

Definition of the present boundary conditions for the near-field model_1

OPERA-PU-TNO421_1

Radioactive substances and ionizing radiation are used in medicine, industry, agriculture, research, education and electricity production. This generates radioactive waste. In the Netherlands, this waste is collected, treated and stored by COVRA (Centrale Organisatie Voor Radioactief Afval). After interim storage for a period of at least 100 years radioactive waste is intended for disposal. There is a world-wide scientific and technical consensus that geological disposal represents the safest long-term option for radioactive waste.

Geological disposal is emplacement of radioactive waste in deep underground formations. The goal of geological disposal is long-term isolation of radioactive waste from our living environment in order to avoid exposure of future generations to ionising radiation from the waste. OPERA (OnderzoeksProgramma Eindberging Radioactief Afval) is the Dutch research programme on geological disposal of radioactive waste.

Within OPERA, researchers of different organisations in different areas of expertise will cooperate on the initial, conditional Safety Cases for the host rocks Boom Clay and Zechstein rock salt. As the radioactive waste disposal process in the Netherlands is at an early, conceptual phase and the previous research programme has ended more than a decade ago, in OPERA a first preliminary or initial safety case will be developed to structure the research necessary for the eventual development of a repository in the Netherlands. The safety case is conditional since only the long-term safety of a generic repository will be assessed. OPERA is financed by the Dutch Ministry of Economic Affairs and the public limited liability company Electriciteits-Produktiemaatschappij Zuid-Nederland (EPZ) and coordinated by COVRA. Further details on OPERA and its outcomes can be accessed at <u>www.covra.nl</u>.

This report concerns a study conducted in the framework of OPERA. The conclusions and viewpoints presented in the report are those of the author(s). COVRA may draw modified conclusions, based on additional literature sources and expert opinions. A .pdf version of this document can be downloaded from www.covra.nl

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Summary

This report describes the execution and results of the first part of Task 4.2.1 of the OPERA research project. The research concerns the present-day hydraulic boundary conditions and properties of host rock for geological disposal of radio-active waste, around a generic repository in that host rock. The Boom Clay (also known as Rupel Clay Member) is studied as a potential host rock.

Two different 3D modelling approaches are used in Task 4.2.1 to obtain information on the boundary conditions and hydraulic properties. Results include maps showing regional variations of properties, such as porosity, permeability, viscosity and temperature, and groundwater flow conditions in the Rupel Clay Member. These modelling results were used to derive properties and boundary conditions for a generic repository in the Rupel Clay Member at a generic depth of 500 m.

Samenvatting

Dit rapport beschrijft de uitvoering en resultaten van het eerste deel van Taak 4.2.1 van het OPERA onderzoeksprogramma. Taak 4.2.1 is gericht op het uitvoeren van onderzoek betreffende de huidige randvoorwaarden en eigenschappen rond een potentiële opbergfaciliteit voor radioactief afval in een gastgesteente. De Boomse Klei (ook bekend als Rupel Klei) wordt hierbij onderzocht als potentieel gastgesteente.

In Taak 4.2.1 is gebruik gemaakt van 3D modelleringen van de ondergrond van Nederland, te weten 3D bekkenmodellering en 3D grondwater modellering. Deze modelleringen geresulteerd kaarten betreffende regionale hebben in de variatie in grondwaterstromingscondities in de Rupel Klei en eigenschappen van de Rupel Klei, zoals porositeit, permeabiliteit, viscositeit van het grondwater en temperatuur. De regionale resultaten van de modelleringen zijn vervolgens gebruikt om randvoorwaarden en eigenschappen rond een potentiële opbergfaciliteit voor berging van radioactief afval in de Rupel Klei op een diepte van 500m, af te leiden.

1. Introduction

1.1.Background

The five-year research programme for the geological disposal of radioactive waste - OPERA- started on 7 July 2011 with an open invitation for research proposals. In these proposals, research was proposed for the tasks described in the OPERA Research Plan (Verhoef and Schröder, 2011).

In OPERA a first preliminary or initial safety case will be developed to structure the research necessary for the eventual development of a repository in the Netherlands. The safety case is conditional since only the long term safety of a generic repository in Boom Clay at a generic depth of 500 m will be assessed (Verhoef and Schröder, 2011). Task 4.2.1 is part of the safety assessment component 'Description of the Disposal system'. It provides input to the 'Formulation and implementation of assessment models' step in the safety assessment.

1.2.Objectives

The research proposed for Task 4.2.1 is described in the Research Plan with the following title: *Definition of boundary conditions for near-field model*.

The main objective of this task is to provide top, lateral and bottom boundary conditions for the near-field area, the undisturbed part of the Boom Clay at present-day and in the future. Thermal and hydraulic boundary conditions and hydraulic parameters for modelling transport processes through the Boom Clay and the overburden are basic conditions defining the OPERA Safety Case.

The proposed modelling and calculations build on findings of Tasks 4.1.1 (*Description of the present geological and geohydrological properties of the geosphere*) and 4.1.2 (*Future evolution of geological and geohydrological properties of the geosphere*) and will serve as direct input to Tasks 6.1.5 (*Non-diffusion related transport processes of solutes in Boom Clay*), 6.2.1 (*Modelling approach for hydraulic transport processes*) and 7.2.5 (*Parameterization of PA models*).

This report describes the execution and results of the research concerning the boundary conditions for the near field area, the undisturbed part of the Boom Clay at present-day. The Boom Clay in the Netherlands is also known as Rupel Clay Member (Vandenberghe et al., 2014).

1.3.Realization

This report has been compiled by TNO with contributions from Deltares. TNO performed a literature study and basin modelling simulations to derive thermal and hydraulic boundary conditions and hydraulic parameters for the near field area in the Rupel Clay Member. Deltares performed gravity-induced groundwater flow simulations, using input data from TNO, to derive present-day hydraulic conditions in the Rupel Clay Member. The developed models are also used in the research concerning the future boundary conditions for the near field area (part 2 of research Task 4.2.1).

1.4.Explanation contents

The general approach and data availability are discussed in Section 1.5. It includes a general introduction into 3D basin modelling. Chapter 2 describes the calculation of hydraulic properties of the Rupel Clay Member by basin modelling. Chapter 3 provides information on the assessment of thermal boundary conditions. Chapter 4 is dedicated to the calculation of hydraulic boundary conditions. Two modelling approaches are used to derive these boundary conditions: groundwater flow modelling and basin modelling.

1.5. General approach

The geological and geohydrological properties of the Rupel Clay Member were investigated in Task 4.1.1 and reported in Vis and Verweij (2014). Vis and Verweij (2014) reported that there are no measured data on pressure and groundwater flow conditions in and around the Rupel Clay Member (where the Rupel Clay Member is located at depths greater than 400 m). Because of this lack of measured data, different modelling approaches are used in Task 4.2.1 to obtain information on the boundary conditions and hydraulic properties for the near-field area, the undisturbed part of the Rupel Clay Member at present-day. The thickness and depth maps of the Rupel Clay Member as well as the limited lithological and calculated permeability properties presented in Vis and Verweij (2014) are used in these modelling approaches.

The following modelling approaches are used:

- 1D and 3D basin modelling (TNO)
- 3D groundwater flow modelling (Deltares)

1.5.1. Basin modelling

Basin modelling is a relatively unknown approach for simulating processes and evolution of properties of rocks and fluids in the shallow part of the subsurface. This section provides information on the methodology.

Originally basin modelling has been developed to reconstruct the evolution of petroleum systems during geological history (generation, migration, accumulation and preservation of oil and gas). Basin modelling results include a lot of implicit results concerning the evolution and present-day properties of the subsurface, such as porosity, permeability and hydraulic conductivity, compressibility, temperature, pore pressure or hydraulic head, viscosity of pore water, groundwater flow. These implicit results of basin modelling are used in this study to provide boundary conditions for the near-field area, the undisturbed part of the Rupel Clay Member at present-day.

The subsurface of onshore and offshore Netherlands has been studied extensively. Since 2006 3D basin modelling (using PetroMod of Schlumberger) was used to integrate the wealth of data and information gathered and mapped in detailed mapping programmes of onshore and offshore Netherlands and to evaluate the interdependencies of the different processes that affect rocks and fluids during its geological history. At this time about 70% of the Dutch subsurface has been studied using basin modelling (Figure 1.1). The results of the basin modelling of the different areas were published over the years either as reports (Abdul Fattah 2012a, 2012c, Nelskamp & Verweij 2012, Verweij *et al.* 2009, 2010, www.nlog.nl) or as scientific papers (e.g., Abdul Fattah 2012b, Nelskamp *et al.* 2012, Verweij *et al.* 2003). Recently these models have been tuned to each other (Nelskamp et al., 2014). The three onshore basin models, after modifications, were used to derive hydraulic properties and thermal and hydraulic boundary conditions for the near field. The

simulations were run separately with each of the basin models. Subsequently, the simulation results were combined in maps.



Figure 1.1: Location of all calibrated 3D basin models in onshore and offshore Netherlands, including the three onshore models used in the present study.

An overview of assumptions underlying the general basin modelling approach, basic data requirements and boundary conditions related to the initial 3D basin models of the Dutch subsurface are described below to provide background information on the applied basin modelling approach.

Basic data requirements for the modelling include present-day geometry, lithologic properties, quantified time sequence of events during geologic history, boundary conditions, and calibration data. The results of the detailed mapping at TNO provided the present-day stratigraphic and structural framework of the sedimentary fill and properties of the rocks and fluids, including lithology and calibration data (temperatures, porosities, permeabilities, pressures, and vitrinite reflectance values) required for the numerical modelling.

General assumptions and conditions inherent in basin modelling:

- Geological history:
 - $\circ\;$ the model is laterally constrained: no horizontal compression or extension of the basin fill is taken into account
 - vertical movement only (no lateral deformation of the sediments in the model, except for salt movement)
 - salt movement has no direct relation to changes in stress
 - compaction of the basin fill/rock matrix is vertical
 - compaction is mechanical according to vertical effective stress-based rock property model (Athy's Law)
 - solid rock is incompressible
- History pore water fluids
 - density of pore water is constant, that is the density of the water is independent of changes in temperature and salinity. The water is incompressible.
- Thermal history
 - conductive heat flow

The basin models of the onshore Netherlands are geological models without faults.

In addition to the above listed general limiting assumptions and conditions, default set-ups of the basin modelling package influence simulation results. Such default set-ups include default relations between standard lithologies and properties through compaction approaches, porosity-permeability relations, thermal models, kinetic models; mixing rules lithology; default mechanical compaction equations and default porosity-permeability relations. The selection of the proper set-up is an important part of the basin modelling workflow. A number of region-specific compaction relations were used in the modelling of the hydraulic properties and boundary conditions for the near field.

Data requirements for basin modelling

The basic data requirements for 3D modelling involve: present-day geometry (stratigraphy; property/facies boundaries within stratigraphic units, water depth); lithological properties (lithological composition of each stratigraphic unit and eroded - part of - unit and of each facies); quantified uninterrupted time-sequence of events during geological history (3D history of sedimentation, uplift and erosion; estimated thickness of erosion; 3D history of water depth, basal heat flow, surface temperature; timing of salt movement); calibration data (such as present-day temperatures, porosities, permeabilities, pressures, vitrinite reflectance measurements).

The results of the mapping of the Dutch subsurface (Duin et al., 2006; Kombrink et al., 2012; see also www.dinoloket.nl) provided the present-day 3D stratigraphic model and the basic conceptual model of the geological evolution for all basin models. The present-day stratigraphic models were improved and extended in the different basin models over the years depending on the focus of the study. The basin models for the shallower parts of the onshore Netherlands were further refined for the purpose of this study. The specific changes to the models will be outlined in the following chapters. The ages assigned to the layers are based on the Geologic Time Scale published by Gradstein *et al.* (2004). For the models different methods of assessing the amount of erosion were used and compared, such as interpolation from areas without erosion, structural reconstruction, calibration using sediment thermal parameters such as vitrinite reflectance or fission tracks or seismic velocity. Table 1.1 shows an example of the timing and duration of periods sedimentation, erosion and nondeposition from Late Carboniferous to present-day for the original onshore basin model of the West Netherlands Basin in the southern parts of the Netherlands.

Table 1.1:Input model of deposition, non-deposition and erosion for the original large scale basin
model in southern part of the Netherlands (from Nelskamp and Verweij, 2012).

Stratigraphic layer	Deposition		Erosion	
	from	to	from	to
Holocene	0.01	0	0	0
Upper Pleistocene	0.13	0.01	0	0
Middle Pleistocene	0.78	0.13	0	0
Base Quatenary	3.1	1.8	0	0
Pliocene	5.8	3.1	0	0
NU	20.1	5.8	0	0
NM	35.4	20.4	0	0
NL	58	40	40	35.4
CKEK	65.5	62	62	58
Top CKGR	73	65.5	0	0
Rest of CK	99.1	80	80	78
KNGL	121.8	99.1	0	0
KNNSL	125.4	124.3	0	0
KNNCU	125.8	125.4	78	76
KNNSY	127.2	125.8	0	0
KNNCA	127.4	127.2	0	0
KNNSB	129	127.4	0	0
KNNSC	131.1	129	0	0
KNNSR	137.4	131.1	0	0
KNNC	138.7	137.4	0	0
S_Jurassic erosion	151	149	149	144
S_Cretaceous erosion	156.4	151	76	74
AT_Jurassic erosion	170	156.4	144	141
AT_Cretaceous erosion	203.6	170	74	73
RNKP and RNMU	244	203.6	141	138.7
RNROF	245.6	244	0	0
RNSO	246.2	245.6	0	0
RBMH	247.2	246.2	0	0
RBMDU	247.6	247.2	0	0
RBMDL	247.8	247.6	0	0
RBMVU	248.5	247.8	0	0
RBM∨L	249	248.5	0	0
RBSH	250	249	0	0
ZE	258	250	0	0
ROCL top	259	258	0	0
ROSL	264	259	0	0
ROCL bot	267.5	264	0	0
DCH	308.7	299	290	285
DCD	311	308.7	285	280
DCCU	312.3	311	280	275
DCCR	313.1	312.3	275	270
DCCB	313.6	313.1	270	268
DCGE2	315	313.6	0	0
DCGE1	316.4	315	0	0
DCGEG	326.4	316.4	0	0

The lithological composition used for the layers is based on the description published by van Adrichem Boogaert & Kouwe (1993) and - when needed - adjusted based on well logs or other more detailed descriptions, especially for the shallower part of subsurface.

Boundary conditions

The boundary conditions such as sediment surface temperature and paleo water depth are based on published data as well as in-house micropaleontological/palynological studies. The present-day ground surface topography is included in the model. For the assessment of basal heat flow boundary conditions the in-house developed tool PetroProb was used (van Wees *et al.* 2009) for several 1D wells as well as 3D models. This tool determines the evolution of the paleo heat flow based on the tectonic subsidence and inferred tectonic history of the studied location. The history of basal heat flow is assigned to the model as a series of paleo heat flow maps. Figure 1.2 shows an example of the boundary conditions for the original basin model of the West Netherlands Basin.



Figure 1.2: Example of boundary conditions for the 3D basin models: history of surface temperature /sediment water interface temperature; paleo water depth; basal heat flow. Input of history of basal heat flow boundary condition into 3D basin models includes a series of maps of regionally varying paleo basal heat flow (examples from Nelskamp, 2015).

1.5.2. Groundwater flow modelling

Deltares performed gravity-induced groundwater flow modelling using a hydrogeological model, covering the entire onshore Netherlands, to simulate the present-day hydraulic conditions in the Rupel Clay Member and the impact of a selection of normal evolution scenario's on these conditions. The basic hydrogeological model is described in detail in Valstar and Goorden (2015) and in Section 4.1.

2. Present-day hydraulic properties of the Rupel Clay Member

2.1.Introduction

The Oligocene Rupel Clay Member is part of the Rupel Formation. The marine sediments of the Rupel Formation were deposited in the southern part of the North Sea Basin. The formation includes three members, from bottom to top: the sandy Vessem Member, Rupel Clay Member and sandy Steensel Member. The Rupel Clay Member consists of clays that become more silty towards the basis and top of the Member (Vis and Verweij, 2014). Texturally, the Rupel Clay Member includes muds, sandy muds and to a lesser extent muddy sands. Vis and Verweij (2014) demonstrated that the Rupel Clay Member shows a spatial variation in lithological composition related to the depositional environment of the sediments: sediments are generally finer grained and show less vertical variation in the northern Dutch onshore corresponding to a more distal part of the paleo basin and are coarser grained and show more vertical heterogeneity in the southern and eastern onshore corresponding to the paleo basin margin. They subdivided the member in three subunits based on grain-size characteristics: the lower subunit shows a fining upward trend, the middle subunit is finest grained and the upper subunit shows a coarsening upward trend. The current burial depth of the Rupel Clay Member varies from close to the surface to about 1500 m (Figure 2.1; Vis and Verweij, 2014). Figure 2.2 shows the thickness map of the Rupel.



Figure 2.1: The depth (in meters relative to m.s.l. = mean sea level ~NAP) of the top of the Rupel Clay Member (From Vis and Verweij, 2014).

Measured hydraulic properties, such as porosity and permeability or hydraulic conductivity data of the Rupel Clay Member in the subsurface of the onshore Netherlands are limited and these data are restricted to shallow depths in the order of tens of meters below surface (Rijkers et al., 1998; Wildenborg et al., 2000; Vis and Verweij, 2014). In NW Belgium, however, the Boom Clay has been studied extensively since more than 30 years, especially at the Mol investigation site (the HADES underground research facility), which has been constructed in the middle part of the Boom Clay at 223 m depth) (Yu et al., 2013).



Clay samples from boreholes at Mol and other locations in NW Belgium have been used for hydraulic conductivity measurement through laboratory experiments and in situ tests were performed to determine the hydraulic conductivity under undisturbed conditions (Wemaere et al., 2008; Yu et al., 2011). Verweij et al. (2015) used the grain sizes measured in samples of the Rupel Clay Member taken from 10 boreholes spread across the Netherlands to calculate porosity and vertical permeability for the Rupel Clay Member located at greater burial depth. They used published measured grain size and vertical hydraulic conductivity data from the Belgium Boom Clay to test and select appropriate input parameters for the grain-size based calculation methods. Comparison of the permeability based on measured hydraulic conductivity of the Belgian Boom Clay with the calculated permeability showed that the calculated vertical permeability slightly overestimates measured vertical permeability by less than 1 order of magnitude for burial depths exceeding 200 m.

Porosity decreases with increasing burial depth. At shallow depths of < 2 km (at temperatures < 70°C) porosity reduction is mainly due to mechanical compaction driven by the increase of effective stress. Compressibility of mud (such as the Rupel Clay Member), and therefore its rate of compaction, is strongly influenced by grain size: finer-grained muds have higher depositional porosities, but their rate of compaction is higher (Yang and Aplin, 2004; Aplin and Macquaker, 2011). At a certain porosity, clay-rich mudstones have smaller pore sizes than silt-rich mudstones (Schlömer and Krooss, 1997; Dewhurst et al., 1998, 1999). Permeability closely relates to pore size and pore-size distribution. At a given porosity, vertical permeabilities vary over orders of magnitude (Neuzil, 1994, Reece et al, 2012; Casey et al., 2013), while clay-rich mudstones have lower permeabilities than clay-poor ones. The burial history of the Rupel Clay Member will have exerted an important influence on its present-day hydraulic properties, such as porosity and permeability.

3D basin modelling was used to provide information on the hydraulic parameters (permeability and porosity).

2.2. Basin modelling approach to calculate hydraulic properties

2.2.1. Input model and boundary conditions

The existing onshore 3D basin models (section 1.5.1) were all extended and refined with the top and base maps of the Rupel Clay Member and the lithological composition of the Rupel Clay Member.

The lithostratigraphic basin model model for the northern part of the Netherlands is more detailed than the other two and includes a combination of maps from different origins. The upper part of the model was refined with:

- 16 layers from the Digital Geological Model (DGMv2; www.dinoloket.nl/ondergrondmodellen)
- 46 layers from the hydrogeological model REGIS II (www.dinoloket.nl/ondergrondmodellen)
- Rupel Clay Member (Vis and Verweij, 2014)

The basin modelling of the hydraulic properties were executed by using newly derived porosity-depth relations for sand and clay derived by using a combination of porosity data from shallow depths (3800 porosity data; depths 0-30 m from DINO database), the Rupel Clay Member (Vis and Verweij, 2014) and porosity data from oil and gas boreholes (Figure 2.3). These new porosity-depth relations were derived by TNO in the context of the

knowledge investment program of the Dutch Geological Survey (KIP GDN 2014 - 4D PetroGIS) (Nelskamp, 2015).



Figure 2.3: Newly derived compaction curves for sand and clay (coloured curves) compared with published ones (From Nelskamp, 2015).

Table 2.1 presents the model stratigraphy and assigned lithologic composition for the shallow part of the model.

Figure 2.4 shows the original 3D lithostratigraphic model for the northern area and a burial history from ca 450 million years ago to present-day. Figure 2.5 presents the lithostratigraphic model with more detailed subdivision of the upper part of the model and an example of the burial history.

Table 2.1:	Lithological composition of the shallow more detailed part of the basin model in North
	Netherlands.

Lithostratigraphic units	New mixed lithologies
Holocene	50% sand 50% clay
Boxtel	50% sand 50% clay
Kreftenheye	100% sand
Eem-Woudenberg	50% sand 50% clay
Kreftenheye-Zutphen	100% sand
Drente	25% sand 75% clay
Drachten	100% sand
Urk-Tynje	75% sand 25% clay
Peelo	50% sand 50% clay
Urk	75% sand 25% clay
Appelscha	100% sand
Peize-Waalre	75% sand 25% clay
Maassluis	50% sand 50% clay
Oosterhout	62,5% sand 37,5% clay
Breda	100% clay
Rupel	5% sand 86.5% clay 8.5% silt



Figure 2.4: Initial 3D basin model covering the northern part of the Netherlands (see Figure 1.1 for location).



Figure 2.5: Example of burial history at 1D extraction of the 3D basin model in northern part of the Netherlands: a) for the complete model and zoomed-in burial history showing in more detail the burial history for the shallow part of the model, including the burial history of the Rupel Clay Member (From Nelskamp, 2015).



Figure 2.6: Example of regional variation in burial history of the Rupel Clay Member: 1D extraction of the 3D basin models in the northern and central part of the Netherlands.

2.2.2. Hydraulic properties

There is a large variation in present-day depth of the Rupel Clay Member (Figure 2.1), resulting from large variation in burial history of the Rupel (Figure 2.6).

The 3D basin modelling results of porosity and vertical permeability of the Rupel Clay Member are shown in maps (Figure 2.7 and Figure 2.8, respectively). The modelled present-day porosity varies between values of less than 18 % in the deeper buried parts of

the Rupel Clay Member in the SE and central parts of the Netherlands and porosity values of more than 36 % where the Rupel is at depths of less than about 400 m in the NE. This regional trend is also apparent in the variation of the vertical permeability from log k of less than -3.75 (corresponding to k = $10^{-3.75}$ mD and 1.75*E-19 m²) for deeper burial depths to log k of more than - 1.9 (corresponding to k = $10^{-1.9}$ mD and 1.24E-17 m²) at relatively shallow depth.

In areas where the depth of the top of the Rupel Clay Member is between 400 and 500 m the porosity is around 32-36% and vertical permeability between 1.24E-17 m² and 6.2E-18 m². These regional magnitudes of the vertical permeability are higher than the grain-size based calculated values of the mudstone parts of the Rupel Clay Member (i.e lithological composition with less than 10% sand) of 5.0E-19 m² to 8.3 E-19 m² for depth range of 428-571 m at boreholes GRD-01, NNE-07. In the basin modelling the input lithological composition of the Rupel Clay Member in the northern part of the Netherlands is 5% sand, 86.5 % clay and 8.5% silt.

The permeability is related to hydraulic conductivity according to the following equation:

k =K ($\mu/\rho g$) where,

 $k = permeability (m^2)$

K = hydraulic conductivity (m/s)

 μ = dynamic viscosity of the fluid (kg/(m·s))

 ρ = density of pore water, assumed to be constant in the modelling (1020 kg/m³)

= the acceleration due to gravity (9.81 m/s^2)

The dynamic viscosity of water is temperature dependent: it decreases with increasing temperature, and therefore with depth. In order to calculate the lateral variation in hydraulic conductivity corresponding to the modelled permeability, the temperature dependence of the dynamic viscosity of the pore water should be taken into account. Figure 2.9 shows the lateral variation in dynamic viscosity of the pore water in the Rupel Clay Member resulting from the basin modelling. The dynamic viscosity varies between less than 0.6 mPa.s (0.0006 kg/m.s) in the SE (Roer Valley Graben) to 0.95-1 mPa.s (0.00095 - 0.001 kg/m.s) in the NE. The dynamic viscosity at a depth of 500 m is about 0.85 mPa.s (0.8 -0.9 mPa.s).







Figure 2.8: Regional variation in vertical permeability (log k; k in mD) in Rupel Clay Member at present-day based on 3D basin modelling of the evolution of permeability of the Rupel Clay Member since its deposition. (Log k = 2 corresponds to permeability k = 10^{-2} mD = 10^{-5} D = 10^{-17} m² and to hydraulic conductivity K = 10^{-10} m/s = 86* 10^{-7} m/day, for μ = 1 mPa.s).



Figure 2.9: Regional variation in water viscosity (mPa.s) in the Rupel Clay Member at present-day, based on 3D basin modelling of the evolution of water viscosity in the Rupel Clay Member since its deposition.

3. Present-day thermal boundary conditions

3.1.Introduction

The 3D temperature distribution in the subsurface is governed by:

- Transport of heat through the subsurface (by conduction; convection, i.e. the transport of heat by groundwater flow)
- Thermal properties of rocks and pore fluids in the subsurface (thermal conductivity and specific heat capacity of rocks and pore fluids)
- Radiogenic heat generation in rocks (heat generated by radioactive isotopes in rocks)
- Input of heat at the base of the rocks considered
- Temperature at the earth surface

The temperature distribution in the subsurface at a certain time during history, assuming steady state conditions, principally depends on the spatial variation in basal heat flow, the distribution of bulk thermal conductivities of the subsurface and the temperatures at the ground surface. The range of thermal conductivities of sedimentary rocks is mostly in the order of $1.5 - 4.5 \text{ Wm}^{-1}\text{K}^{-1}$, while the thermal conductivity water is around $0.6 \text{ Wm}^{-1}\text{K}^{-1}$ and the thermal conductivity of oil or gas is less than $0.2 \text{ Wm}^{-1}\text{K}^{-1}$. The presence of pore fluids in the rocks reduce the bulk thermal conductivity. Hence, porosity has a significant influence on the bulk thermal conductivity and therefore on the temperature distribution. Bulk thermal conductivities of clastic lithostratigraphic units and carbonates broadly range between values of $1.5 \text{ and } 3.5 \text{ Wm}^{-1}\text{K}^{-1}$. The bulk thermal conductivities of halites and anhydrites vary between approximately $2.8 \text{ and } 5 \text{ Wm}^{-1}\text{K}^{-1}$. Salt diapiric structures can significantly disturb heat flow. Focussing of heat flow through salt structures will increase temperatures in the top part of the salt structures and in adjacent lithostratigraphic units.

Present-day temperature conditions in the subsurface may not be in equilibrium with current boundary conditions and are in a transient state reflecting in greater or lesser extent paleo boundary conditions (e.g. paleo surface temperatures).

3.2. Temperature data and information

Bonté (2012; Bonté et al., 2012) investigated the temperature distribution in the subsurface of onshore Netherlands, using a dataset of 4276 measurements of bottom hole temperature (BHT) from 456 oil and gas boreholes and 52 temperature measurements from drill stem tests at 24 boreholes. After quality control and correction of the temperature data, Bonté (2012; Bonté et al., 2012) calculated an average geothermal gradient of 31.3° C for the corrected data with a surface temperature of 10.1° C (Figure 3.1). Figure 3.1 shows that most of the temperature data are from depths exceeding 1km.

Different studies have shown that the thermal gradient in onshore Netherlands is not constant, but varies spatially (Bonté et al, 2012; Luijendijk, 2012; Verweij et al., 2005) resulting in lateral variation of temperatures at the same depth as shown on different isodepth temperature maps published since 1980 (Haenel et al., 1980; RGD, 1984; Hurtig et al., 1992; Rijkers and Van Doorn, 1997; Hurtel and Haenel, 2002; 3D web based geothermal information system at www.thermogis.nl). This is not surprising since the lithostratigraphic build-up of subsurface of the Netherlands is not layer-cake, and both the lithostratigraphy and the associated bulk thermal conductivities vary spatially over short

distances due to differences in lithological composition as well as differences in burial history.



Figure 3.1: Average geothermal gradient and regional distribution of temperature measurements (From Bonté, 2012).

In addition to bulk conductivity, groundwater flow may affect the present-day temperature distribution in different areas of the Netherlands. The isotherm map of onshore Netherlands at a depth of 250 m below ground surface clearly shows the cooling effect of groundwater flow in the area of the Veluwe and Utrechtse Heuvelrug (Van Dalfsen, 1983). Luijendijk (2012) investigated the thermal influence of topography-induced groundwater flow during the Neogene and Quaternary. He showed that topography-induced flow through the Roer Valley Graben has a clear cooling effect. The modelled flow is confined to the upper 1000 m and the associated advective cooling of this part also affected even deeper parts of the model by conduction.

Ter Voorde et al (2014) used a numerical model to study the effect of the surface temperature history of the past 130000 years in the Netherlands on present-day subsurface temperatures. The modelling shows that this paleo temperature history resulted in a decreased geothermal gradient in the upper kilometer of the Dutch subsurface, and a slightly increased gradient at depths between 1 and 3 km. Hence, the present-day temperatures in the realm of the Rupel Clay Member are still in a transient state, to a greater or lesser extent.

Temperature data for the Dutch subsurface are available from measurements in groundwater wells at very shallow depths of ten to a few hundred meters and from measurements in oil and gas boreholes at greater depths mostly exceeding 1000 m. The

regional distribution of the deeper temperature measurements is quite uneven (Figure 3.1). The Rupel Clay Member in the Dutch subsurface occurs at burial depths from close to the surface to about 1500 m. The depth of the safety case of a generic repository in the Rupel Clay Member concerns a generic depth of 500 m, i.e. at depths where temperature measurements are very limited.

Present-day temperature is one of the implicit results of basin modelling. Basin modelling of the temperature takes important processes and factors into account that influence the present-day temperature condition in the Rupel Clay Member, such as its burial and porosity history, bulk thermal conductivity of the sedimentary fill of the Dutch subsurface (as related to lithological composition and porosity), basal heat flow and surface temperature as well as radiogenic heat generation in rocks and transient effects of paleoboundary conditions. Measured temperatures at different depths and different locations are important calibration data for basin modelling in general (e.g. Nelskamp and Verweij, 2012). Bonté et al. (2012) used a thermal-tectonic modelling method, calibrated with temperature measurements to calculate and investigate the temperature distribution of the sedimentary basin fill of the Netherlands, taking into account the basin evolution of the past 20 million years and thermal properties and processes of the whole lithosphere. Here we focus on modelling the present-day temperature condition in the upper part of the sedimentary sequence in the Dutch subsurface.

3.3.Basin modelling approach to calculate thermal boundary condition

3.3.1. Input model and boundary conditions

The same input model as used for calculating the porosity and permeability (Chapter 2) was used for the temperature calculations. The top and bottom thermal boundary conditions include the history of surface temperature and basal heat flow, respectively, and the side boundaries are no flow boundaries for heat. The thermal conductivity (vertical~) is calculated using the Sekiguchi model (Sekiguchi, 1984). The heat capacity is based on the empirical property database of Waples and Waples (2004). Basin modelling is calibrated with temperature data from oil and gas boreholes. The influence of groundwater flow on the temperature distribution is not taken into account in the basin modelling.

3.3.2. Thermal boundary condition

Figure 3.2 shows the simulated present-day temperature distribution in the Rupel Clay Member. The map shows that the temperature in the Rupel Clay Member varies from less than 22°C to more than 50°C. The first order influence of burial depth on the present-day temperature is clearly visible: the highest temperatures occur in the SE, where burial depth reaches depths of more than 1500 m, while temperatures of less than 22°C occur in the NE corresponding to burial depths of less than 300 m. In areas where the top of the Rupel is at depth of 400-500 m, the temperature map at 500 m depth extracted from the 3D web based geothermal information system ThermoGIS (www.thermogis.nl): most of the temperatures at 500 m are between 22 and 26°C (higher temperatures occur only locally on top of salt structures).

The basin modelling does not include the effects of groundwater flow on the temperature distribution. Given the findings on the cooling effects of groundwater flow through the Roer Valley Graben of Luijendijk (2012), the present-day temperatures derived by basin modelling in the SE of the Netherlands might be too high.



Figure 3.2: Regional variation in temperature (°C) in the Rupel Clay Member at present-day based on 3D basin modelling of the evolution of water temperature in the Rupel Clay Member since its deposition.

4. Present day hydraulic boundary conditions

The driving forces for water flow through the subsurface are gradients in hydraulic potential, water density differences, and also gradients in salt concentration and electrical potential. All these driving forces are active in the Rupel Clay Member in the Netherlands to a greater or lesser extent (Vis and Verweij, 2014). Here focus is on hydraulic potential gradients and related water flow through the Rupel Clay. The present-day hydraulic potential gradients and water flow are genetically related to two main influencing mechanisms; 1. Infiltration of meteoric water into the subsurface generating gravity induced flow systems/topography induced flow systems; 2. Sedimentary loading. The hydraulic potential gradients together with the hydraulic properties of the Rupel Clay Member determine the water flow through the Rupel. There are no measurements of hydraulic potential gradients over the Rupel Clay at depths of \geq 500 m.

Two modelling approaches were used to provide information on the present-day hydraulic boundary conditions:

- 3D steady state groundwater flow modelling
- 3D basin modelling of groundwater flow induced by the combined influence of sedimentary loading and topographic relief of the water table.

4.1.Hydraulic boundary conditions derived from groundwater flow modelling

Deltares performed the gravity-induced groundwater flow modelling. The geohydrological model used to assess the present-day hydraulic conditions in the Rupel Clay Member are described in detail in Valstar and Goorden's report on OPERA task 6.2.1. (2015). The main characteristics of the geohydrological model given below are based on this report.

The geohydrological model consists of layers from the existing shallow groundwater flow model NHI (Netherlands Hydrological Instrument). The base of the NHI model reaches a maximum depth of approximately 300 m. In order to incorporate the Rupel Clay Member and some underlying units, the model was extended to greater depth with information from:

- Digital Geological Model DGM 1.3 (2009) (DGM model is available at www.dinoloket.nl/ondergrondmodellen; Gunnink et al., 2013)
- Hydrogeological model REGIS II.1 (REGIS II model is available at www.dinoloket.nl/ondergrondmodellen; Vernes and Van Doorn, 2005)
- Geological model of the deep subsurface (model available at www.dinoloket.nl/digitaal-geologisch-model-dgm-diep; Kombrink et al., 2012)
- Top and bottom of Rupel Clay Member (Vis and Verweij (2014)

Figure 4.1 shows the SN and WE cross sections of the model.



Figure 4.1: West-East and North-South cross sections showing the geometry of the hydrogeological model of the Netherlands (from Valstar and Goorden, 2015).

The horizontal and vertical hydraulic conductivity of the Maassluis and Oosterhout Formations and part of the Breda Formation were taken from the REGIS II.1. The hydraulic conductivities for the older lithostratigraphic units were calculated using the lithological compositions of the units and new porosity-depth and porosity-permeability relations for different lithologies recently derived by Nelskamp (2015). These new relations are based on an extensive new dataset (approximately 3800 porosity and 1650 permeability measurements for the very shallow subsurface of the Netherlands recorded in combination with depth, stratigraphy, lithology and lithofacies) in combination with calculated porosity and permeability for the Rupel Clay Member (from Vis and Verweij, 2014) and data from greater depths oil and gas wells. The calculated permeabilities were converted to hydraulic conductivity taking the depth dependence (actually the depth related temperature dependence) of water viscosity into account. Figure 4.2 shows the variations in vertical hydraulic conductivity for the Rupel Clay Member used in the modelling. The influence of faults is not explicitly included in the modelling. The new model is a steady state model for saturated groundwater. The influence of differences in groundwater density on groundwater flow is not taken into account and nor are the influences of sedimentary loading. Yearly averaged boundary conditions from the NHI model area used for the NHI layers in the top part of the model. The boundary conditions for the deeper layers were chosen as fixed hydraulic heads with the same values as the deepest layers of the NHI model. No flow boundaries were assigned for the deeper model layers in the coastal areas. Scenarios were run for two different hydraulic conductivity of the Rupel Clay Member: scenario 1 for the hydraulic conductivities calculated using the grain-size based method outlined above and shown in Figure 4.2 and scenario 2 for hydraulic conductivity values that are 100 times lower; these lower values correspond better to the values for the mud part of the Rupel Clay Member given in Vis and Verweij (2014).

The results for scenario 1 are described here. Figure 4.3 shows the modelled present-day variation in hydraulic head at the top of the Rupel Clay Member. The modelled difference in hydraulic head over the Rupel Clay Member and the associated groundwater flux are presented in Figure 4.4 and Figure 4.5, respectively. Hydraulic head differences over the Rupel Clay Member show a large variation in the eastern part of the country: from a downward decrease of hydraulic head that varies between > 0.7 m and 0 m, and a downward increase in hydraulic head between > 0.7 m and 0 m. In the low lying western and northern parts of the Netherlands the hydraulic head difference is between -0.1 and 0.1 m. The associated modelled steady state vertical cell flux varies between an upward directed flux of 0 to more than 0.8 m³/day (corresponding to a Darcy velocity between 0 - 1.28E-5 m/day) and downward directed flux between 0 and 0.7 m³/day (corresponding to a Darcy velocity between 0 - 1.12E-5 m/day).

At about 500 m depth the Rupel Clay Member is mostly in the realm of downward increasing hydraulic heads and associated vertical upward directed flow, vertical cell flux of 0.01-0.3 m3/day, corresponding to 1.6E-7 to 4.8E-6 m/day (~0.06 - 1.75 mm/year).

The vertical flow velocities of the modelled gravity-induced groundwater flow through the Rupel Clay Member can be considered as maximum values. This is, amongst other things, because: 1. The modelling scenario 1 uses a relatively high value for the vertical hydraulic conductivity of the Rupel Clay Member; Valstar and Goorden (2015) also performed simulations of hydrological transport using about 100 times lower values for the hydraulic conductivity of the Rupel and found that the residence time in the Rupel increased significantly; 2. the differences in groundwater density are not taken not account, while in reality the density of the groundwater increases with depth (the fresh-brackish groundwater interface is well above 400m depth except in the Roer Valley Graben, e.g. Dufour 2000; Luijendijk, 2012); the increasing density with depth counteract the infiltration of groundwater and would diminish the maximum depth of penetration of the gravity-induced groundwater flow.



Figure 4.2: Regional variation in input of hydraulic conductivity of the Rupel Clay Member in the hydrogeological model of the Netherlands (Figure 4.1).



Figure 4.3: Regional variation in hydraulic head at top of the Rupel Clay Member at present-day: result of steady state gravity-induced groundwater flow modelling using the hydrogeological model of the Netherlands (Figure 4.1).



Figure 4.4: Regional variation in vertical difference in hydraulic head over the Rupel Clay Member: result of steady-state gravity-induced groundwater flow modelling using the hydrogeological model of the Netherlands (Figure 4.1).



Figure 4.5: Regional variation in steady state vertical cell flux through the Rupel Clay Member (m³/day) at present-day: result of steady-state gravity-induced groundwater flow modelling using the hydrogeological model of the Netherlands (Figure 4.1).



Figure 4.6: Regional variation in vertical difference in overpressure over the Rupel Clay Member (in MPa) at present-day: combined result of 3D basin modelling of the evolution of topography-induced flow and compaction flow since deposition of the Rupel Clay Member. Positive values indicate an increase of overpressure with depth.

4.2. Hydraulic boundary conditions derived from basin modelling

4.2.1. Input model and boundary conditions

The same input models as used for calculating the porosity and permeability and thermal boundary conditions was used to study the combined influence of gravity-induced groundwater flow and sedimentary loading on the present-day hydraulic boundary conditions and flow conditions in the Rupel Clay Member. The lateral boundaries of the three basin models are no flow boundaries. The hydraulic top boundary condition for simulating gravity-induced groundwater flow is the present-day surface topography. This simplified approach assumes that the groundwater table approaches the ground surface: this approach will overestimate the height of the groundwater table in areas such as the Veluwe, Utrechtse Heuvelrug, dune areas, where the groundwater table is known to be well below the ground surface. The thus simulated groundwater flow is induced by the current topography in the model area only. Transient effects of paleo and present-day sedimentation are included in the modelling.

The vertical Darcy flow velocity was calculated using the difference in simulated overpressure at the top and bottom of the Rupel Clay Member (Figure 4.6, taking into account its thickness (Figure 2.2), permeability and water viscosity (Figures 2.8 and 2.9). Overpressure (P_{excess}) is related to hydraulic head (h_w):

 $h_w = -z + (p_w / \rho_w g) (m)$

 $\rho_w g h_w = p_w - \rho_w g z = P_{excess}$

 $h_w = P_{excess} / \rho_w g$

For ρ_w = seawater density = 1020 kg/m³:

 $P_{excess} = 9.81*1020* h_w (kg/m.s^2)$

The simulation results show that vertical upward flow through the Rupel Clay Member prevails outside the Veluwe and Utrechtse Heuvelrug and dune areas with Darcy velocities between 0 and \geq 50E-11 m/s (corresponding to ~ 4.32E-5m/day). This range of vertical flow velocities are comparable in magnitude with those resulting from the gravity-induced groundwater flow modelling (Section 4.1). The lowest upward flow velocity of around 0.5E-11m/s (corresponding to ~ 4.32E-7m/day) occurs in the area where the Rupel is at greatest depth, i.e. in the Roer Valley Graben. At about 500 m depth the vertical upward flow through the Rupel Clay Member is about 2E-11 m/s - 5E-11 m/s (0.63E-6 m/day - 4.32E-6 m/day, corresponding to 0.63-1.57 mm/year).

The 3D basin modelling of groundwater flow induced by the combined influence of sedimentary loading and topographic relief (of the water table) has a number of limitations, including the above outlined assumption that the topographic relief of the ground surface corresponds to the relief of the water table; the closed boundaries of the basin models; the constant density of the groundwater. The results of the basin modelling with respect to the upward vertical flow velocities do not allow to differentiate between areas where the vertical flow is part of the topography-induced flow system and areas where the flow is induced only by sedimentary loading.

5. Conclusions

Two 3D modelling approaches were used to calculate thermal and hydraulic boundary conditions and hydraulic properties for the near field area at present-day. It was decided to use these modelling approaches because of a lack of measured data on hydraulic properties and groundwater flow conditions in and around the Rupel Clay Member at depths relevant for the assessment of long term safety of a generic repository (500m).

The 3D basin modelling covers large part of the Netherlands and the 3D groundwater flow modelling covers even the whole of the Netherlands. The model-based calculations provide insight into the regional variations of hydraulic properties and thermal and hydraulic conditions in the Rupel Clay Member in the Netherlands. These results are presented in maps.

The following hydraulic parameters and thermal boundary conditions for a generic repository in the Rupel Clay Member at a generic depth of 500 m were derived from the regional 3D basin modelling results:

-
m²
0.9 mPa.s)
п -

The hydraulic boundary conditions and groundwater flow conditions in the Rupel Clay Member were simulated with both basin modelling and groundwater flow modelling. The results of both types of simulation show that at depths of the Rupel Clay member around 500 m there are areas where groundwater flow is directed vertically downwards and other areas where the flow is upwards. Downward directed flow is related to groundwater recharge areas in topography driven flow systems and upward directed flow is related to discharge areas of gravity-induced flow systems, compaction flow systems and combination of these two.

Upward directed flow and related hydraulic head differences can be considered as a less desirable hydrodynamic condition compared with downward directed flow. The hydraulic boundary and groundwater flow conditions related to upward directed flow for a generic repository in the Rupel Clay Member at a generic depth of 500 m are:

•	Hydraulic head difference	: 0.015 m - 0.003 m (between bottom and top of
	a 100 m thick layer)	

• Upward directed groundwater flow : 0.06 mm/year - 1.75 mm/year

The modelling approaches have increased our understanding of lateral variations of hydraulic parameters and thermal and hydrodynamic conditions in the Rupel Clay Member in the Netherlands. Limiting assumptions and conditions underlying the approaches affect the simulation results. Measured calibration data of permeability and pressure/hydraulic head in Rupel Clay Member will decrease uncertainty in simulation results.

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