg m}^{-3}$,
• $\mu = 0.001 \text{ Pa s}$.

Tab. 12 Overview of basic fracture parameters in a vtk file created for hydrogeological models in NAPSAC

<table>
<thead>
<tr>
<th>VTK attribute</th>
<th>Attribute description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFN_IDSUBLFRAC</td>
<td>fracture ID in the model</td>
</tr>
<tr>
<td>DFN_IDMACROFRAC</td>
<td>original fracture ID – corresponds to fracture ID prior to removal of non-connective fractures</td>
</tr>
<tr>
<td>DFN_SET</td>
<td>fracture population ID</td>
</tr>
<tr>
<td>DFN_SF_L1</td>
<td>fracture size, i.e. length of square edge (L1=L2) for square fractures</td>
</tr>
<tr>
<td>DFN_SF_AreaL1xL2</td>
<td>fracture area</td>
</tr>
<tr>
<td>DFN_SF_Aper</td>
<td>fracture hydraulic aperture</td>
</tr>
<tr>
<td>DFN_SF_AperTransport</td>
<td>fracture transport aperture</td>
</tr>
</tbody>
</table>

The final HydroDFN fracture networks for simulations of flow and transport were distributed for each model version in the vtk format to other investigators. These networks were also re-imported to NAPSAC so that the unanimous fracture input to all SW is guaranteed.

5.3.1 Version v0

The model version v0 was used to test a procedure of HydroDFN model preparation in detail. The GeoDFN fracture network was for time reasons at first generated directly in NAPSAC. The v0 fracture network model parameters are adopted from parameter values documented in SKB report R-09-20 (Joyce et al. 2010). The fracture set count (5), their orientation and power function exponent $k_r$ were adopted without change. The value of parameter $P_{32}$ defining fracture area per unit volume in a model was adjusted – for model version v0 it was increased 1.5 times so that a connective network of fractures would be generated in a model domain of $100 \times 100 \times 100$ m. Fracture population parameters used for GeoDFN generation in NAPSAC are shown in Tab. 13. In a near-field within 10 m of the disposal borehole the square fractures with minimal equivalent radius of 0.25 m ($r_1$) were generated; in the far-field the minimum equivalent radius was 1 m ($r_2$). The maximum equivalent radius of fractures in the model domain was 50 m ($r_3$).
In total, 24933 fractures were generated in the GeoDFN model – 18685 fractures with $r_{eq}>1.0$ m and 6248 fractures with $r_{eq}<1.0$ m (i.e. in the near-field 20x20x20 m). During the connectivity analysis 18183 non-connective isolated fractures that do not take part in flow or transport were removed from the GeoDFN model. The resulting HydroDFN network (see Fig. 10 and Fig. 11) consisted of 6750 fractures - 5901 fractures with $r_{eq}>1.0$ m and in the near-field furthermore also 849 fractures with $r_{eq}<1.0$ m. This connective network was then used for simulation of flow and transport in NAPSAC, Flow123d and ADFNE. For these simulations the fracture network is further discretized to computational elements (specific to each SW used) – the computational mesh characteristics are shown in Tab. 14.
Fig. 11 Vertical cross-section through GeoDFN and HydroDFN version v0 fracture network (NAPSAC) – connective HydroDFN fractures in yellow, isolated fractures removed from GeoDFN in black

Tab. 14 Characterization and discretisation of computational mesh in individual SW

<table>
<thead>
<tr>
<th>PROGEO ConnectFlow - NAPSAC</th>
<th>TUL Flow123d</th>
<th>FJFI ADFNE</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Source fracture intersecting disposal borehole – square sub-fractures with size 0.2x0.2 m</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Other fractures – square sub-fractures with maximum size 2x2 m (i.e. fractures smaller than 2x2 m are further divided)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• In total 62096 fractures and sub-fractures and 124233 sub-fractures intersections</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Irregular triangular mesh</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• In total 361673 elements</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Element size in source fracture – 2.13e-5 to 2.31m² (mean 0.206 m²)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Maximum element size – 3.08 m² (mean 0.396 m²)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Triangulation method on network of fractures and intersections</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• For transport - transfer of fractures with “non-zero” flux to GoldSim – necessary to input fracture width parameter, respectively length of intersection</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Aside from preparation of unanimous fracture network other types of tasks were performed and evaluated in NAPSAC within the framework of testing of v0 network generation:

• Optimization of output format (vtk file) of fracture network generated in DFramM for import into NAPSAC and other SW,
100 various realizations of stochastic DFN networks (but with same input parameters) – on each network the connectivity analysis was performed, the HydroDFN model was prepared and flow and transport were simulated:
- The cross-connection of fracture network and disposal borehole was evaluated – all 100 HydroDFN networks were transmissive on a model domain level (i.e. they connected model boundaries); only 42 networks were connected to the disposal borehole – i.e. almost 60% of disposals holes were „safe“ as far as the advective transport goes, for the rest it was necessary to evaluate transmissivity, respectively the borehole influx,
- Fluxes in the models were evaluated and the breakthrough curves were processed (particle delay times) along with particle trajectory lengths (see chapter 5.4.1),

Testing of fracture shape influence on flow and transport – in the DFraM SW the GeoDFN with v0 parameters was prepared with the shape of fractures being an octagon inscribed into ellipse:
- Import of such a network into NAPSAC was tested including preparation of HydroDFN model and simulation of flow and transport – it all worked without a problem,
- Cross-comparison of results for octagonal, square and rectangular network (fractures had same centers, slopes and areas) – it was concluded that the results are quite different; outputs were different connective networks with different path trajectories, see Fig. 12.

![Pathlines](image)

**Fig. 12** Testing of fracture shape influence on flow and transport – HydroDFN network with octagonal fractures (upper right); relation between octagonal, square and rectangular fracture shape (lower right); comparison of particles trajectories (left)
5.3.2 Version v1

The GeoDFN network generated in DFraM served as input for HydroDFN network of model v1. The GeoDFN network was prepared based on measured data from URF Bukov. The GeoDFN contained 2435000 fractures within the model domain of 100x100x100 m. This fracture count was undervalued (probably by up to 20-30 %) because of the discrepancies in sizes of observational frames (this was accounted for in proposed methodology for data processing and parameter calibration but not included in models v1 and v2).

Model v1 HydroDFN preparation in NAPSAC:

- Removal of fractures with sizes outside of considered value extent – 874370 fractures with an area less than 0.5x0.5 m² were removed from GeoDFN along with 18 fractures with an area more than 50x50 m²,
- Removal of non-conductive fractures with transmissivity index TI=0 – in the GeoDFN all conductive and potentially conductive fractures were kept (transmissivity index TI=1 and TI=2 defined by CGS) – 241437 remained in the reduced GeoDFN model,
- Connectivity analysis in NAPSAC and removal of isolated and dead-end fractures and clusters – resulting v1 HydroDFN network for flow and transport simulations had 4678 fractures.

The Tab. 15 summarizes the basic characteristics of the input GeoDFN model (GeoDFN imported into NAPSAC) and the output HydroDFN model (after connectivity analysis in NAPSAC) of fracture networks for individual model versions.

Tab. 15 Basic summary of GeoDFN a HydroDFN model characteristics

<table>
<thead>
<tr>
<th>Model version</th>
<th>v0</th>
<th>v1</th>
<th>v2</th>
<th>v2-EDZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model volume</td>
<td>[m³]</td>
<td>100x100x100</td>
<td>100x200x100</td>
<td></td>
</tr>
<tr>
<td>GeoDFN model – reduced network with potentially conductive fractures</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total number of fractures</td>
<td>[-]</td>
<td>24933</td>
<td>241437</td>
<td>762599</td>
</tr>
<tr>
<td>Number of fractures per unit volume (P_{30})</td>
<td>[m⁻³]</td>
<td>2.49·10⁻²</td>
<td>2.41·10⁻¹</td>
<td>3.81·10⁻¹</td>
</tr>
<tr>
<td>Fracture surface area per unit volume (P_{32})</td>
<td>[m².m⁻³]</td>
<td>2.79·10⁻¹</td>
<td>3.19·10⁻¹</td>
<td>5.54·10⁻¹</td>
</tr>
<tr>
<td>Porosity of fractures</td>
<td>[-]</td>
<td>4.27·10⁻⁶</td>
<td>3.37·10⁻⁶</td>
<td>6.32·10⁻⁶</td>
</tr>
<tr>
<td>HydroDFN model – after analysis of fracture connectivity</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total number of fractures</td>
<td>[-]</td>
<td>6750</td>
<td>4678</td>
<td>60352</td>
</tr>
<tr>
<td>Number of fractures per unit volume (P_{30})</td>
<td>[m⁻³]</td>
<td>6.75·10⁻³</td>
<td>4.68·10⁻³</td>
<td>3.02·10⁻²</td>
</tr>
<tr>
<td>Fracture surface area per unit volume (P_{32})</td>
<td>[m².m⁻³]</td>
<td>1.62·10⁻¹</td>
<td>8.41·10⁻²</td>
<td>2.71·10⁻¹</td>
</tr>
<tr>
<td>Porosity of fractures</td>
<td>[-]</td>
<td>3.06·10⁻⁶</td>
<td>1.67·10⁻⁶</td>
<td>4.65·10⁻⁶</td>
</tr>
</tbody>
</table>
The resulting network for model v1 was overall on the connectivity limit (so called percolation threshold). This consequence of this being that the fracture network had no fracture within the volume of set disposal borehole – the source point for transport simulations was hence moved within the borehole axis to the nearest conductive fracture, i.e. to the 12 m distance. The input GeoDFN and output HydroDFN networks for unanimous model specification for flow and transport simulations are shown in Fig. 13.

Fig. 13 GeoDFN (left) a HydroDFN (right) fracture network for model v1

### 5.3.3 Version v2

Fracture network for model v2 is based on measured data from URF Bukov (as is model v1) with some errors in the fracture population parameters optimization process fixed in the DFraM SW. The v2 model domain is twice as big compared to model v1 – reason for this being an inclusion of line of 11 disposal boreholes interconnected by a tunnel.

One GeoDFN fracture network with updated fracture population parameter set was generated for model v2 – the stochastic fracture network contained 5124000 fractures. Within GeoDFN, individual fractures were assigned transmissivity index based on percentage representation proposed by CGS. HydroDFN network was then prepared using the same methodology as in model v1 – i.e. fractures with sizes outside the defined interval were removed from the GeoDFN and only conductive and potentially conductive fractures were kept. In total, 462690 remained in the GeoDFN model.

Through NAPSAC connectivity analysis the isolated and dead-end fractures and clusters were removed. Resulting v2 HydroDFN model contained 11380 fractures (Fig. 14) and similarly to model v1 it was not connective enough. Evaluation of the HydroDFN connection to disposal holes showed that not a single disposal hole communicates with this network nor is it intersected by a fracture (see model cross-section in Fig. 15).
The HydroDFN network (11380 fractures) prepared this way contains only 0.22 % of fractures from the GeoDFN (5124000 fractures) – this value is very low, about ten times lower compared to values stated in the SKB reports for Swedish sites. The cause of this might be in the methodology of random assignment of transmissivity index to fractures in the GeoDFN:

1. Percentage representation of conductive features was only estimated because representation of conductive fractures was not yet conceptually measured and evaluated at any site in the CR,
2. The random assignment of transmissivity index is problematic by itself – conductive features constitute a mutually connective network as opposed to generated GeoDFN where the vast majority of fractures is isolated – from the estimated ratio of conductive fractures many were removed because the transmissivity indexes were assigned also to isolated fractures during GeoDFN generation.
The methodology for fracture network generation was modified for model v2 so that the total number of connective fractures in HydroDFN is increased:

- 10% of fractures with TI=0 (non-conductive fractures) were reclassified (randomly selected) as potentially conductive – in total, the modified GeoDFN contained 462690 fractures with TI=1 and TI=2 from the original model and 299909 new fractures (10% of TI=0),
- During the connectivity analysis 593091 isolated and 109156 dead-end fractures were removed from the model – resulting HydroDFN v2 model (Fig. 16) contains 60352 connective fractures (i.e. 1.5% of the GeoDFN – value that corresponds to SKB measurements evaluated by the PFL method),
- 9 of 11 disposal boreholes were connected to the HydroDFN through 22 fractures in total.

![Fig. 16 Resulting v2 HydroDFN model – vertical cross-section through the disposal holes line](image)

Model version v2 simulations were performed also on a variant that included the tunnel EDZ:

- The tunnel EDZ in the model was realized using a single continuous fracture with transmissivity of $1 \times 10^{-7}$ m².s⁻¹, thickness of 0.3 m and porosity of 0.01% (Joyce et al. 2010) – fracture is situated in the tunnel floor and connects individual disposal boreholes,
- After an extension of input GeoDFN network of stochastic fractures by one fracture representing the EDZ the connectivity analysis was again performed – 592701 isolated and 109420 dead-end fractures were removed from the model. The resulting HydroDFN v2-EDZ model (Fig. 17) had 60479 connective fractures (i.e. 127 more than the variant without EDZ),
- All 11 disposal boreholes were connected to the HydroDFN v2-EDZ fracture network through 38 fractures in total.
5.4 Results and comparison – flow and transport simulation

This chapter summarizes the results of flow and transport simulations for individual model versions. Model versions v0 and v1 were processed in all three software programs – NAPSAC, Flow123d, and ADFNE. Models v2, respectively v2-EDZ were completely (both flow and transport) performed in NAPSAC program only; Flow123d enabled only the simulation of flow, ADFNE had problems with the size of the computational network and modelling of the task turned out to be impossible.

5.4.1 Version v0

Basic parameters were evaluated within the framework of processing the results of flow and transport simulation in model version v0 (more details in Tab. 16, Fig. 18 and Fig. 19):

- Size of the overall flow through the model – a very good agreement was reached in all used programs for the uniform assignment of the fracture network – the values range between $1.43 \times 10^{-8}$ and $1.52 \times 10^{-8}$ m$^{3}$.s$^{-1}$,
- Mean time of tracer travel (advective transport) – unlike for the flows, the difference between these values (1.6 to 5.5 years) is more significant across the software packages; the result calculated in ADFNE is characterized by the greatest deviation.
- The specific flow at the intersection of the fracture with the deposit borehole refers to the advective flow rate at the source (ratio of the specific flow and the aperture of the source fracture) or the amount of water flowing through the source area (product of the specific flow and the intersection lengths – in ADFNE it is possible to determine only the flow at the intersections of fractures, not directly at the location of the borehole (due to simpler fracture discretization in ADFNE).
Tab. 16 Overview of flow and transport simulation results – common assignment, model v0

<table>
<thead>
<tr>
<th>Model v0</th>
<th>PROGEO</th>
<th>TUL</th>
<th>FJFI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of fractures/intersections</td>
<td></td>
<td>6750/9221</td>
<td></td>
</tr>
<tr>
<td>Software</td>
<td>ConnectFlow – NAPSAC</td>
<td>Flow123d</td>
<td>ADFNE</td>
</tr>
<tr>
<td>Total flow through the fracture network</td>
<td>1.52E-08 m$^3$.s$^{-1}$</td>
<td>1.45E-08 m$^3$.s$^{-1}$</td>
<td>1.43E-08 m$^3$.s$^{-1}$</td>
</tr>
<tr>
<td>Specific flow in the intersection of fracture and disposal borehole</td>
<td>6.90E-11 m$^2$.s$^{-1}$</td>
<td>5.77E-11 m$^2$.s$^{-1}$</td>
<td>not determined</td>
</tr>
<tr>
<td>Advektive transport - characteristics of the breakthrough curve:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Minimum</td>
<td>1.2 years, 74.8 m</td>
<td>0.7 years, 64.0 m</td>
<td>1.2 years</td>
</tr>
<tr>
<td>• Median</td>
<td>2.0 years, 100.5 m</td>
<td>1.6 years, 89.2 m</td>
<td>5.5 years</td>
</tr>
<tr>
<td>• Maximum</td>
<td>22.3 years, 149.5 m</td>
<td>17.24 years, 120.2 m</td>
<td>20.0 years</td>
</tr>
</tbody>
</table>

Fig. 18 Breakthrough curves of advective transport – common assignment of model v0
Simulations of flow and transport for 100 various versions of the stochastic fracture network (with the same parameters describing the fracture populations) were performed in NAPSAC software within the framework of model version v0 processing:

- Fracture networks interconnected in all 100 versions were generated at the level of the entire model domain. Depending on the network connectivity, the flow through the model varied within the range of 2 orders of magnitude – $7.0 \times 10^{-10}$ to $5.0 \times 10^{-8} \text{ m}^3\text{s}^{-1}$, mean value of the flow was $1.8 \times 10^{-8} \text{ m}^3\text{s}^{-1}$, see Fig. 20,
- when placing the disposal borehole into the center of the model domain, the fracture network intersected with the disposal borehole in 42 versions – trajectories and delay times of particles were evaluated for these models, see Fig. 21 and Fig. 22,
- lengths of the trajectories vary between 55 and approx. 300 m, with mean length of 95 m,
- delay times vary between 0.3 and 2000 years, with mean travel time of 7 years,
- Based on these results, it is quite important to avoid executing only one variant of the stochastic network but rather carry out simulations at several different fracture networks – for model v0, it was appropriate to simulate at least 10 versions (preferably 20-25 versions), however, the minimal number of versions depends on the total number of fractures in the model and on the overall connectivity – fracture networks with a higher number of fractures and better interconnection have more homogeneous character and a smaller number of versions is sufficient; on the contrary, more simulations are required for less connective networks.
Fig. 20 Evaluation of the overall flow through the model for 100 various realizations of the fracture network – NAPSAC

Fig. 21 Evaluation of the lengths of trajectories for 100 different fracture network versions – NAPSAC – the graph shows results for 42 disposal boreholes which were interconnected with the fracture network
5.4.2 Version v1

Basic parameters were evaluated within the framework of processing the results of flow and transport simulation in model version v1 (more details in Tab. 17, Fig. 23 and Fig. 24):

- Size of the overall flow through the model – a very good agreement was reached in all used programs for the uniform assignment of the fracture network – the values range between $3.35 \times 10^9$ and $3.95 \times 10^9$ m$^3$.s$^{-1}$,
- Mean time of tracer travel time (advective transport) – unlike the flow values, these values range between 100 and 1200 years and differ considerably across individual software types – the differences are clearly caused by very slow flow in the source fracture intersecting the disposal borehole (see Fig. 25) and by differences in the velocities calculated by individual software packages. The fastest flow and the shortest delay time were calculated in ADFNE for which it is not possible to specify the source directly in the intersection of the fracture and disposal borehole but only in the nearest intersection of fractures. The longest delay time was calculated in Flow123d, and this difference (compared to the NAPSAC results) was caused by a lower velocity calculated by Flow123d in the area of the disposal borehole (approximately 4 times lower velocity compared to that obtained in NAPSAC). Calculation accuracy in areas with less connective fracture network, which are thus characterized by a very low

![Fig. 22 Evaluation of the delay times for 100 different fracture network versions – NAPSAC – the graph shows results for 42 disposal boreholes which were interconnected with the fracture network](image-url)
Transport of radionuclides from deep geological repository/Testing of conceptual and numeric models – Final report

pressure gradient, will play an important role here. These cases would require a more detailed comparison and analysis as to which solution is more accurate because they significantly influence the results of the transport.

Tab. 17 Overview of flow and transport simulation results – common assignment, model v1

<table>
<thead>
<tr>
<th>Model v1</th>
<th>PROGEO</th>
<th>TUL</th>
<th>FJFI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of fractures/intersections</td>
<td>4678/8017</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Software</td>
<td>ConnectFlow – NAPSAC</td>
<td>Flow123d</td>
<td>ADFNE</td>
</tr>
<tr>
<td>Total flow through the fracture network</td>
<td>3.95E-9 m³s⁻¹</td>
<td>3.76E-9 m³s⁻¹</td>
<td>3.35E-9 m³s⁻¹</td>
</tr>
<tr>
<td>Specific flow in the intersection of fracture and disposal borehole</td>
<td>4.0E⁻¹⁵ m³s⁻¹</td>
<td>1.11E⁻¹⁵ m³s⁻¹</td>
<td>not determined</td>
</tr>
<tr>
<td>Advective transport - characteristics of the breakthrough curve:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Median</td>
<td>500 years, 135 m</td>
<td>1200 years, 116 m</td>
<td>100 years</td>
</tr>
</tbody>
</table>

Fig. 23 Breakthrough curves of advective transport – common assignment of model v1
5.4.3 Version v2

Determination of geometry and computational network for Flow123d was very difficult with the existing SW equipment due to a high number of fractures in model v2. Although the network
was created (the generated computational network consisted of 2755800 triangular elements) and flow simulations were performed in this network, the results were not quite correct, probably due to presence of degenerated elements or incorrect representation of fractures connectivity in parts of the computational domain (results of follow-up analyses, i.e., determination and description of transport routes are thus not mentioned). Water flow through the domain amounts to $5.8 \times 10^{-8} \text{ m}^3 \text{s}^{-1}$ (for the gradient in the direction of axis $x$) and $3.3 \times 10^{-8} \text{ m}^3 \text{s}^{-1}$ (for the gradient in the direction of axis $y$). These values are slightly higher than the flows calculated in NAPSAC (see below).

![Fig. 26 Model v2 – results of flow simulation in Flow123d, gradient in the direction of axis x on the left, gradient in the direction of axis y on the right](image)

Calculation of model version v2 in ADFNE was modified against the previous simulations – results obtained directly from NAPSAC (flows and pressures in fracture intersection points) were used for model processing due to problems with a high number of fractures, which were implemented in the DFN model in ADFNE by first creating a "pipes" network in the ADFNE using the central method, and then assigning a volume flow to each intersection of each "pipes".

Flow and transport calculation were carried out on 4 models in total within NAPSAC software – for basic version v2 without the tunnel and version v2-EDZ with the influence of the tunnel. Two variants of boundary conditions were further simulated for each of these versions – with constant gradient of $0.05 \text{ m.m}^{-1}$ in the direction of axis $x$ (perpendicular to the line of disposal boreholes – head boundary conditions 405 m and 400 m) and in the direction of axis $y$ (parallel with the line of disposal boreholes – head boundary conditions 395 m and 405 m). A slightly higher flow was calculated in the direction parallel with the line of disposal boreholes (in the direction of axis $Y$).

Calculated flows in model v2 without the tunnel:

- gradient $X \approx 3.97 \times 10^{-8} \text{ m}^3 \text{s}^{-1}$ (the flow area of the model is double in this direction),
- gradient $Y \approx 2.33 \times 10^{-8} \text{ m}^3 \text{s}^{-1}$.

Calculated flows in model v2-EDZ with the tunnel are slightly higher:
- gradient X – 4.08x10^{-8} \, \text{m}^3\text{s}^{-1} (the flow area of the model is double in this direction),
- gradient Y – 2.54x10^{-8} \, \text{m}^3\text{s}^{-1}.

Tab. 18 lists the values of specific flows at source points of the intersections of the disposal boreholes and the fracture network. These values are important from the perspective of transport – the performed simulations in all model versions show that the flow velocity in the close vicinity of the disposal boreholes has the greatest influence on the overall delay time. Zero values in the table represent connection of the disposal borehole to so called dead-end fracture which has only one intersection point and does not contribute to the flow within the remaining part of the fracture network.

<table>
<thead>
<tr>
<th>#</th>
<th>WDP</th>
<th>MACROFRAC</th>
<th>X FLUX(m^2/s)</th>
<th>Y FLUX(m^2/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>5145</td>
<td>4.49E-11</td>
<td>6.22E-12</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>8658</td>
<td>1.74E-12</td>
<td>2.58E-13</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>13880</td>
<td>9.73E-15</td>
<td>2.93E-15</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>17618</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>13794</td>
<td>8.47E-13</td>
<td>8.75E-13</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>32363</td>
<td>5.87E-14</td>
<td>8.57E-14</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>46416</td>
<td>1.38E-12</td>
<td>8.12E-12</td>
</tr>
<tr>
<td>8</td>
<td>7</td>
<td>4441</td>
<td>8.72E-13</td>
<td>1.10E-12</td>
</tr>
<tr>
<td>9</td>
<td>7</td>
<td>22403</td>
<td>3.75E-13</td>
<td>1.20E-12</td>
</tr>
<tr>
<td>10</td>
<td>7</td>
<td>24878</td>
<td>5.39E-12</td>
<td>1.83E-11</td>
</tr>
<tr>
<td>11</td>
<td>7</td>
<td>36133</td>
<td>8.41E-14</td>
<td>1.29E-13</td>
</tr>
<tr>
<td>12</td>
<td>7</td>
<td>42203</td>
<td>8.00E-13</td>
<td>7.47E-13</td>
</tr>
<tr>
<td>13</td>
<td>7</td>
<td>51648</td>
<td>9.00E-14</td>
<td>4.52E-14</td>
</tr>
<tr>
<td>14</td>
<td>8</td>
<td>2633</td>
<td>1.08E-12</td>
<td>5.14E-14</td>
</tr>
<tr>
<td>15</td>
<td>9</td>
<td>21503</td>
<td>9.19E-12</td>
<td>6.29E-12</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
<td>14919</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>17</td>
<td>10</td>
<td>23700</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>18</td>
<td>10</td>
<td>25188</td>
<td>1.89E-15</td>
<td>1.83E-15</td>
</tr>
<tr>
<td>19</td>
<td>10</td>
<td>32653</td>
<td>3.89E-13</td>
<td>3.80E-13</td>
</tr>
<tr>
<td>20</td>
<td>11</td>
<td>23682</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>21</td>
<td>11</td>
<td>25885</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>22</td>
<td>11</td>
<td>26335</td>
<td>1.49E-15</td>
<td>3.92E-16</td>
</tr>
</tbody>
</table>

Charts in Fig. 27 and Fig. 28 document the breakthrough curves (delay times) for the advective transport from individual disposal boreholes (for model v2 without a tunnel), respectively the comparison of summary breakthrough curves for all executed model variants. Results show a relatively homogeneous course of the curves for both variants of the specified gradient (x, y) – groundwater flow direction (perpendicular to or parallel with the line of disposal boreholes) thus did not have a substantial impact on the results of the transport in the performed simulations. A more significant impact on the resulting delay time was encountered for EDZ fracture inclusion into the model – the mean delay time in model v2-EDZ decreased to about
a half – from 8 years for model v2 without the tunnel to 3.5 years for model with the tunnel. Fig. 29 and Fig. 30 show particle trajectories for individual model variants. In case of the version with EDZ, there is an obvious interconnection with the fracture network and creation of a preferential route within the tunnel line (it issues from the defined EDZ concept, multiple scenarios will, however, have to be prepared for the safety assessment).

Fig. 27 Model v2 – NAPSAC – delay times (breakthrough curves) for advective transport from individual disposal boreholes – gradient X (left) and gradient Y (right)

Fig. 28 Comparison of summary breakthrough curves for the model variants executed in NAPSAC
Fig. 29 Model v2 – particle tracking simulation in NAPSAC – gradient in the direction of axis x – version without tunnel on the left, version with EDZ on the right

Fig. 30 Model v2 – particle tracking simulation in NAPSAC – gradient in the direction of axis y – version without tunnel on the left, version with EDZ on the right
5.5 Export of results from NAPSAC to GoldSim

NAPSAC software primarily exports only the basic summary information into its output files – usually the statistically evaluated and summary data regarding the fracture network, flow through the model, transport paths, etc. Implemented commands enable export of additional files with highly detailed model results for individual fractures, intersection points of the fractures, computational nodes, sections of transport paths, etc. These files are exported in text format, however, they are quite large for models with higher numbers of fractures or defined particles due and this makes them less suitable for direct upload into (or into another program). Scripts have been therefore created in Python language, which process the exported files from NAPSAC and convert them into format suitable for retrieval into GoldSim, Excel, Matlab, etc. After discussions with the experts from ÚJV and FJFI, the results from NAPSAC are delivered in 5 files in total:

- *.sum – basic output file with summary information for individual particles. Raw SUM file coming directly from NAPSAC.
- *.list – extended output file with detailed information about particle tracking in subfractures (the subfractures represent refinement of discretization of the main macrofractures for more accurate flow and particle tracking calculations). Modified export from PTV file from NAPSAC.
- *.MACROFRACTURES_Q.list – extended output file with detailed information about particle tracking in macrofractures - information from flow calculation is added, i.e., the water balance in macrofractures and volume flows through intersection points of the macrofractures. Modified export from PTV, DFN, and PIPE file from NAPSAC.
- *.vtk – file for transport paths visualization in PARAVIEW software,
- *.SAVEVALUES.txt – file with calculated pressure values in all “global nodes” (usually centers or end points of the intersection lines of fractures).

Detailed description of parameters in particle tracking output files from NAPSAC is available in the following tables.

Tab. 19 Structure of *.sum output file

<table>
<thead>
<tr>
<th>Parameter description</th>
<th>Parameter description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PARTICLE NUMBER [-]</td>
<td>particle number, trajectory number</td>
</tr>
<tr>
<td>TRAVEL TIME [year]</td>
<td>total travel time of the particle within the model</td>
</tr>
<tr>
<td>PATHLENGTH [m]</td>
<td>total length of the trajectory</td>
</tr>
<tr>
<td>AV. PORE VEL. [m.s⁻¹]</td>
<td>average transport velocity, i.e., ratio of PATHLENGTH/TRAVEL TIME</td>
</tr>
<tr>
<td>INITIAL VEL. [m².s⁻¹]</td>
<td>specific flow at the point of particle release (at the starting point)</td>
</tr>
<tr>
<td>F QUOTIENT [year.m⁻¹]</td>
<td>summary value of F-factor</td>
</tr>
<tr>
<td>ARRIVAL POSITION [-]</td>
<td>internal designation of the point at which the particle leaves the model (intended for checking whether the particle arrived to the boundary condition (SURFACE) or whether the particle was lost during the calculation (LOST))</td>
</tr>
</tbody>
</table>
Tab. 20 Structure of *.list output file

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PART NUMBER</td>
<td>particle number, trajectory number</td>
</tr>
<tr>
<td>STEP ID</td>
<td>transport step number</td>
</tr>
<tr>
<td>cumulTIME</td>
<td>cumulative travel time of the particle within the model</td>
</tr>
<tr>
<td>cumulLENGTH</td>
<td>cumulative length of the trajectory</td>
</tr>
<tr>
<td>APER</td>
<td>hydraulic aperture of the subfracture</td>
</tr>
<tr>
<td>APERTRANS</td>
<td>transport aperture of the subfracture</td>
</tr>
<tr>
<td>FFAKTOR</td>
<td>value of F-factor for relevant transport step</td>
</tr>
<tr>
<td>GRADIENT</td>
<td>hydraulic gradient in relevant transport step</td>
</tr>
<tr>
<td>SPECIFIC FLUX</td>
<td>specific flow in relevant transport step</td>
</tr>
<tr>
<td>SUBFRAC NUMBER</td>
<td>number of the subfracture in which the particle moves in given transport step</td>
</tr>
<tr>
<td>MACROFRAC NUMBER</td>
<td>number of the macrofracture in which the particle moves in given transport step</td>
</tr>
</tbody>
</table>

Tab. 21 Structure of *.MACROFRACTURES_Q.list output file

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PART NUMBER</td>
<td>particle number, trajectory number</td>
</tr>
<tr>
<td>STEP ID</td>
<td>number of transport step in which the particle leaves the macrofracture and moves to another macrofracture</td>
</tr>
<tr>
<td>cumulTIME</td>
<td>cumulative travel time of the particle within the model</td>
</tr>
<tr>
<td>cumulLENGTH</td>
<td>cumulative length of the trajectory</td>
</tr>
<tr>
<td>APER</td>
<td>hydraulic aperture of the macrofracture</td>
</tr>
<tr>
<td>APERTRANS</td>
<td>transport aperture of the macrofracture</td>
</tr>
<tr>
<td>cumulFFAKTOR</td>
<td>cumulative value of F-factor</td>
</tr>
<tr>
<td>MACROFRAC NUMBER</td>
<td>number of the macrofracture in which the particle moves in given transport step</td>
</tr>
<tr>
<td>MACROFRAC AREA</td>
<td>total area of the macrofracture within the model (if the macrofracture is located at the border of the model, it means the current cut area in the model and not the original generated size)</td>
</tr>
<tr>
<td>MACROFRAC TOTAL_Q</td>
<td>balance of the total water quantity in the macrofracture, i.e., the total inflow into the macrofracture through all intersection points with other macrofractures, respectively the total discharge leaving the macrofracture through all intersection points with other macrofractures</td>
</tr>
<tr>
<td>MACROFRAC INTERSECTION_Q_OUTFLOW[+]</td>
<td>water quantity leaving through intersection point with connected macrofracture in the direction of particle movement. Non-zero difference between TOTAL_Q and INTERSECTION_Q_OUTFLOW produces discharge through other intersection points on the macrofracture.</td>
</tr>
</tbody>
</table>
Due to the computational network refinement to subfractures, there may be a situation when water leaves the macrofracture in one part of the intersection point (with particle moving through this part of the intersection point) while there is water flowing into the macrofracture in the other part of the intersection point. If this two-sided flow occurs on an intersection point, the size of INFLOW is non-zero.

<table>
<thead>
<tr>
<th>MACROFRAC</th>
<th>INTERSECTION_Q</th>
<th>INFLOW[-]</th>
<th>[m³.s⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>MACROFRAC</td>
<td>INTERSECTION_L</td>
<td>OUTFLOW/INFLOW</td>
<td>[m]</td>
</tr>
</tbody>
</table>

Length of the intersection point (OUTFLOW) through which the particle is moving and through which water is discharged into follow-up macrofracture. If a water inflow into the macrofracture takes place at the intersection point at the same time, the INFLOW length is non-zero. Total length of the intersection point corresponds to the sum of OUTFLOW and INFLOW lengths.

5.6 DFN model upscaling into CPM

DFN model upscaling into CPM (sometimes also designated as equivalent CPM, i.e., ECPM) is a process during which characteristics of a discrete fracture network from HydroDFN model are recalculated into continuous network of model cells, respectively into a 3D grid. The main parameters assigned to individual cells within the CPM model during upscaling are:

- hydraulic conductivity tensor (for flow and transport calculation),
- porosity (for advective transport calculation),
- wetted surface of fractures (for inclusion of the influence of rock matrix into transport calculation).

DFN model upscaling into CPM usually results in an overall simplification and schematization of model geometry – depending on suitably selected discretization of the CPM model (cell size), the number of computational elements is reduced, demands on the calculation decrease considerably, and the calculation thus allows for efficient simulation of tasks that would be too complex in the original DFN concept due to a network with excessive number of fractures and intersection points that would render it numerically unsolvable. At the same time, a suitably chosen discretization of CPM model (and suitably chosen upscaling method) do not cause a large impact and simplification of the heterogeneity of hydraulic or transport properties (interconnection of fractures from DFN model is converted into interconnection of adjacent cells in CPM model) and the flow results, respectively the results of transport in DFN and CPM model, should be comparable (equivalent).

5.6.1 Upscaling methodology in NAPSAC software

Upscaling from HydroDFN into CPM was performed in NAPSAC software during the T8 project as this software has its own tool implemented for this purpose. Upscaling is not quite a trivial process, mainly the hydraulic conductivity tensor calculation for individual cells of the CPM model can be time consuming depending on the parameters defined in the upscaling settings and chosen model discretization.

The procedure to be followed during the upscaling of DFN model parameters into CPM in NAPSAC is as follows:
1. Created HydroDFN model with defined parameters of fractures represents the input into the entire process (neither flow nor transport have to be calculated in advance for the model).

2. Selection of discretization of the future CPM model (regular grid or possibility of irregular grid retrieval from a file).

3. Upscaling settings (size of buffer around the cells, definition of properties to be calculated from the DFN model).

4. Calculation of properties for individual cells – NAPSAC first “cuts” the DFN model of the fracture network to relevant cell size (it is advisable to use a buffer around the cell so that the calculation is performed for a slightly bigger area due to elimination of possible errors for fractures connected in cell corners) and performs hypothetic flow calculation in this segment of the fracture network (possibly also the advective transport calculation) with gradient in the direction of main axes x, y, z – such calculated flows (and possibly also the transport results) are then used to determine the hydraulic conductivity tensor (6 values in total – K_{xx}, K_{xy}, K_{xz}, K_{yy}, K_{yz}, K_{zz}), porosity (from the opening of individual fractures in the segment), etc., gradually for all cells according to the discretization.

5. Output of the entire process are the calculated properties exported into discrete files (in the format used by NAPSAC; a Python script enables data conversion into vtk file).

Exported upscaled parameters are then input during CPM model creation. Within the framework of T8 project, PROGEO tested 2 programs using the CPM concept:

1. specialized software NAMMU from ConnectFlow package which supports direct upload of upscaled parameters (it is capable of working with the complete hydraulic conductivity tensor),

2. MODFLOW and MT3DMS programs which are commonly available and used for solving hydrogeological tasks (they, however, work only with the main hydraulic conductivity directions (K_{xx}, K_{yy}, K_{zz}).

### 5.6.2 Results and comparison of models

Several upscaling variants with different input DFN fracture network and different size of CPM model cells were tested on model v0.

The simplest and basic upscaling variant was to convert the DFN model to a single CPM cell with the size of 100 x 100 x 100 m. This size, among others, corresponds to the size of the cell used in regional models within the “HG models" project. Flow through HydroDFN model version v0 calculated in NAPSAC (1.84x10^{-8} m^3.s^{-1}), defined gradient (0.05), and cross-section area of the model (100 m^3) input into the Darcy’s law enable simple derivation of the value of hydraulic conductivity of this CPM cell K_{xx,100}=3.7x10^{-11} m.s^{-1}. This value represents an average hydraulic conductivity of given rock block (equivalent for given generated fracture network; another realization of stochastic fracture network would result in a different flow value and thus also a different equivalent value of hydraulic conductivity). Transport apertures and sizes of individual fractures then again enable simple determination of average porosity of given rock block ε_{100}=2.3x10^{-6}. This value represents only the specified “open” volume of fractures available for advective transport through the fracture network, it thus does not include the porosity of the rock matrix which is the order of magnitude higher. If we simulate the advective transport in this CPM cell (from the disposal borehole in the center of the cell towards the model boundary, i.e., for the trajectory length of 50 m), we get the advective travel time of 2.0 years.
Fig. 31 shows the hydraulic conductivity of CPM model (red to light blue cells, blue color indicates the areas with zero permeability, black color indicates remaining parts of fractures) obtained by upscaling of DFN model v0 in NAPSAC for regular grid variant with cell size 5 x 5 x 5 m.

Graph in Fig. 32 compares the resulting breakthrough curves of the tracer calculated for DFN model v0 (gray curve) and for corresponding upscaled CPM model with cell size of 5 m. The graph shows a relatively significant difference in the breakthrough times:

- 20 to 60 years in DFN model v0,
- 0.8 to 3 years in CPM model v0.

The difference in this case is clearly caused by the CPM model discretization – cells with the size of 5 x 5 x 5 m in the closest vicinity of the disposal borehole cannot sufficiently and equivalently describe the character of the fracture network in this area which would require a much finer discretization (smaller cell size). The “DFN*” breakthrough curve then corresponds to the variant of tracer source shifting by 5 m further away from the disposal borehole where the fracture network is more interconnected and the breakthrough curves mutually correspond much better. Mean travel time of 2 years also very well corresponds to the calculated value of the model with cell size of 100 m.
Fig. 32 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v0 calculated in NAPSAC and NAMMU, regular grid of CPM model with the cell size of 5x5x5 m

Comparison of results between DFN model (for various variants of size of the calculation elements, i.e., for various variants of fractures division into subfractures) and equivalent CPM model with finer discretization and smaller cell size of 2 x 2 x 2 m is in Fig. 33. This is a slightly different version of the input fracture network v0 compared to the previous (above-mentioned) models. The graphs however show a very good conformity of results between input HydroDFN model and upscaled CPM model.

Fig. 33 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v0 calculated in NAPSAC and NAMMU, regular grid of CPM model with the cell size of 2x2x2 m

Comparison of the results of DFN and CPM models v1 provided a slightly worse conformity compared to model v0. Upscaling of the uniform fracture network in model v1 was performed only for the cell size of 2 x 2 x 2 m. However, model v1 showed that even this relatively fine discretization was not sufficient for equivalent calculation of flow character in the nearest vicinity of the defined disposal borehole. Detailed analysis revealed very slow flow in DFN
model in the fracture intersecting with the disposal borehole which resulted in a significant prolongation of tracer penetration time to 500-1000 years, see Fig. 34. Results of the transport in CPM model v1 (this time calculated in both MT3D and NAMMU with comparable breakthrough curves; full transport used in MT3D in addition to the particle tracking method) show travel times lower in the order of magnitude: 45-55 years. A better agreement could of course be reached by even more detailed discretization of the CPM computational network, oh the other hand, we would get more or less to the size of the computational element used in DFN and the method of upscaling to CPM would no longer be effective from the calculation perspective. Based on this experience, it seems to be more convenient to simulate the nearest vicinity of the disposal boreholes and tunnels with DFN method. CPM approach can be used in greater distances.

Fig. 34 Comparison of breakthrough curves of tracer in DFN and CPM model – model version v1 calculated in NAPSAC (DFN) and MT3D (CPM), regular grid of CPM model with the cell size of 2x2x2 m
6 GoldSim

In addition to calculating the flow and transport of trackers in the specialized hydrogeological programs NAPSAC and Flow123D, the transport of the tracker was also simulated in the GoldSim program in the framework of the project. One of the main objectives of these simulations was to prepare and verify procedures for the transfer and use of simulation results from hydrogeological programs for safety analyses performed in GoldSim. The model used for safety analyses (not the subject of this project) contains hundreds of parameters and rock transport is an important retardation medium. For these reasons, it is necessary that the rock transport (whether in the immediate vicinity of the storage boreholes, which is part of a near field or distant far field) should be clearly and credibly described in GoldSim.

Simulations in GoldSim program (in current version 12.0.0) were realized in two workplaces - FJFI a ÚJV. Three final versions of data v0, v1 and v2 were available to track the trackers. Due to the limited duration of the project, the “working” version of v0 was also used to test the data transfer between the NAPSAC (PROGEO) and GoldSim (ÚJV) programs.

6.1 GoldSim input parameters, transfer of data from HydroDFN models and data processing

Within the solution of data transfer from HydroDFN model („Particle tracking“) to model, which was created in GoldSim, transport path data were exported from program NAPSAC and handed in form of four files. Three of those were standard text files (for possibility of batch processing or loading into program EXCEL) and one in form of „vtk“ file. The last mentioned file is used to display 3D transport paths, which is possible e.g. in free software ParaView (see Fig. 35).

![Fig. 35 Visualisation of 100 transport paths (with one starting point) exported from HydroDFN model. Sections of macrofractures are distinguished in colour according to the value of transport aperture](image-url)
Individual particles occur in the segments of transport paths, which are shown in Fig. 35. Those segments correspond to „subfractures“, which result from finer discretization of the NAPSAC model. The length of the transport path segments can vary in the same macrofractures. Also, it is not possible to replace or combine transport paths, which go through the same macrofractures (in the same order), because their parameters (e.g. length or F-quotient) can be significantly different.

Detailed characteristic of the transport paths in the first data file contains all computational steps of each transport path. Unique identification numbers of all particles, computational steps with coordinates and identification numbers of subfractures and macrofractures are included in the data file.

Following parameters for each computational step are listed in the first data file:

- cumulative time (year),
- cumulative length (m),
- F-quotient (year·m⁻¹),
- hydraulic aperture (m),
- transport aperture (m),
- gradient (m·m⁻¹),
- specific flux (m²·s⁻¹).

F-quotient was calculated from the results of the NAPSAC simulations according to equation (6.2) and is stated in units (year·m⁻¹). More details about the F-quotient are described later in the text. Each segment of the transport path is also classified by value of hydraulic and transport aperture, which are constant in whole macrofractures.

After an agreement between researchers was the second data file made in form of summary information of transport paths in macrofractures. In this file, the values of parameters listed above are compiled into segments of the transport paths, which correspond to individual macrofractures, because in GoldSim model, one segment of the transport path is matched to one macrofracture.

This data file contains additional parameters:

- macrofracture area (m²),
- total flow rate (m³·s⁻¹) in each macrofracture,
- flow rate (inflow and outflow) in macrofracture intersections (m³·s⁻¹),
- length (m) of macrofracture intersections.

The third data file contains a summary of all transport paths and is consisted mainly of:

- total time of each transport path (year),
- total length of each transport path (m),
- average transport velocity for each transport path (m·s⁻¹),
- initial specific flow (m²·s⁻¹) of each transport path (i.e. at the source point),
- total F-quotient (year·m⁻¹) of each transport path.

In this GoldSim model concept, in which one model segment of the transport path corresponds to part of the transport path in one macrofracture, choice of following parameters is key:

- length of transport path section in each macrofracture,
- length of each macrofracture intersection – considered as modelled width (W),
transport aperture – by using multiplication of transport aperture and width (W) is determined a flux area,

- F-quotient – with use of F-quotient is according to equation (6.1) calculated flow rate Q.

Coefficient $WL/Q$ or F-quotient (also transport resistance) is one of the descriptive factors of 1D transport path. Authors differ in technical terms for this parameter in literature:

- FWS/q (Neretnieks 2002),
- $\beta$ (Cvetkovic et al. 1999),
- F-quotient (Andersson et al. 1998),
- WL/Q (Vieno a Nordman 2000)

F-quotient is defined by following equation:

$$FWS = \beta = F = \frac{2WL}{Q}$$ (6.1)

where $L$ represents the length of the path (or segment of the path), $Q$ is the flow along the channel, $W(s)$ is the width of the channel.

For advective transport time is applied:

$$F = \sum_f 2t_f e_f$$ (6.2)

where $t_f$ represents a tracer arrival time of $f^{th}$ transport path segment and $e_f$ is a transport aperture (radius) of $f^{th}$ transport path segment. Real residence time of radionuclide in the transport path through the geosphere ($t_R$) can be determined according to Vieno and Nordman (1999) as a sum of time, which a particle spends by moving of radionuclide in groundwater $t$ (advective transport time), and a residence time of radionuclide influenced by matrix diffusion and sorption by equation $u$:

$$t_R = t + \frac{2}{3} u^2$$ (6.3)

parameter $u$ is expressed by:

$$u = \frac{WL}{Q} \in \sqrt{D_p R_p}$$ (6.4)

Where parameter $D_p$ is rock matrix pore diffusivity and $R_p$ is rock matrix retardation coefficient.

Definition of the transport resistance (so called F-quotient) and advective transport time used in Finnish and Swedish reports is in agreement with geosphere parameters as are defined in program GoldSim (GoldSim 2014) and how these parameters were used in previous calculations within the project SÚRAO „ Research support for the safety assessment of a deep geological repository “, e.g. within the project Transport 2 (Trpkošová et al. 2016) and Transport 7 (Trpkošová et al. 2018).

### 6.2 Selection of transport path (particle trajectory)

To describe a transport path, which occurs in observed part of the deep repository, there was 100 trajectories available. Transport paths lengths and their arrival times were calculated in
program NAPSAC (using particle tracking method). All 100 particles were released from one point in modelled area and differ in their arrival (drainage) locations at the end of modelled area (Fig. 35).

Transfer of these transport paths (more precisely their selection) into subsequent GoldSim simulations occurred in more developmental steps. At first and analogous to Finnish and Swedish concept to choose the position of defected canister, there was an effort to select only part of particles of all observed canisters. That would reduce quantity of particles and computational requirements. To characterise a transport path was used F-quotient and radiological criteria, so called „performance measures” R₁ and R₂ (Posiva 2012a, Posiva 2014). These criteria quantify a value of maximal release rate from geosphere to biosphere from a certain position of the deep repository with respect to their radiological toxicity.

\[ R_1 = \max_{0 < t < 15000 \text{ years}} \left[ \frac{R_{1-129}(t)}{H_{1-129}} + \frac{R_{36Cl}(t)}{H_{36Cl}} + \frac{R_{14C}(t)}{H_{14C}} \right] \]  

and

\[ R_2 = \max_{0 < t < 15000 \text{ years}} \left[ G_{1-129}R_{1-129}(t) + G_{36Cl}R_{36Cl}(t) + G_{14C}R_{14C}(t) \right] \]

where \( R_N(t) \) [Bq·a⁻¹] represents „release rate“ of radionuclide \( N \) into surface environment in time \( t \), \( G_N \) [Sv·Bq⁻¹] is an ingestion dose coefficient of certain radionuclide and \( H_N \) [Bq·a⁻¹] means a restriction, which specifies a release of radionuclides into environment. This restriction is defined for each radionuclide within the Finnish regulations.

Values of parameters \( G_N \) and \( H_N \) for three radionuclides, which were included into the base case scenario (BS-ALL) simulation are listed in Tab. 22. Due to the computational requirements were not simulated radiological criteria for all monitored radionuclides, but only for critical radionuclides of certain scenario. Nuclides \(^{129}\)I, \(^{36}\)Cl and \(^{14}\)C were selected, because of their high amount to dose contribution (Posiva 2014). These nuclides are also significant in Czech concept and therefore were used within this project for calculations of radiological criteria \( R_1 \) and \( R_2 \).

<table>
<thead>
<tr>
<th>Radionuclide N</th>
<th>Parameter ( G_N ) [Sv·Bq⁻¹]</th>
<th>Parameter ( H_N ) [Bq·rok⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{129})I</td>
<td>1.1E-07</td>
<td>1E08</td>
</tr>
<tr>
<td>(^{36})Cl</td>
<td>9.3E-10</td>
<td>3E08</td>
</tr>
<tr>
<td>(^{14})C</td>
<td>5.8E-10</td>
<td>3E08</td>
</tr>
</tbody>
</table>

A transport model of all 100 particles was created in program GoldSim with aim of calculating the radiological criteria \( R_1 \) and \( R_2 \). The model does not differ from model, which was used to simulate transport of selected tracers (see chapter 6.5), only the input data were from the interim version of model v0, before the final version of model v0 was finished. Given the fact, that computations in program GoldSim are relatively time consuming, the aim was to correlate calculated radiological criteria \( R_1 \) and \( R_2 \) with total values of F-quotient for certain particle.
Difference between these parameters is (besides other things) in incorporation of transport and retardation processes. F-quotient covers only simulation of transport by advection and can be calculated from data obtained by particle tracking method, while the radiological criteria \( R_1 \) and \( R_2 \) include all transport and retardation processes along the transport path, such as rock matrix diffusion, dispersion in rock environment, sorption or radioactive decay, and those need to be computed with use of program, that is specialised for these simulations. In this case, program GoldSim is used. For all particles were besides radiological criteria \( R_1 \) and \( R_2 \) (Fig. 36, Fig. 37) calculated also values of F-quotient (Fig. 38). These parameters were subsequently correlated. Particles were sorted by ascending F-quotient. In the same order are particles displayed in Fig. 36 and Fig. 37. As it is possible to see in graphs, with a few exceptions, the higher the F-quotient, the smaller the value of criteria \( R_1 \) and \( R_2 \). There is a tight correlation between these parameters and because of that, just F-quotient was used in data versions v0 and v1 to select particles, those were intended for further comparison of calculations in program NAPSAC and GoldSim.

![Fig. 36 Radiological criterion \( R_1 \), order of particles is based on ascending F-quotient](image1)

![Fig. 37 Radiological criterion \( R_2 \), order of particles is based on ascending F-quotient](image2)
With use of F-quotient were selected particles, whose mass flow rate and total balance were obtained from NAPSAC (or MODFLOW for interim model version v0) and GoldSim simulations, and subsequently were mutually compared (see chapter 6.4). Due to different results, which are described in chapter 6.4, the aim to achieve similar results from programs was abandoned. GoldSim simulations were used as another method to compare transport of selected radionuclides without calibration of transport path parameters to results of 3D transport model (see chapter 6.5).

6.3 Parameters and description of transport path

In program GoldSim was created a model of radionuclide transport in area of interest. All 100 particles were simulated, each particle represents one transport path. The transport path is consisted of that many parts, how many of macrofractures were intersected by a particle on its way (Fig. 39). Transport path of each particle is made of twenty parts (Pipes) and if certain particle does not intersect that many macrofractures, attributes of the last part of the path, which were calculated based on NAPSAC data, are prescribed to the excess parts of the path with a minimal value of length.
In program GoldSim, it is necessary to define each part of the transport path by:

1. Dry bulk density (kg·m⁻³), according to the tracer
2. $D_e$ (m²·s⁻¹), according to the tracer
3. $D_w$ (m²·s⁻¹), according to the tracer
4. $K_d$ (m³·kg⁻¹), according to the tracer
5. Initial volume of tracer (g·year⁻¹), according to the tracer
6. porosity (-), according to the tracer
7. thickness of the matrix diffusion zone (m), according to the tracer
8. length corresponding to path of a particle in certain macrofracture $L$ (m), (Fig. 40)
9. flow (m³·s⁻¹), defined according to equation $Q = (W \times 2L) / FF$
10. flow area (m²), calculated by multiplication of width $W$ by transport aperture $e_t$ (Fig. 40)
11. width $W$ (m), chosen the value of macrofracture intersection length (Fig. 40)
12. dispersivity (-), corresponds to amount of macrofractures, those are intersected by particle on its transport path

Fig. 39 Selection of transport paths and macrofractures intersected by certain particles

A selection of input parameters is shown in Tab. 23 and Tab. 24

Fig. 40 Parameters of the transport path segment
Tab. 23 Example of transport parameters. Parameters with label PipeX are parameters corresponding to certain transport path segment for one certain particle, parameters with label s pathX apply to all parts of the transport path of one particle

<table>
<thead>
<tr>
<th>Materials</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry bulk density [kg·m⁻³]</td>
<td>2741</td>
</tr>
<tr>
<td>Reference diffusivity [m²·s⁻¹]</td>
<td>2.30E-09</td>
</tr>
<tr>
<td>Nuclides</td>
<td></td>
</tr>
<tr>
<td>Solubility [mol·dm⁻³]</td>
<td>-1.00E+00</td>
</tr>
<tr>
<td>De [m²·s⁻¹]</td>
<td>5.00E-15</td>
</tr>
<tr>
<td>Dw [m²·s⁻¹]</td>
<td>2.30E-09</td>
</tr>
<tr>
<td>Kd [m³·kg⁻¹]</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>Initial concentration [g·yr⁻¹]</td>
<td>0.3027456</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transport_paths_geometry</th>
<th>PIPE01</th>
<th>PIPE02</th>
<th>PIPE03</th>
<th>PIPE04</th>
<th>PIPE05</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Skin thickness layer [m]</td>
<td>path1</td>
<td>path2</td>
<td>path3</td>
<td>path4</td>
<td>path5</td>
</tr>
<tr>
<td>Initial concentration ratio</td>
<td>0.5499</td>
<td>0.5231</td>
<td>0.9099</td>
<td>0.8447</td>
<td>2.2265</td>
</tr>
<tr>
<td>Dispersivity [m]</td>
<td>13</td>
<td>17</td>
<td>17</td>
<td>11</td>
<td>14</td>
</tr>
</tbody>
</table>

Tab. 24 Length (in metres) of selected transport path segments of particles 1 – 5 (each transport path is consisted of total 20 segments)

<table>
<thead>
<tr>
<th>Part number</th>
<th>PIPE01</th>
<th>PIPE02</th>
<th>PIPE03</th>
<th>PIPE04</th>
<th>PIPE05</th>
<th>PIPE06</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.537</td>
<td>5.043</td>
<td>1.358</td>
<td>16.813</td>
<td>4.683</td>
<td>5.976</td>
</tr>
<tr>
<td>2</td>
<td>2.375</td>
<td>4.663</td>
<td>1.358</td>
<td>12.68</td>
<td>4.683</td>
<td>5.6</td>
</tr>
<tr>
<td>3</td>
<td>8.421</td>
<td>4.107</td>
<td>7.309</td>
<td>4.683</td>
<td>4.756</td>
<td>5.891</td>
</tr>
<tr>
<td>4</td>
<td>2.713</td>
<td>4.737</td>
<td>1.988</td>
<td>15.582</td>
<td>4.683</td>
<td>6.121</td>
</tr>
<tr>
<td>5</td>
<td>2.444</td>
<td>4.573</td>
<td>1.359</td>
<td>15.602</td>
<td>4.683</td>
<td>7.792</td>
</tr>
</tbody>
</table>

6.4 Model calibration

The intention to calibrate the transport path parameters in program GoldSim to achieve the maximal conformity with results of MODFLOW (NAPSAC) model was based on previous work carried out in projects Transport 2 (Trpkošová et al. 2016) and Transport 7 (Trpkošová et al. 2018). For this purpose, total F-quotient for every particle was calculated, then 10 particles (Fig. 41) were selected. For those ten particles were available additional data (mass flow rate) from transport MODFLOW model of interim version v0. Value of total balance of the model was also available. The particles were selected with regards to cover critical transport paths with the smallest value of F-quotient, but also with regards to include transport paths with higher value of F-quotients, which are more favourable from point of view of the deep repository safety.
The values of mass flow rate for selected particles were computed in program GoldSim. Parameters in GoldSim were not calibrated, those parameters were obtained by calculations described in chapter 6.1. The results of GoldSim and MODFLOW models are in a good agreement in case of total mass balance. The total mass balance, that is displayed in Fig. 42, is in the results of GoldSim model labelled “GS”, in MODFLOW model is total mass balance called “Mass_OUT”.

The values of mass flow rate resulting from MODFLOW and GoldSim simulations are not in very good agreement in case of selected particles. The MODFLOW value of mass flow rate is higher than the result from GoldSim model (Fig. 43, Fig. 44). If single mass flow rates of all selected particles from MODFLOW were summed, the value of mass flow rate should be lower or equal to total value of mass flow rate (called Mass_OUT) of the model. However, the value of mass flow rate, that was mentioned above (marked as Sum_PB_DFN), is higher than total
mass flow rate of the model. In Fig. 45 is displayed the value of mass flow rate calculated in program MODFLOW for transport paths with very similar values of F-quotient. Transport paths, that are characterised by very similar F-quotient, in GoldSim simulations result into very similar values of mass flow rate, while in MODFLOW model, the values of mass flow rate vary even in several orders.

These differences originate from matching of the transport paths, which were calculated in DFN model (by particle tracking method in NAPSAC), to mass flow rates, which were computed in EPM model (using advective transport in MODFLOW).

Fracture network of EPM model is discretised into squared cells, thereby transport paths from two different concepts (DFN and EPM) do not fully correspond. Methodology to transfer DFN model to EPM was not possible to perfectly solve within the project Transport 8. Because of that reason, transport path parameters in program GoldSim were not calibrated with aim of a maximal conformity in values of total mass balance or mass flow rate, which were calculated in EPM transport model (MODFLOW).

In program GoldSim the model was simulated with parameters, which were based on particle tracking method from DFN model (NAPSAC). The model with those parameters was then used to compare transport of selected radionuclides (see chapter 6.5).

**Fig. 43 Comparison of mass flow rate from MODFLOW and GoldSim simulations for two selected particles 46 and 54**
6.5 Transport computations - results of model versions v0 and v1 with use of four tracers

Four fictional tracers, labelled A, B, C, D, were chosen in order to compare results of the transport task. Transport parameters of those tracers are displayed in Tab. 25 – A represents non-sorbing tracer, B slightly sorbing tracer, C medium sorbing tracer and D strongly sorbing tracer. Effective diffusion coefficients and porosity of tracers B, C, D are the same, only tracer
A, which represents an anion, differs. The value of longitudinal dispersivity was considered the same (1 m) in all fractures and the thickness of rock matrix was also 1 m. Radioactive decay was not considered in this task. As a boundary condition was chosen a source with constant flow. The outflow from the domain, which was normalised with respect to inflow, was monitored.

**Tab. 25 Transport parameters of four fictional tracers used in comparative computation**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_d$ (m$^3$·kg$^{-1}$)</td>
<td>0</td>
<td>1.00·10$^{-4}$</td>
<td>1.00·10$^{-3}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Porosity ()</td>
<td>0.00044</td>
<td>0.0065</td>
<td>0.0065</td>
<td>0.0065</td>
</tr>
<tr>
<td>$D_w$ (m$^2$·s$^{-1}$)</td>
<td>2.3·10$^{-9}$</td>
<td>2.3·10$^{-9}$</td>
<td>2.3·10$^{-9}$</td>
<td>2.3·10$^{-9}$</td>
</tr>
<tr>
<td>$D_e$ (m$^2$·s$^{-1}$)</td>
<td>5.00·10$^{-15}$</td>
<td>1.83·10$^{-13}$</td>
<td>1.83·10$^{-13}$</td>
<td>1.83·10$^{-13}$</td>
</tr>
</tbody>
</table>

For each model of versions v0 and v1 were in FJFI performed two computations. In the first computation was used a solution of flow, which was gained by use of center method in ADFNE (the blue line in Fig. 46 and Fig. 47), in order to create an input file of object *Network Pathway*. Because of the finding, that the calculation of flow in ADFNE does not have to provide correct results (see 7.4), in case of the second computation, the flow results from NAPSAC (green lines in Fig. 46 and Fig. 47) were used to make the input file. It applies especially to model version v1, in which the source element is located on a large fracture with a small difference of pressure on individual lines of intersection.

From the comparison of the breakthrough curves in Fig. 46 we can state, that the results of the model version v0 are similar. Breakthrough curves from ÚJV model (red lines) and FJFI model with use of NAPSAC flow results (green lines) correspond better than results of FJFI model, which is based on flow, that was calculated in ADFNE (blue lines). One of possible reasons for the difference between curves is a method of the flow wetted surface determination, which can vary. In case of FJFI model, the flow wetted surface is defined as a double of product of the intersection line length and the distance from the centre of the line of intersection to centre of the fracture.

The difference between the curves in Fig. 47 is more obvious. It is caused by specificity of the task in flow calculation of model version v1, in which case a delay occurs, particularly in the first fractures with a large area together with a small difference of pressure between the lines of intersection. In this case, dependence of breakthrough curves on the way of the flow wetted surface determination is even more critical.
Fig. 46 Transport model version v0 – comparison of results. Red lines - ÚJV, blue lines – FJFI with use of ADFNE flow results, green lines – FJFI with use of NAPSAC flow results

Fig. 47 Transport model version v1 – comparison of results. Red lines - ÚJV, blue lines – FJFI with use of ADFNE flow results, green lines – FJFI with use of NAPSAC flow results
6.6 Sensitivity

As mentioned before, the model of radionuclide transport, that was created in program GoldSim, is based on simulation of 100 particles, whose transport data were obtained. Number of particles was chosen due to experience of working with aim to cover complex properties of the rock environment, so the transport data gained by simulations represent critical, but also more favourable (from point of view of safety) transport paths. The reduction of point amount could prioritize certain characteristics of the rock environment and suppress the others. Because of that reason, particles were randomly divided into ten groups and were not sorted by their F-quotient. In Fig. 48 - Fig. 51 are displayed unit mass flow rates (input/output amount of tracer) of each group together with mass flow rate of 100 particles from version v0, in Fig. 52 - Fig. 55 are shown these unit mass flow rates from version v1. From the graphs is apparent, that the amount of 100 particles can complexly describe the rock environment, the mass flow rate curves of 100 particles occur usually in the middle of mass flow rate curves, which represent individual groups of particles.

Fig. 48 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer A, model v0

Fig. 49 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer B, model v0
Fig. 50 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer C, model v0.

Fig. 51 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer D, model v0.

Fig. 52 Comparison of mass flow rate of 100 particles with mass flow rate, that was combined into groups of ten particles. Model parameters correspond to input parameters for tracer A, model v1.
Besides the different number of simulated particles, the attention was also paid to various fracture widths, because the width of the fracture is a significant retardation parameter from point of view of rock matrix diffusion and sorption. In case of tracers A, B, C, (D is not able to transport itself through the model area in a reasonable time), of version v0 were simulated 4 variants of fracture width. In two variants was a width of the fracture smaller (5x and 10x) than the width, which was calculated from particle tracking data. In another two variants was value...
of the fracture width higher (5x and 10x) than the width, which was obtained by calculations of results from the particle tracking. Final curves of unit mass flow rate are shown in Fig. 56 - Fig. 58. The curves are in accordance with expectation, that grow of the fracture width results in grow of the rock matrix diffusion area and amount of material available for process of sorption. As a result of that, transport of tracer in rock environment towards the drainage base is more gradual.

Fig. 56 Comparison of unit mass flow rate of tracer A in case of different fracture width, model v0

Fig. 57 Comparison of unit mass flow rate of tracer B in case of different fracture width, model v0

Fig. 58 Comparison of unit mass flow rate of tracer C in case of different fracture width, model v0.
7 Assessment, experience, problems with tasks processing and project resolution

Works performed within the framework of Transport 8 project focused on the description of fracture systems and DFN modelling were highly specific in a number of cases and the prepared general project methodology had to be often modified (or completely changed) and elaborated into further detail – this chapter thus summarizes the experience collected during the project resolution and also the recommendations for changes to the methodology.

7.1 Structural data measurement and processing

Structural geological (SG) documentation must be carried out using a uniform methodology. It is also necessary to count with the collection of field data, or supplement the existing documentation so that the SG dataset is as large as possible and allow the best possible statistical processing. However, the use of archive SG data from e.g. CGS databases or previous projects that did not take into account the subsequent DFN modelling is complicated and results are often not representative, because it is not possible to reconstruct traces of individual fractures or to create a statistically representative sample of data.

When revalidating, extending or modifying primary geological documentation, the use of 3D photogrammetric models or similar technological procedures seems to be a good choice. In the case of documentation of underground spaces with a lot of iron reinforcements, they are a useful tool for enabling correction of terrain data based on the influence of local magnetic anomalies affecting the geological compass. However, the use of these models has the disadvantage of their often small scale (scale of the outcrop / wall of corridor).

In terms of fracture populations, an increase of their number does not seem necessary for the purposes of the GeoDFN calculation. Depending on the size of the acquired dataset, it is possible to work with a smaller number of populations, which will facilitate subsequent optimization processes and computational iterations. Optimized parameters of the data dispersion and its principal vector are sufficient for the creation of the DFN network. Further data separation can take place on the basis of supporting parameters like transmissivity index type, character and fill type, etc.

According to the research carried out within the framework of this project, it is clear that applying knowledge of the stress state for the determination of the conductivity of structures seems to be a suitable way to approach the issue of determining the permeability potential of individual structures. Although this problem was solved within the project using a not quite ideal dataset, it is possible to separate from SG data based on the orientation of the assumed stress tensor such as a fracture that can lead water. In case of obtaining a disproportionately large SG dataset, e.g. from deep boreholes and the interval stress measurement performed there, e.g. by borehole-breakout or overcoring methods, these procedures can be fully applied.

7.2 Construction of GeoDFN, DFraM

In the present chapter, we further elaborate the recommendations for the field survey and primary analysis of the recorded trace lengths. We also present a preliminary proposal of enhanced methodology for parameter optimization with DFraM v.2 program. It is noted,
though, that the methodology has not been fully verified and in the course of its implementation and verification it still may undergo further modifications.

7.2.1 Recommendations regarding the mapping of fracture networks and processing of the data

The fact that the observation windows (surfaces on outcrops, tunnel walls, etc.) are the primary source of information, which serves as the basis for identification of the 3D model of the fracture network within the entire volume of the rock mass body, should be taken into account as early as in the phase of the observation windows selection and traces mapping. The windows should be selected so as to comprise representative samples of the rock mass, especially as far as spatial arrangement, orientation, density, and size of brittle structures are concerned. The geometric shape of each window is defined by a polygon with vertices specified in the file xxxyyyyya_BB.xlsx. These polygons must not overlap and they should circumscribe all recorded points defining the traces, which are listed in the files xxxyyyyya.xlsx. The larger the windows' dimensions are, the higher moves the limit trace length beyond which the data bias due to the true ends of the fractures being not invisible occurs. All traces longer than the chosen minimum recorded trace length $l_{r,\text{min}}$ must be recorded as systematically as possible to minimize the data bias due to neglecting short traces.

While developing the SG dataset according to the methodology by Kabele et al. (2018), attention is paid to choosing the observation windows so as to be close to planes. In spite of that, we noticed that due to the inherent unevenness of outcrops and tunnel walls, the recorded windows’ vertices and traces’ endpoints passed on through the xxxyyyyya_BB.xlsx and xxxyyyyya.xlsx files did not lie in a perfect plane. However, during the DFN model identification, the mapped traces are compared with the model traces, which were generated as intersections of planar polygons (fractures) with planar windows. Therefore, the mapped points should be projected to the mean plane of the corresponding window. This functionality will be implemented in the DFraM v.2 software with the next update.

As it is mentioned in Chapter 3, when estimating fractures' transmissivity index (TI), we considered the relative orientation of the fractures with respect to the rock-mass principal stress directions. In order to perform this calculation systematically in the future, the SG dataset should include the information about the rock mass stress state, in particular, about the magnitudes and directions of all three principal stresses.

7.2.2 Recommendations for the primary analysis of recorded trace lengths

The automatic identification of parameters describing the distribution of fracture size and density ($x_{\text{min}}, \alpha, P_{30}$) in DFraM v.2 program is based on an iterative solution of a nonlinear problem arising from the minimization of objective functions. As the data entering the objective functions are randomly generated, the minimized functions are noisy and may exhibit false local minima. Therefore, it is important to ensure that the initial values of the parameters, from which the iterative calculations start, are not set “blindly”, but they should be chosen as close to the sought optimum as possible. To this end, we recommend to carry out a primary analysis of the trace lengths, which is based on the OSM (outcrop scale modelling) concept described in the report by Hartley et al. (2018).
First, depending on the nature of the fracture system and the amount of the available data, it is necessary to decide if it is appropriate to identify parameters $x_{\text{min}}, \alpha, P_{30}$ individually for each population or if they should be determined overall across all fractures regardless of their populations. The former approach is suitable when a sufficiently large dataset is available for each population or when individual populations differ not only by the dominant orientation but also by the trace length distribution. This may be the case, for example, when a significant proportion of fractures belonging to one population terminates on fractures of another population.

The chart of the complementary cumulative frequency of fracture length $l$ plotted in log-log scale (see example in Fig. 59) is the basis for the primary analysis. In the log-log scale, the ideal power-law distribution appears as a descending straight line. As it is obvious from Fig. 59, the measured data can be fitted by a straight line in a certain interval of trace length $(l_{r,1}, l_{r,2})$, that is, they can be approximated by the power law distribution. Even though the minimum recorded trace length $l_{r,\text{min}} = 0.2$ m was specified for the present survey campaign, the deviation from the power-law distribution is obvious up to the value $l_{r,1} > l_{r,\text{min}}$. This effect may be attributed to the fact, that many short traces might have been poorly visible and thus they were not recorded. The frequency of the traces deviates from the power-law distribution also on the right side of the chart, that is, for the lengths larger than $l_{r,2}$. This type of deviation is a consequence of the finite size of the observation windows, which causes that for some traces only a portion of their whole length is visible and recorded.

As shown by Darcel et al. (2003), in the ideal case, when traces are generated as intersections of circular fractures, whose radii follow the power-law distribution with exponent $\alpha$, with a plane, the trace length distribution is also power law, but with exponent $\alpha_t = \alpha - 1$.

The above facts can be utilized for the initial estimate of parameter $\alpha$. In the log-log graph of the trace length complementary cumulative frequency, we approximate the data in the interval $(l_{r,1}, l_{r,2})$ by a straight line. From the slope of this line ($s_t = 1 - \alpha_t$) we determine the exponent of the trace length distribution $\alpha_t$ and, subsequently, the exponent of the fracture size distribution $\alpha = \alpha_t + 1$.

The said graph can be also used to estimate the appropriate value of the location parameter $x_{\text{min}}$ for the 3D fracture network model. As noted by Hartley et al. (2018), if a DFN consists of fractures whose equivalent radii $r_{\text{eq}}$ follow the power-law distribution with the value of location parameter $r_{\text{eq,\text{min}}}$, then traces generated on 2D observation window exhibit deviation from the power-law distribution for lengths $l < l_{m,1} = 2 r_{\text{eq,\text{min}}}$. The cause of this deviation is not “overlooking” the short traces as in the case of the field data, but the fact that even though all fractures in the model have a diameter larger or equal than $2 r_{\text{eq,\text{min}}}$, they can still produce traces shorter than $2 r_{\text{eq,\text{min}}}$. This is documented in Fig. 59, where we additionally plotted complementary cumulative frequencies of trace length, which was identified from two realizations of a DFN model. The model consisted of square fractures, whose circumscribed circles’ radii followed the power-law distribution with parameters $x_{\text{min}} = 0.15$ m and $\alpha = 3$, for which the corresponding values are $r_{\text{eq,\text{min}}} = \sqrt{2/\pi} x_{\text{min}} \approx 0.12$ m and, thus, $l_{m,1} \approx 0.24$ m.

Considering that the cause of the left-side bias for the filed data and for the model is different, it is appropriate to choose the value of $x_{\text{min}}$ in such a way, that $l_{m,1} = l_{r,1}$ and to ignore all measured and modelled traces with $l \leq l_{m,1} = l_{r,1}$, whose frequency is affected by the bias. It is obvious in Fig. 59 that even the model trace lengths exhibit bias on the right side of the chart. This deviation, however, has the same origin as in the case of measured traces, that is, the
total lengths of the fractures' intersections with the window plane exceeding its size. If the observation windows in the field survey and in the model are geometrically identical and the maximum size of the modelled fractures is significantly larger than the windows' size, then this effect manifests itself in the observation and model data in the same way and occurs beyond the same trace length \( l > l_{r,2} \equiv l_{m,2} \).

In the course of the primary analysis, it is also useful to evaluate the areal fracture density \( P_{20} \) on the observation windows for traces with length larger than \( l_{r,1} \). These values then can be used for the initial guess of the volume density \( P_{30} \) as discussed hereafter.

![Complementary cumulative frequency of trace length obtained from the survey and from the model. Colour dashed lines correspond to power-law distribution](image)

Fig. 59

### 7.2.3 Preliminary proposal of refined methodology for parameter optimization with DFraM v.2 program

Upon performing the primary analysis of the measured data, a refined parameter identification can be carried out using the DFraM v.2 program as follows:

1. DFraM v.2 is executed in the mode "Task: DFN optimization" with the option "Calculate only directional statistics: yes". This way, the parameters of Fisher distribution of the fracture orientation are quickly obtained.

2. Using the parameters of Fisher distribution from point 1, the values of parameters \( x_{\min} \) and \( \alpha \) determined according to section 7.2.2 and the value of density \( P_{30,\text{try}} \) based on an expert estimate, DFN model is generated by running DFraM v.2 in mode "Task: DFN generation". In this model, areal density \( P_{20,\text{try}} \) is evaluated for all traces with length larger than \( l_{m,1} \) identified on virtual windows, which have the same geometry and orientation as the windows surveyed in the field.

3. The final optimization of parameters is performed by executing DFraM v.2 in mode "Task: DFN optimization" with options "Calculate only directional statistics: no" and "Optimized parameter (1 - a alpha, 2 - x_min): 1". To this end, the values of \( x_{\min} \) (as a fixed value) and \( \alpha \) (as an initial value) estimated according to section 7.2.2 are used. The initial value of fracture volume density is determined based on the previously obtained values as \( P_{30,\text{try}} \cdot \frac{P_{20,\text{try}}}{P_{20,\text{try}}} \). While minimizing the objective functions, only traces
longer than \( l_{r,1} \) (input as “Minimum recorded size of fracture traces on virtual outcrops”) are taken into account.

### 7.3 Processing of HydroDFN models

Use of vtk file format proved to be useful for HydroDFN models processing requiring mutual data communication across various software packages and/or for storage of uniform definition of the fracture network (this file format also allows for simple data visualization in freely accessible ParaView software). The vtk file format has a clearly defined structure and it is relatively easy to prepare conversion scripts for internal formats of imported and exported files used in individual software packages (when direct data import/export in form of vtk files is not available). Use of the vtk file format is also implemented in DFraM software for GeoDFN models generation.

Preparation of HydroDFN model, which is created by reduction of fractures from GeoDFN model on the groundwork of fracture network interconnection analysis, was successfully executed in NAPSAC software during the project as this software contains suitable tools implemented directly for this purpose. It is partly possible to remove isolated fractures directly in the DFraM software, however, development of this tool is not yet fully completed. Flow123d does not allow for analysis of fracture network connectivity and it only operates with imported fracture network. Network connectivity analysis is available in ADFNE according to its documentation (Alghalandis 2017), however, it was neither used nor tested during the project.

Need for division (discretization) of generated fractures to smaller computational elements, which will enable a more accurate calculation of flow and/or transport appears to be an important point for assurance of representative resolution of HydroDFN model in the nearest vicinity of disposal boreholes (implemented in NAPSAC and Flow123d). Refinement of the fractures will have to be included also in the cases when simulation of preferential flow through fractures (channeling) will be required.

### 7.4 ADFNE/GoldSim

In the initial phase, DFNs with a relatively small number of fractures (in the order of 100) were generated in ADFNE. The created routines for DFN generation and its conversion to the input file of the Network Pathway object were verified on these networks, as well as the implementation of the DFN model in GoldSim itself. After successfully completing this step, they were implemented in ADFNE DFN based on a common network specification for version v0. Even under these conditions, the input file of the Network Pathway object was successfully generated in ADFNE and then the transport task in GoldSim was solved. This verified the functionality of the ADFNE / GoldSim link and the subsequent use of the Network Pathway object.

In order to compare the results from ADFNE with the results obtained by other modelling groups, a function has been implemented in ADFNE that allows uploading of common DFNs stored in vtk files. By comparing the results with the results from NAPSAC, it can be said that ADFNE provides equivalent results for finding intersections. This cannot be said about the solution to the flow problem. In ADFNE, the calculated pressures, volumetric flows and total flows through the domain differ from the results in NAPSAC. The GoldSim calculated
breakthrough curves then differ from those calculated in NAPSAC and Flow123d. This can be attributed to the ADFNE flow problem calculation methodology, which is more suitable for 2D DFN flow calculation (Priest 1993). The central method used is certainly suitable for idealized 3D cases where the fractures intersect with only two adjacent fractures, as in Fig. 9. In these cases, the 3D model is equivalent to the 2D model in terms of intersection complexity. In a more complex case, which corresponds to a situation where a large number of small fractures intersects one large fracture, flow between the intersection points may be distorted; the central method implicitly assumes that there is a flow from the center of the intersection to the center of the fracture and from there to the center of another intersection with less pressure. The results of the simulations in NAPSAC, however, show that in such complex cases, an outlet at the intersection with a higher pressure than that at an intersection with the inlet may occur, which the central method does not allow.

For the 3D case, it is better to use the triangulation method. Since the triangulation method is not part of the ADFNE package available (version 1.5), this method has been implemented - the Delaunay triangulation function available in MATLAB (DelaunayTriangulation, MathWorks 2017) was used. Using the triangulation method we encountered two problems. The first, a technical one, is in the increase in the number of pipes that model the DFN, and the second in determining the hydraulic conductivity of the pipes and the conversion of the pipes into the DFN model in GoldSim. The first problem led to an increase in computational demands for solving the flow problem, for which it is necessary to solve a system of linear equations in the form $A\mathbf{x} = \mathbf{b}$ in MATLAB. For a large number of pipes (over fifty thousand), the amount of memory necessary to allocate matrix $A$ exceeds the memory capacity available on a regular MATLAB PC. The second problem led to an increase in flow through the domain if we attributed each pipe to direct correlation to the crack size ($T = ar^b$) according to the common network. This flow exceeded the flow calculated in NAPSAC and Flow123d. Furthermore, in Priest (1993), it is stated that it is preferable to use a finite-element 2D model of each fracture, such as used in NAPSAC and Flow123d, to solve the flow problem in 3D DFN. Based on these arguments, we decided to take over the solution to the task, i.e. the volume flows in Pipes objects from the results of NAPSAC.

NAPSAC results were provided in the form of average volume velocities and pressures at each intersection. The results from NAPSAC were implemented by creating a pipe network in the ADFNE using a central method, and then each pipe was assigned a volume flow corresponding to the intersection. At the same time, the direction of flow was taken into account by arranging the endpoints in the flow direction and the endpoints lying on the intersection were assigned the pressure that was used to determine connectivity. A downstream connection between two pipes fulfills the condition that the pressure at the start point of the first pipe is greater than the pressure at the end point of the second pipe. The introduction of this condition prevented the formation of closed flow loops that the Network Pathway object does not allow. Taking the results from NAPSAC, we eliminated the differences in the intersection curves obtained for flow and transport simulation.

7.5 ConnectFlow (NAPSAC, NAMMU)

From the perspective of the topics covered by project T8, it was possible to execute all planned works in NAPSAC software without any major problems. This is mainly due to the long-term development and use of this software in resolution of complex projects at sites in Sweden and Finland. Partial problems were associated with some less frequent functions associated with
detailed data export that was required for uniform assignment of tasks or as the input data for GoldSim (export of a detailed geometric fracture model for determination of fracture intersection points, export of detailed “pipe” model for the determination of flows through the intersection points, import/export of vtk file, etc.) – all these problems were successfully resolved thanks to active technical support for ConnectFlow software and/or by creation of conversion scripts in Python language.

Newly developed functions of NAPSAC software include simulation of full transport directly in DFN fracture network without need for upscaling into CPM model. This function was tested within the scope of T8, however, the currently incorporated transport processes are oriented rather to the aspects of Swedish and Finnish repositories (situated in the vicinity of the sea) as they support mainly tasks with variable density of saline solutions. Moreover, it is not possible to simulate sorption in the rock matrix but only diffusion. The “particle tracking” method was therefore used in NAPSAC for advective transport in the fracture network; this method is very fast from the perspective of calculation efficiency and provides results comparable with the outputs of full transport tested on equivalent CPM model.

Based on the experience with upscaling and DFN model conversion to CPM, it seems to be more convenient to simulate the nearest vicinity of the disposal boreholes and tunnels with DFN method. CPM approach can be used in greater distances. High accuracy of a flow solution in the vicinity of the disposal boreholes is important from the perspective of transport – the simulations performed on all model versions show that the flow velocity in the nearest vicinity of the disposal boreholes is most influenced by the overall delay time, mainly in fractures with low gradients and slow flow where low network connectivity was generated. It is therefore important to choose suitable and sufficiently small discretization of the computational network in the vicinity of disposal boreholes, i.e., divide (refine) the specified fractures into smaller subfractures.

The problem with specification of starting positions of particles for transport nodes of the fracture network had to be resolved in NAPSAC software in connection with network connectivity – transport (particle tracking) in NAPSAC takes place between “transport nodes” in the intersection points of fractures (and at the connection lines of subfractures in case of macrofractures refinement). If the specified source point (disposal borehole) does not have any intersection with the fracture network, such source is automatically moved even by several meters and assigned to the nearest transport point (to the nearest “conductive” intersection of the fracture network). On one hand, this approach is conservative (the particle would get to the conductive fracture for example by diffusion), on the other hand, it considerably distorts the results of the transport. The resulting methodology of transport calculation was thus modified so that the particles “start” only in the intersection points of the disposal boreholes and fractures. This also enables evaluation of a share of “safe” disposal boreholes which are not connected to the conductive network of fractures.

NAPSAC software offers a function for creation of a “pipe model” – tubular model which interconnects the conductive intersection points of fractures. This model basically serves as the groundwork for transport calculation using the “particle tracking” method – output is in form of detailed information about flows between individual connecting lines of fracture intersection points. Scripts have been created in Python language, which process these detailed outputs from NAPSAC and convert them into format suitable for retrieval into GoldSim.
7.6 Flow123d

The use of Flow123d for simulations within this task may be assessed ambivalently. The simulator itself works very well; simulations of both flow and advective transport (after identification and rectification of minor glitch in mass balance calculations) run without any problem. Even the computational mesh with nearly 3 million elements in case of model v2 didn't pose a problem for ordinary (albeit powerful) desktop computer. The program for identification and evaluation of transport paths based on a construction and analysis of weighed directed graph may also be valued positively. It is very efficient and capable to identify fastest paths from a source to each of the elements that are a part of the graph structure. It is worth noting that it is not a particle tracking method; outputs of the implemented SW are not directly comparable to the results of particle tracking. Both approaches, in principle, provide similar information about the computational domain function as a geo-barrier. Available tools for preparation of geometry and computational mesh need to be valued slightly negatively; for models v0 and v1 they worked just fine (even though the computations were time demanding) but for model v2 they more or less failed.

7.7 GoldSim

The data transfer from DFN models to program GoldSim was solved by the research team during this project for the first time. In the future, it will be necessary to focus on connection of results from the tracer transport, which were calculated by using programs NAPSAC or Flow123D, with GoldSim model, because conformity among these programs is helpful for verification of radionuclide transport parameters in the rock environment during the safety analysis of DGR.

Another comparison was implemented by part of the research team (ÚJV and FJFI) at the GoldSim program level. The simulations of four tracers for the final data version v0 and v1 were compared, in which case both models were based on different conceptual models. During the comparison, the results from both programs were in a good agreement for data version v0 and in a less good agreement for the data version v1. In the future it will be necessary to pay attention also to this topic.
8 Conclusion and proposed next steps

Within the Transport 8 project, conceptual and computational models for simulating flow and transport of radionuclides in fracture systems of the isolating part of the rock massif were tested. In the introductory phase, search of archive materials Posiva and SKB was carried out. Based on the data taken from the Forsmark site (the parameters of the fracture sets were adopted), the GeoDFN and HydroDFN fracture network for the initial model version v0 was generated in the NAPSAC program. In the NAPSAC, Flow123d and ADFNE programs, a hydraulic and transport model was developed and the methodology of preparation and transmission of data between different software was tested.

In the selected part of the URF Bukov, characterization of fracture systems was performed. Based on the measured data, two other versions of the model were realized – v1 and v2. For the processed data from URF Bukov, the parameters of fracture populations were optimized in the DFraM program and the geological GeoDFN model of the fracture network was generated (in model version v2, optimized population parameters were updated). The fracture network model represented the hypothetical volume 100x100x100 m³ of the rock mass near the disposal borehole outside the regional conductive structures (model volume of 100x200x100 m³ in the v2 model version with multiple boreholes). Fractures were generated stochastically in the models, fracture size (equivalent radius) ranged from 0.25 m to 50 m. In the NAPSAC program, the GeoDFN connectivity was analysed and a uniform HydroDFN fracture network was prepared. The flow and advective transport in the NAPSAC, Flow123d and ADFNE programs were calculated and the simulation results were processed and evaluated. In the v2 version, the tunnel and effect of the EDZ on the flow velocity and advective travel time was also evaluated.

In parallel, the procedure for linking output and input data between NAPSAC and ADFNE/GoldSim programs was prepared and tested. The results from NAPSAC and ADFNE were further used to simulate transport in GoldSim – 4 fictitious tracers with different diffusion and sorption parameters were simulated.

The following points summarize the recommendations for next steps (follow-up works) that resulted from the works performed as a part of the Transport 8 project and that relate to the problem of fracture networks, data collection and evaluation, DFN modelling, and safety assessment.

Structural data collection:

- A suitable extension of existing documentation will include the possibility of statistic data set extension by 1D data from boreholes and/or planar 2D data (see the following point); it will be necessary to resolve the interconnection of such data with 3D data collected by standard methods.
- Estimate of lengths of individual faults currently represents the greatest limitation besides the availability of rock outbursts. It is apparent that the structures propagate further into the rock massif, however, their real length often cannot be determined. At least for the surface data, a solution could be to use remote surveying methods and detection of morpholineaments or waterlogged linear zones. In a well mapped terrain (or its part) with sufficient number of rock outbursts, these could be correlated on the groundwork of their directional analysis with the data measured at outbursts, thus
enabling better quantification of the size of brittle failures and thus allow DFN construction with better boundary conditions.

**DFraM and DFN models generation:**

- Completion of development of a computational tool for primary statistical analysis of data from SG measurements (outbursts, tunnels, borehole surveys).
- Verification of innovated methodology for DFN parameters identification and implementation of supporting functions into DFraM software.
- Development and implementation of algorithms for calculation of fractures’ transmissivity on the groundwork of rock massif’s stress condition.
- Development and implementation of methods for RM stress calculation using the DFN models (also for application in EDZ).
- Grown DFN approach utilization for efficient generation of DFN models considering the genesis and connectivity characteristics of fracture populations (e.g., termination of fractures).
- Considering the spatial variability of the fracture network (e.g., due to depth, in the vicinity of large faults, or in EDZ). Sufficient information would have to be obtained by structural-geological surveys for this purpose.

**Flow123d:**

- Development of software tools for rock environment and transport effects modelling – development of SW packages that would enable creation of stochastic 3D models of discrete fracture networks (DFN) on the groundwork of structural-geological data and that would also enable (as a superstructure to the existing Flow123d software) simulation of transport processes at these networks including retention in the adjacent rock matrix.
- Resolution of problems with computational network creation and further development of program for determination and rating of transport paths into a complex tool that would not only determine the transport path on the groundwork of known velocity field (output from Flow123d) but also work as a full-feathered transport model.
- MLMC (MultiLevel Monte Carlo) method implementation, usage of which could simplify the discrete fracture network to a computational network comprising only the most significant fractures while the remaining fractures would be represented as equivalent porous medium with its hydraulic and transport parameters set using the MLMC method so that the simulation results on both computational networks would be close to each other.

**GoldSim:**

- When working on common tasks, it appeared that the Network Pathway object in GoldSim software represents an efficient tool for transport task resolution in DFN. As the next proposed step, we propose creating a set of routines that would enable interconnection between NAPSAC and Network Pathway object in GoldSim.
- Focus on the model calibration methodology in GoldSim – achieving a better conformity with HydroDFN model results (NAPSAC, MODFLOW, Flow123d, etc.).
- Optimization of data export from HydroDFN models for “Pipe” model compilation.
HydroDFN modelling:

- From the perspective of the hydrogeological modelling, we consider very important to focus on DFN models of regional scale – they represent an important groundwork for smaller scale models due to specification of representative boundary conditions; at the same time, the tracer movement through conductive structures of regional character forms a substantial part of the transport path.

- On the other hand, it is necessary to focus also on the detail of interface between the disposal borehole and fracture. This is important for the determination of flow velocities and size of the source which comes out of the engineering barrier (primarily the diffusion motion) into isolating part of the rock massif (primarily advective motion through the fracture network with inclusion of transport processes into the rock matrix).

- Models for a limited number of scenarios were processed during works on T8 project due to limited project duration – usually only the basic model variants (one stochastic network realization, one disposal borehole, one EDZ variant, etc.). The safety assessment will require work with a much broader assignment and higher variability of input data.

- Measured hydrogeological data (permeability measurement in boreholes, water pressure tests, tracer tests, etc.) is absolutely crucial for a representative hydrogeological model creation – this data can be utilized for HydroDFN model calibration. Any other assignment of hydraulic parameters, e.g., only from geological mapping, is insufficient.

Other recommendations:

- For works on similar tasks and projects, we recommend parallel solution in multiple software packages at multiple workplaces – this is important especially in the phase when any of the software packages is continuously developed and its functionality is not fully verified. On the other hand, even commercially available software packages have some of the declared functions “on paper only” as they have been verified only on simple tasks and they fail to process more complex tasks without any limitations. Functional technical support for the software is very important in this respect. This recommendation does not relate only to HydroDFN modelling but generally to all project phases where solution methodology is not clearly defined in advance.

- The project schedule should comprise time allowance for completion of partial phases, optimization and verification of proposed procedures, and possibility of schedule updating according to the achieved results.

- As regards the planned works, we recommend clear definition of software packages preferred by SÚRAO for the area of DFN modelling (GeoDFN, HydroDFN, safety assessment, etc.). Viewed from the perspective of software, the DFN issue is highly specific and requires certain experience that cannot be simply transferred or applied to a different software type (due to different character of input and output data, different control structure, different numeric methods, hardware demands, etc.).

- Within the framework of the T8 project, the flow and transport calculations were demonstrated for each model version on one fracture network realization. It is, however, necessary to emphasize that the DFN models are stochastically generated by their nature. This means, that each DFN model realization will have a different connectivity and different critical transport path even if the same values of probability distribution parameters are used for creation of fractures. HG simulations should thus
be performed on a statistically meaningful number of DFN realizations and results should be interpreted in statistical sense.
9 Literature


NAŠE BEZPEČNÁ BUDOUCNOST

SÚRAO

Správa úložišť radioaktivních odpadů
Dlazděná 6, 110 00 Praha 1
Tel.: 221 421 511, E-mail: info@surao.cz
www.surao.cz