DANMARKS OG GRØNLANDS GEOLOGISKE UNDERSØGELSE **RAPPORT 2022/13**

Effective porosity and hydraulic conductivity of fractured chalk and limestone aquifers

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1. Dansk sammenfatning

Baggrund og formål

Grundvandsstrømning og stoftransport tæt på kildepladser og indvindingsboringer som oppumper vand fra opsprækkede porøse kalk-formationer (f.eks. Skrivekridt, Danien kalk mm.) er karakteriseret ved, at strømningen primært foregår i sprækkerne. Pga. den konvergerende strømning tæt på og mod indvindingsboringen stiger strømningshastigheden markant, jo tættere man kommer på boringen. En eventuel forureningstransport i dette 'boringsnære miljø' vil primært foregå i selve sprækkerne. Da bjergarten, som omslutter sprækkerne (dvs. matrix), har en høj porøsitet, vil der samtidigt ske en diffusion af opløste stoffer fra sprækkerne til matrix, som har voksende betydning i større afstand fra boringen. Pga. de høje transporthastigheder i boringsnære sprækker vil der normalt ikke optræde ligevægt mellem stofkoncentrationen i hhv. sprækker og matrix. Denne ligevægt er en principiel forudsætning for at beskrive transporten ved anvendelse af en traditionel strømnings- og transportmodel, også benævnt den ækvivalente porøse medium model (eller enkeltporøs model), som typisk benyttes i grundvandskortlægningens modelopsætninger (MODFLOW/MT3D og MIKE SHE).

I de tilfælde, hvor der ikke når at indstille sig en ligevægt mellem stofkoncentrationen i sprækker og matrix, er det ud fra en teoretisk betragtning mere optimalt at benytte en diskret modelformulering, med adskilt beregning og fysisk beskrivelse af stoftransport i hhv. sprækker og matrix. Den diskrete model har desværre så store krav til den fysiske beskrivelse af sprækketæthed, sprækkeplacering og størrelsen af sprækkernes åbninger (apertur), modsat den enkeltporøse model, at den i praksis også er meget usikker grundet manglende viden om disse parametre. Alternativt til den diskrete model kan en såkaldt dobbelt porøs model benyttes. Selvom den dobbelt porøse model ikke stiller samme krav til viden om sprækkernes dimensioner m.m., forudsætter modellen kendskab til forhold som sprækkeporøsitet, matrixporøsitet samt udvekslingskoefficienten mellem sprækker og matrix. Desuden har ikke alle modeller mulighed for at benytte en dobbelt porøs løsning. Til beregning af BNBO (den afstand hvorfra grundvand kan transporteres til indvindingen på et år) er det derfor relevant at vide, om beregningen med god tilnærmelse kan foretages i en enkelt porøs model, med en beregningsmæssig repræsentativ værdi for porøsiteten af sprække-matrix systemet, en såkaldt effektiv porøsitet.

Formålet med projektet er at give et videns-baseret estimat på den effektive porøsitet for de relevante danske kalktyper til brug for beregning af BNBO. Herunder at undersøge, om de danske kalktyper, med baggrund i eksisterende data og litteratur for relevante parameterværdier, kan opdeles efter geologiske enheder og regional placering (kalk-provins). Projektet skal også lave nyt kortmateriale omkring hvor og hvilke danske kalkenheder, der benyttes til indvinding af grundvand, samt geografisk beskrive, hvor karst-dannelse er observeret i Danmark.

Fremgangsmåde og resultater

Opgaven er løst ved en to-trins indsats, der i første trin består af et litteratur- og data studie, hvor eksisterende viden fra rapporter og videnskabelige undersøgelser er sammenholdt med data fra danske boringer i kalken (databasen JUPITER), efterfulgt af konceptuel modellering af transporttid og afstand med dobbelt- og enkeltporøse modeller med parameterværdier fundet i litteraturstudiet. Det blev tidligt i undersøgelsen klart, at en teoretisk gennemgang af strømning i et opsprækket kalkmedie og modellering af dette var nødvendigt, for at skabe en fælles forståelse for projektets elementer og samtidig definere relevante begreber der benyttes i modellering af strømning i opsprækket kalk. En nærmere gennemgang af relevante parametre og begreber for beregning af stoftransport i opsprækket kalk kan findes i tabel 2.1. Samtidigt har det indledningsvist også været nødvendigt, at gennemgå den danske kalkstratigrafi for at kunne teste en eventuel underinddeling af de danske kalk- og kridt-enheder, som er aktuelle i forbindelse med grundvandsindvinding. På baggrund af den første screening af litteratur og data for danske kalk-grundvandsmagasiner, blev de første konceptuelle stoftransport-modeller defineret og en følsomhedsanalyse af relevante parametre gennemført. De konceptuelle modeller er 3D-MODFLOW (vandstrømnings model) og MT3D (stoftransport model) modeller med cellestørrelsen 10x10x2 m (x, y, z). Ved følsomheds-analysen vurderedes hvordan BNBO-afstanden, dvs. afstanden, eller distancen, for en administrativt forudsat 1 års stoftransporttid af en konservativ forurening mod en indvinding, påvirkes af henholdsvis; indvindingsmængde, hydraulisk ledningsevne, dispersion (spredning af forureningsfane), udvekslingskoefficienten mellem sprækker og matrix, samt sprække- og matrix-porøsiteten. De testede intervaller for nævnte parametre og indvindingsmængder kan ses i tabel 5.3. Resultatet af følsomhedsanalysen viser entydigt (figur 5.3.2, 5.3.3), at den hydrauliske ledningsevne er den mest følsomme parameter i forhold til simulering af den 1-årige transportafstand fra indvindingen med en variation fra 145 m til mere end 14 km (1-årig BNBO transportafstand). Udvekslingskoefficienten mellem matrix og sprækker var den næstmest følsomme parameter med en 1-årig transportafstand mellem 172 til 2155 m, mens variation af de resterende parametre medførte 1-årige transportafstande mellem 240 til 565 m. Det store udfaldsrum, specielt for hydraulisk ledningsevne viser, at parametrisering af modellerne er meget afgørende for usikkerheden på estimatet af den 1-årige transportafstand.

For udvekslingskoefficienten udgør manglende viden en stor erkendt usikkerhed baseret på to forhold. For det første viser følsomhedsanalysen, at udvekslingskoefficienten har betragtelig indflydelse på estimering af den 1-årige transportafstand. For det andet er der meget få estimater af udvekslingskoefficienten fra eksisterende studier. Derfor er det testet, hvad en forøgelse og reduktion af den valgte parameterværdi med en faktor 10 medfører for henholdsvis en beregnet 1-årig transportafstand, samt med hvilken effektiv porøsitet, denne 1-årige transportafstand kan simuleres i en enkelt porøs model. Den store spændvidde i testen (+/- faktor 10) er valgt, da der ikke findes viden og en mere reel spændvidde for parameteren (som f.eks. for hydraulisk ledningsevne). For en reduktion af udvekslingskoefficienten fra 3,5 x 10^{-3} 1/d til 3,5 x 10^{-4} 1/d forøges transportafstanden fra 180 m til 480 m, mens den effektive porøsitet i EP-modellen reduceres til mellem 3 og 4 % (figur 5.5.2) ved 3,5 x 10^{-4} 1/d. Modsat og med en forøgelse af udvekslingskoefficienten fra 3,5 x 10^{-3} 1/d til 3,5 x 10^{-2} 1/d, reduceres transportafstanden fra 180 m til 120 m, mens den effektive porøsitet i EP-modellen estimeres til 26 % (figur 5.5.1). Eksemplet viser, at en parameterændring kan have betydelig effekt på den simulerede transportafstand, samt at den anvendte effektive porøsitet i en enkelt-porøs modellering også påvirkes (i dette tilfælde fra 3-26 %).

Følsomhedsanalysen viste som nævnt ovenfor, at den hydrauliske ledingsevne er den mest afgørende parameter for de beregnede transportafstande i den dobbelt porøse modellering og understreger vigtigheden af, at indhente alt tilgængelig information om denne. Det var muligt via JUPITER, den nationale boringsdatabase, hvor 9107 boringer filtersat i de 6 danske kalkenheder (Skrivekridt, Bryozokalk, Kalksandskalk, Slamkalk, Grønsandskalk og Kerteminde mergel) blev vurderet efter geografiske kalk-provinser (Falster, Lolland, Sjælland, Falster, Fyn, Djurs – Himmerland og Vendsyssel). Hydraulisk ledningsevne blev estimeret ud fra transmissiviteten divideret med længden af den i kalken åbne del af boringen, eller filtersatte del. Middelværdier for kalktyperne i de forskellige kalk-provinser (med 18 underinddelinger) viste hydrauliske ledningsevner mellem 0,33 og 3,39 x 10^{-4} m/s, hvor de fleste ligger tæt på middelværdien for det samlede datasæt på 1,34 x 10^{-4} m/s (app. E). Ud fra signifikans-tests (bekræftelse eller afvisning af nul-hypotese, app. E) adskiller de fleste af middelværdierne sig statistisk set fra hinanden. Dette billede var dog ikke entydigt, da flere middelværdier for de 6 landsdækkende enheder ikke adskilte sig signifikant fra hinanden. For at undgå inddeling i mere end 10 forskellige grupper med baggrund i kun en lille forskel i hydraulisk ledningsevne, blev enhederne inddelt i 3 grupper. En gruppe (med kalktyperne Bryozokalk, Kalksandskalk, Slamkalk, og Kerteminde mergel) med middel hydraulisk ledningsevne omkring den samlede medianværdi (50 % percentilen) på 1,35 x 10^{-4} m/s; en gruppe (med kalktypen Skrivekridt) omkring 25 % percentilen på 0,36 x 10^{-4} m/s, og en gruppe (med kalktypen Grønsandskalk) omkring 75 % percentilen på 5,11 x 10^{-4} m/s. Udover grupperingen af kalkenhederne i en høj, median, eller lav hydraulisk ledningsevne, blev det ud fra analysen af de hydrauliske ledningsevner samtidig klart, at indvinding af grundvand fra kalk og kridt altid foregår i opsprækkede magasiner, da den hydrauliske ledningsevne for matrix i sig selv er for lav til at kunne opretholde indvinding derfra. For at modellere stoftransport er det således nødvendigt at benytte et dobbelt porøs modellerings-setup, eller sikre at der anvendes en effektiv porøsitet, der vil give tilnærmelsesvis samme resultat i beregningen af BNBO arealet som ved anvendelse af en dobbelt porøs model.

Regional variation af parameterværdier kan kun understøttes, hvis tilstrækkeligt mange data er tilgængelige. Derfor er det i første omgang valgt at differentiere i forhold til regionale værdier for hydraulisk ledningsevne, hvor en regional værdi baseret på mere en 50 observationer vurderes som valid. Med hensyn til porøsitet for sprække og matrix, udvekslingskoefficienten og dispersivitet, er data ikke tilgængelige i et omfang, der kan retfærdiggøre regionalt fordelte værdier. For nogle bjergarter er der ingen parameterværdier tilgængelige og her anbefales det, at der anvendes værdier observeret for andre danske kalkbjergarter. F.eks. er der kun tilgængelige data for udvekslingskoefficienten for Skrivekridt og Bryozokalk.

Matrix-porøsiteten, oftest bestemt ved udtagelse af et mindre bjergarts-volumen, er beskrevet med et relativt stort antal observationer. For Skrivekridt med et gennemsnit på 38 %, Bryozokalken på 26 %, og kalksandskalken på 25 %. Middelværdien for alle observationerne for kalkbjergarterne er 30 %.

Sprækkeporøsiteten for de danske kalkmagasiner er beskrevet (hydrauliske test og modellering) ved langt færre observationer fra litteraturgennemgangen med en middelværdi på 0,8 % og et typisk interval mellem 0,1 og 1,6 %.

Udvekslingskoefficienten mellem sprækker og matrix er indtil videre kun bestemt ved modellering og fuldskala tracer-forsøg. Således findes der meget få værdier for denne parameter, begrænset til enkelte studier i hhv. Skrivekridt og Bryozokalk med en samlet middelværdi på 3,5 x 10^{-3} 1/d.

Mens det for den hydrauliske ledningsevne har været muligt, på baggrund af et omfattende dataset, at differentiere imellem forskellige kalktyper og kalk-provinser, vurderes det ikke rimeligt at tildele forskellige værdier for porøsitet og udvekslingskoefficient. Derfor er værdierne 3,5 x 10^{-3} 1/d (udvekslingskoefficient), 0,8 % (sprækkeporøsitet) og 30 % (matrix porøsitet) benyttet til den efterfølgende konceptuelle modellering.

Den konceptuelle stoftransportmodellering er bygget således op, at der benyttes en konceptuel, dobbelt porøs model, DP- model, til at simulere et gennembrud ved en indvinding. Metodisk betragtes denne herefter som det 'sande' gennembrud. Det tilstræbes her at ramme et gennembrud ved indvindingen efter 365 dage. Således er et spild (forurening) 1 år om at nå til indvindingen fra en given placering opstrøms i oplandet. Den eksakte placering er fundet iterativt ved at flytte placeringen frem og tilbage indtil det præcise sted, der giver et gennembrud efter 365 dage, er fastlagt. Nærmere beskrivelse af de konceptuelle stoftransportmodeller findes i afsnit 5.1 og illustreres i figur 5.1.1.

Efter de 'sande' afstande er fundet i den dobbelt-porøse model, er en tilsvarende enkel porøs model opsat, hvor den eneste forskel er, at stoftransporten ikke beskrives i et dobbelt, men enkelt porøst domæne (kontinuum) ved én effektiv porøsitetsværdi. I den enkelt-porøse model er placering af potentielt spild således det samme som fundet i den dobbelt porøse model (med et gennembrud efter 365 dage). I stedet for at ændre på distancen for at opnå det rigtige tidspunkt for gennembruddet (fra DP-modellen), er den effektive porøsitet således ændret i den enkelt porøse model for at matche både timing og distance simuleret ved den dobbelt porøse model. Således er der fundet effektive porøsiteter (n_{eff}) for kalkmagasiner med den høje, den mellemliggende og den lave hydrauliske ledningsevne.

Tabel 1.1 Parametre til BNBO modellering

Bjergart	K	n_f	n_m	n_{eff}	β
	m/s	%	%	%	1/d
Skrivekridt	3,60 x 10^{-5} (3 m/d)	0,8	30	17	3,5 x 10^{-3}
Bryozokalk Kalksandskalk Slamkalk Kerteminde mergel	1,35 x 10^{-4} (12 m/d) Middelværdi	0,8	30	13	3,5 x 10^{-3}
Grønsandskalk	5,11 x 10^{-4} (44 m/d)	0,8	30	11	3,5 x 10^{-3}

K er hydraulisk ledningsevne, n_f er sprække porøsitet, n_m er matrix porøsitet, n_{eff} er effektiv porøsitet og β er udvekslingskoefficienten mellem sprække og matrix.

Tabel 1.1 viser de anbefalede parametre for de danske kalkbjergarter ved henholdsvis dobbelt (K, n_f, n_m, β) og enkelt porøs modellering (K, n_{eff}).

Den beregnede effektive porøsitet ligger mellem 11 og 17 % hvilket viser, at der ikke er opnået ligevægt i udvekslingen mellem sprækker og matrix under den givne simuleringsperiode og afstand. Hvis der var opnået ligevægt ville den effektive porøsitet være lig matrix porøsiteten. Tidspunktet og afstand, hvorover der er opnået ligevægt mellem sprækker og matrix kaldes t-eq.. t-eq. findes i den enkelt porøse model ved den transport-afstand og tidsperiode, hvor den effektive porøsitet er lig matrixporøsiteten, dvs. ved 30 % porøsitet (se yderligere i kapitel 3, Teori). For den hydrauliske ledningsevne, som anbefales for de fleste kalktyper (50 % percentilen), er t-eq. beregnet til at indtræde efter 85 år med en transportafstand på 1450 m. Således er tidshorisonten langt udover BNBO-perspektivet på 1 år, men nærmer sig den administrativt fastlagte tidsramme for afgrænsning af indvindingsoplandet, svarende til transporten fra hele indvindingsoplandet (grundvandsdannende områder) til en indvindingsboring.

Som det fremgår af tabel 1.1, varierer den effektive porøsitet relativt meget, når den hydrauliske ledningsevne ændres. Det viser, som også illustreret ved følsomheds-analysen, at de fundne effektive porøsiteter skal benyttes ved den parametersætning for de øvrige parametre og modelforhold, som de er fundet ved (konceptualisering af stoftransport, sektion 5.1). Herunder er det vigtigt at understrege, at forudsætningen for simulering i hhv. dobbelt og enkelt porøse medier, er laminar strømning jf. den teoretiske gennemgang i kapitel 3. Laminar strømning er typisk ikke til stede ved strømning i makro-sprækker (kanal strømning) påvirket af indvinding, hvor turbulente strømningsforhold forventes at gøre sig gældende boringsnært. For indvindings-boringer eller kildepladser med tydelig indikation af turbulent strømning (f.eks. ved meget høje hydrauliske ledningsevner eller fra borehulslogging - videolog eller forskellige typer flowlog) for strømning i makro-sprækker, kan de anbefalede effektive hydrauliske ledningsevner og den stedfortrædende enkelt porøse modellering ikke benyttes. Makro-sprækker er defineret som større enkeltsprækker (centimeter til decimeter apertur) eller opsprækkede zoner (decimeter til meter tykkelse).

For nogle områder i Danmark er der observeret karstificering af kalken (sektion 6.2). Karstificering kan indikere, at strømningen foregår i mere gennemgående/forbundne makrosprækker. Det er derfor relevant, hvor der er observeret karst og makro-sprække strømning, da dette kan give en indikation af, om en given indvinding kan være påvirket af ikke-laminar strømning i makro-sprækker. En anden indikation af strømning i makro-sprækker er høje observerede hydrauliske ledningsevner (> 10^{-3} m/s). Følsomhedsanalysen (figur 5.5.3) af de hydrauliske ledningsevner viste endvidere, at med en hydraulisk ledningsevne over 10^{-3} m/s (590 m/d), forøges den 1 årige BNBO-transportafstand hurtigt fra < 500 m ved en hydraulisk ledningsevne på 10^{-3} m/s til > 14 km ved en hydraulisk ledningsevne på 6,8 x 10^{-3} m/s. Det vurderes, at observerede hydrauliske ledningsevner over 10^{-3} m/s er en klar indikation på makrosprækker og dermed turbulente flow forhold nær ved indvindingsboringen. Ved mange indvindingsboringer ses indstrømningen til boringen igennem enkelte makro sprækker over et vertikalt interval på f.eks. 10-30 m af grundvandsmagasinet. Under disse forhold foregår grundvandstrømningen, i en meget lille del af magasinet. Strømningshastigheden vil som resultat af det lille volumen, hvor strømningen foregår i, blive meget høj (turbulent), og kan ikke beskrives ved en Darcy-baseret beregning af grundvandsstrømningen. Vurderes den hydrauliske ledningsevne kun for det specifikke interval i boringen (f.eks. henover en 10 cm "tyk" sprække), hvor indstrømningen i praksis foregår, vil den hydrauliske ledningsevne være større end 10^{-3} m/s. Da observationer omkring hydrauliske ledningsevner for indvindingsboringer (f.eks. i JUPITER) for det meste er angivet i forhold til hele den åbne del af boringen (filtersatte del), vil en værdi på 10^{-3} m/s eller højere altså indikere, at der findes nogle meget vandførende horisonter i boringen med turbulente forhold. Derfor anbefales det ikke at benytte enkelporøs modellering ved indvindingsboringer, eller horisonter af disse, hvor der er kendskab til hydrauliske ledningsevner over 10^{-3} m/s. Der er således to overordnede argumenter for ikke at anvende enkelt porøse modeller med hydrauliske lednings evner over 10^{-3} m/s til modellering af BNBO. For det første vil der typisk foregå turbulent strømning (ikke laminar). For det andet ses ved den konceptuelle modellering, at 1-års transportafstanden bliver meget stor med hydrauliske ledningsevner over 10^{-3} m/s. Det medfører kilometer lange, men meget "tynde" BNBO-områder, som sandsynligvis ikke dækker den præcise placering af det aktuelle sprække-system, der giver vand til indvindingen. Ved hydrauliske ledningsevner mindre end 10^{-3} m/s, vil BNBO-arealet være mere cirkulært omkring indvindingen.

For at kunne benytte de anbefalede parametre for de forskellige bjergartstyper fordelt over Danmark, er der lavet et kortmateriale der angiver, hvor de forskellige kalk-bjergarter benyttes som grundvandsmagasiner. Hvis der ved en indvindingsboring ikke er kendskab til hvilken kalk-bjergart der indvindes fra, kan kortet bruges som støtte til bestemmelse af denne. Kortmaterialets datagrundlag er baseret på kalk-lithologier i JUPITER ud fra hvilke afgrænsende polygoner er tolket. Kortmaterialet beskrives nærmere i kapitel 6 og viser udbredelsen af danske grundvandsmagasiner af kalk og kridt (karbonat-bjergarter). De relevante magasiner er: Skrivekridt, Bryozokalk, Slamkalk, Kalksandskalk, Grønsandskalk og Kerteminde mergel.

Praktisk anvendelse af parametre
De fundne effektive porøsiteter relaterer sig til den hydrauliske ledningsevne, de er estimeret sammen med. Derfor bør de fundne effektive porøsiteter kun benyttes med de samme hydrauliske ledningsevner ved estimering af BNBO-områder. Det anbefales at vælge en af de 3 effektive porøsiteter med tilhørende hydrauliske ledningsevner. Det kan gøres på to måder afhængig af eksisterende lokal viden:

1) Der er ingen tilgængelig information om K-værdier i JUPITER eller ingen viden om eksisterende makrosprækker i lokalområdet. I dette tilfælde skal parametrene tildeles i henhold til kalktypen ved indvindingsboringens indtag. Kortet over de danske kalkbjergarter, kapitel 6, og borehulsbeskrivelser i JUPITER, kan hjælpe med dette valg. Afhængigt af kalktype vælges en af de tre parametergrupper, jævnfør tabel 1.1.
2) Der er pålidelig viden om K-værdier i JUPITER eller fra lokale undersøgelser og denne er under 10^{-3} m/s, og der er ingen indikation af makrosprækker. I dette tilfælde bør BNBO-estimeringsmodellen tildeles n_{eff}- og K-værdierne fra den gruppe (25, 50 eller 75 % percentil), som den stedspecifikke K-værdi ligger tættes på. De stedspecifikke K-værdier bør ikke bruges direkte i modellen, men bruges til at vælge parametre fra en af de tre parametergrupper. Hvis der er mere end én kendt og troværdig K-værdi for en model med mere end én indvindingsboring, kan et gennemsnit af de kendte K-værdier bruges til at identificere en af de tre parametergrupper. Troværdige K-værdier er fra hydrauliske test, der er velbeskrevne og dokumenterede (f.eks. i konsulentrapporter ved den givne indvindingsboring).

Opsummering

- Grundvandsstrømning i danske kalk og kridt magasiner foregår i et forbundet sprække-matrix-system, hvor porøsiteten i matrix indeholder størstedelen af grundvandet, mens selve strømning fra opland til indvinding sker via sprækkerne, som medfører den høje hydrauliske ledningsevne.
- Den hydrauliske ledningsevne er den modelparameter, som påvirker den 1-årige (BNBO) transportafstand mest.
- Det er muligt at simulere 1 års gennembrud med en effektiv porøsitetsværdi i en enkelt-porøs model.
- De effektive porøsiteter bør kun anvendes under forhold, som svarer til dem, de er fundet under, da ligevægt i udveksling mellem matrix og sprækker ikke er opnået under BNBO forhold.
- I områder med meget høj ledningsevne (>10^{-3} m/s) med makrosprækker eller karstlignende strømningsforhold, anbefales udpegning af BNBO baseret på effektive porøsitetsværdier / enkelt porøse modeller ikke.
- Tabel 1.1 angiver de anbefalede parametre for beregning af BNBO-områder for de danske kalkbjergarter.

2. Terms and notations

The below table offers a list of important notions and concepts and a Danish translation including a description of the terms.

Table 2.1 Concepts and notions used for working with transport in fractured porous carbonate rocks together with a translation to Danish

English	Danish	Notation/unit	Dansk beskrivelse af term
Mass transfer coefficient	Udvekslings-koefficient	β [1/t]	Definerer hastighed af udveksling af opløst stof mellem matrix og sprækker
Matrix	Matrix		Kalken består af hhv. matrix og sprækker
Aperture	Apertur	2b	Tykkelse af sprækkeåbning
Spacing	Sprækkeaf-stand	2B	Afstand mellem sprækker
Representative Elementary Volume	Repræsentativt elementær volumen	REV	Det volumen en given parameterværdi repræsenterer.
Equivalent Porous Media	Ekvivalent porøs media-/model	EPM	Ofte anvendes også betegnelsen EP model, Equivalent Porous model i rapporten
Dual Continuum	Dobbelt porøsitet	DC	Dual continuum. Generel betegnelse for media eller model som indeholder to værdier for samme parameter, fx porøsitet eller hydraulisk ledningsevne
Double Porous model	Dobbelt porøs	DP	Dobbelt porøs, som dual continuum, men hvor parameteren er porøsitet. Ofte anvendt som beskrivelse af model, DP model, dobbelt porøs model
Dimensionless number	Dimensionsløst tal	F_s	Værdi der beskriver om der findes ligevægt mellem koncentrationer i sprække og matrix
Discrete Fracture	Diskret sprække	DF	Betegnelse som angiver at akkurate mål for sprækker
Dispersion	Dispersion	α	Kontrollerer spredningen på stof
Longitudinal dispersivity	Langsgående dispersivitet	α_L [L]	Spredning af opløst stof i langsgående retning set i forhold til advektiv strømningsretning
Transversal dispersivity	Tværgående dispersivitet	α_T [L]	Spredning af opløst stof normalt på langsgående retning set i forhold til advektiv strømningsretning
Diffusion coefficient	Diffusionskoefficient (effective)	D or D_{eff}	Kontrollerer diffusion af opløst stof, hastighed af udligning af koncentrationsgradienter
Conservative transport	Konservativ transport		Stoftransport hvor der ikke optræder nedbrydning eller sorption
Diffusion distance	Diffusionsaf-strand	L_d	Afstanden for en given diffusion

Hydraulic conductivity	Hydraulisk ledningsevne	K [L/t]	De hydrauliske ledningsevner kan opdeles i en horisontal (Kh) og vertikal komponent (Kv)
Hydraulic conductivity for the matrix	Hydraulisk ledningsevne for matrix	K_m [L/t]	Hydrauliske ledningsevne for matrix (for opsprækket domæne med angivelse af separate værdier for matrix samt sprække)
Hydraulic conductivity for the fractures	Hydraulisk ledningsevne for sprækker	K_f [L/t]	Hydraulisk ledningsevne for sprække (for domæne med angivelse af separate værdier for matrix samt sprække)
Effective hydraulic conductivity	Effektiv hydraulisk ledningsevne	K_{eff} [L/t]	Hydraulisk ledningsevne (for domæne med angivelse af én værdi for matrix samt sprække K)
Hydraulic gradient	Hydraulisk gradient	J	Hydraulisk gradient er trykfald over afstand
Porosity	Porøsitet	n	n angiver porøsitet generelt
Porosity of the matrix	Matrix porøsitet	n_m	Porøsitet af matrix i opsprækket domæne
Porosity of fracture	Sprække porøsitet	n_f	Porøsitet af sprække i opsprækket domæne
Effective porosity	Effektiv porøsitet	n_{eff}	Den porøsitet, der benyttes i EP modeller for opsprækkede kalksystemer
Equilibrium transport distance	Ligevægtstransport afstand	L_{eq} [L]	Afstand hvorefter der ved opløst transport er opnået ligevægt i konc. mellem sprækker og matrix
Transmissivity	Transmissivitet	T [L^2/t]	Transmissiviteten angiver raten som vand passerer gennem en enhed bredde L^2 af et grundvandsmagasin ved en hydraulisk gradient.

3. Theory

3.1 Modelling concept for describing flow and solute transport in fractured porous media

In this chapter, as well as in the entire report, the migration of a conservative substance contained in a single phase (water) is described. It is assumed that the flow and solute transport takes place in a fractured porous medium, e.g. fractured chalk, limestone or marl. The fractures are conceptualized as the space between two parallel plates that are embedded in a so-called matrix being the porous medium surrounding the fractures. Flow in the fractures is assumed to be so slow that laminar flow conditions exist, and that Darcy's law is valid for groundwater flow in a saturated, rigid medium described as:

$$q = -K\frac{dh}{dx} \tag{1}$$

where x is the coordinate [m], and q is the Darcy flux [m/s]. The resistance to flow is described by the permeability (k) [m] or the hydraulic conductivity (K) [m/s], and h is the hydraulic head [m]. In the following, it is assumed that flow is at steady-state, i.e., no changes with time. If the flow in the fractures is assumed to be described as flow between two parallel plates the hydraulic conductivity of the fracture is given by:

$$K_f = \frac{\rho g(2b)^2}{12\mu} \tag{2}$$

where ρ is the density of the fluid [kg/m^3], g is the gravitational acceleration [m/s^2], μ is the dynamic viscosity [kg/m/s], and 2b is the distance between the parallel plates [m], also referred to as the fracture aperture. Equation (1) describes the flow in both a porous medium and fractures if it is parameterized according to Eq. (2).

Modelling of flow and transport in fractured porous media may be carried out using three different approaches: The discrete fracture method (DF), the dual continuum method (DC) or the equivalent porous medium method (EPM), Figure 3.1. The three methods are described by e.g. Bear (1992).

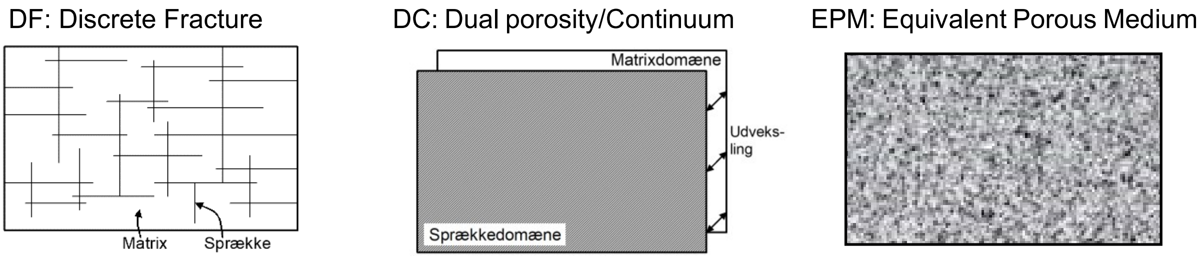


Figure 3.1 Three approaches to model transport in fractured porous media

In a discrete fracture model, the individual fractures and their connection are described explicitly. This approach is unattractive for two reasons. First, it is computationally demanding if the scale of interest is large compared to the fracture density, which is typically the case in BNBO investigations. Second, it is problematic to estimate the location of the fractures and the hydraulic conductivity of the fractures, as this requires detailed knowledge about the fracture location and aperture distribution, see Eq. (2). Therefore, the discrete fracture approach will not be used in the present study. Instead, it is often more suitable to model flow and transport in a fractured medium using a continuum approach (DC or EPM in Figure 3.1) as this does not rely on detailed information on the fracture system. This requires, however, that a macroscopic representative elementary volume (REV) can be defined.

3.2 Continuum modelling: REV

According to Bear (1992), the size of the REV should be much larger than the spacing between the fractures, but significantly smaller than the length characterizing the domain of interest. In Figure 3.2, an illustration of the REV is presented, where the red magnifying glass represents the area (volume) considered. The smallest glass only captures the matrix and will clearly not represent the sum of fractures and matrix. The largest circle, on the other hand, may be large enough to represent a REV, as it will integrate over both matrix and fractures, and the macroscopic quantities found within the glass may stay relatively independent of location. Assuming that the average distance between the fractures (2B) is one meter, then the radius of the REV may be on the order of five to 10 meters, depending on the geometry of the fracture network.

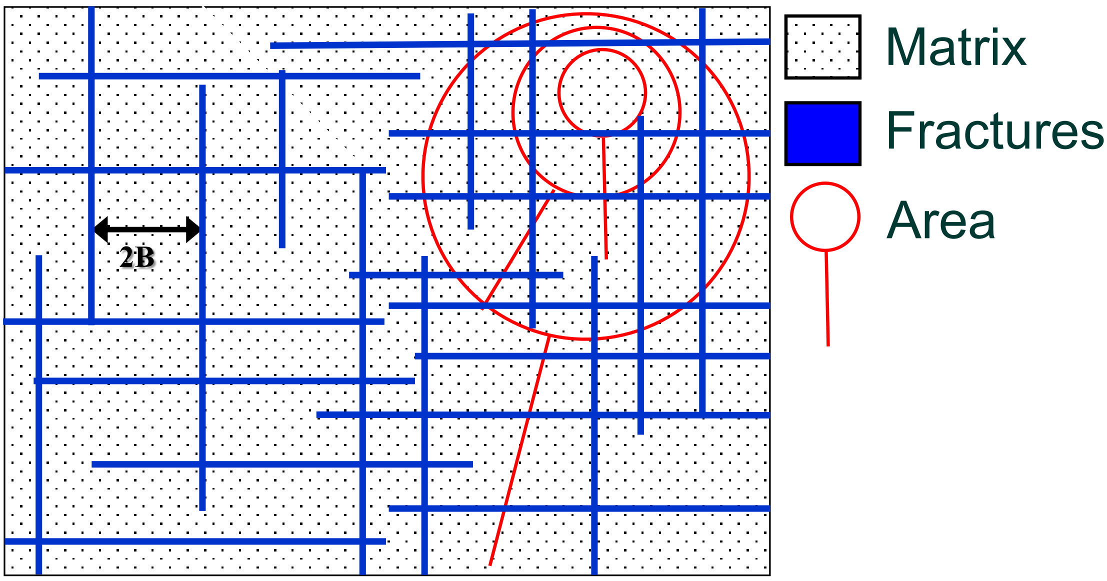


Figure 3.2 Illustration of the size of the REV (three red circles, each representing an estimate of REV) for a fractured medium, where the blue lines represent fractures located perpendicular to the orientation of the page.

3.3 EPM/DC: Equilibrium between fractures and matrix

In the EPM approach, the fractures and the matrix are described as a single continuum with one set of parameters (hydraulic conductivity, porosity, etc.). This is in contrast to the DC approach, where fractures and matrix are described as separate domains with their own set of parameters. The choice between the EPM and the DC approach depends on the transport characteristics of the problem. The application of the EPM approach requires that equilibrium conditions exist between the fractures and the matrix with respect to solute concentration. van der Kamp (1992) suggests that this requirement can be examined using the dimensionless number F_s:

$$F_s = \frac{t_d}{t_a} = \frac{(2B)^2 K_{eff} J}{L_t n D_{eff}} \quad (3)$$

where t_d is the time scale for diffusion from the fractures to the centre of the matrix elements, and t_a is the arrival time or travel time to the point of interest. 2B is the fracture spacing, Figure 3.2, L_t is the travel distance, n is the total porosity, K_{eff} is the effective hydraulic conductivity, J is the hydraulic gradient and D_{eff} is the effective diffusion coefficient of the matrix (see below for definition of “effective” values). For small values of F_s equilibrium between the matrix and the fractures can be assumed while for large values of F_s, non-equilibrium conditions exist between the two domains. van der Kamp (1992) suggests that $F_s < 0.1$ should be fulfilled for equilibrium conditions to be assumed and the EPM approach can be applied. In that case, no benefits are obtained using a dual-continuum approach compared to the simpler EPM approach.

3.4 EPM - Equivalent porous medium model

In the equivalent porous medium model (EPM) it is assumed that fractures and matrix can be described as one united porous medium using one set of parameters. Hence, it is assumed that the aquifer behaves like a normal porous medium, and therefore it is described using the same principles as, e.g., used for a sand aquifer. The application of this type of model requires that effective parameters can be defined, e.g., effective hydraulic conductivity or effective porosity. Effective parameters are upscaled quantities that can capture the impact of small-scale heterogeneity on large-scale flow and transport. Hence, effective parameters describe the combined effect of heterogeneities, in the present case fractures and matrix, on the flow and transport. Effective hydraulic conductivity is also referred to as “bulk” hydraulic conductivity (e.g., Nilsson et al., 2001). The effective hydraulic conductivity is estimated as:

$$K_{eff} = n_f K_f + n_m K_m \quad (4)$$

where n_f and nm are the porosities of fractures and matrix, respectively, and K_f and K_m are the hydraulic conductivities of fractures and matrix, respectively. K_{eff} is expected to be a parameter that is constant in time and unaffected by changes in flow and transport conditions. The effective porosity, n_{eff}, on the other hand, depends on the time scale and the transport properties of the problem at hand, see Figure 3.3.

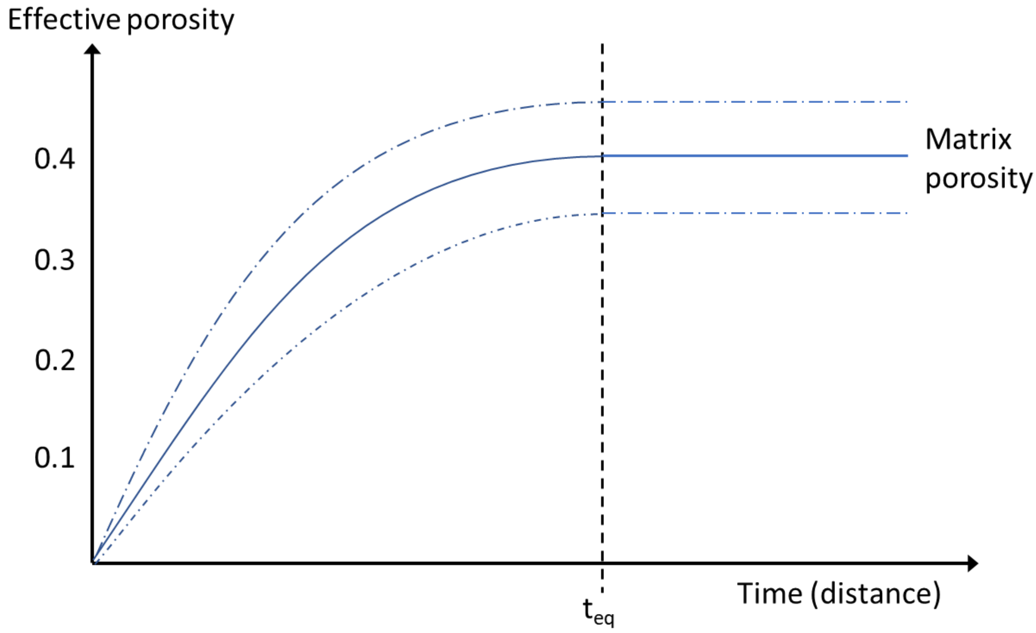


Figure 3.3 Sketch of how the effective porosity varies with transport time. The real relation between time and effective porosity is unknown and the example above is only for illustration – not for use.

If the time scale is small and the exchange of solute between fracture and matrix is relatively slow, the transport through the fractures will dominate and the fractured medium can be described as an equivalent porous medium, where the effective porosity equals the fracture porosity which is expected to have a value in the order of magnitude of about 1%. After some time, molecular diffusion between fracture and matrix will be more significant and will affect the solute concentration in the fractures as well as in the matrix. After a sufficiently large transport time, it may be assumed that the diffusion from the fractures to the matrix is fully developed and the effective porosity will therefore be at its maximum, equivalent to the matrix porosity. This corresponds to the time it takes to reach equilibrium between matrix and fracture, t-eq in Figure 3. It should be noticed that the shape of the curves in Figure 3.3 should only be considered as an illustrative example. The EPM model with effective porosity equal to the matrix porosity can be applied at times equal to T-eq or higher. In between these to end-points, it is necessary to use an effective porosity that lies in between the fracture and the matrix porosity, meaning that the effective porosity will change when the travel distance or time, over which the transport is taking place, changes. As a result, it is problematic to use the EPM method in intermediate situations since the value of the effective porosity will change in unknown ways.

An estimate of the equilibrium transport distance may be obtained from Eq. (3). Rearranging the formula by van der Kamp (1992) yields:

$$L_t = \frac{(2B)^2 K_{eff} J}{0.1\, n\, D_{eff}} = \frac{(1)^2 \cdot 1 \cdot 10^{-5} \cdot 1 \cdot 10^{-3}}{0.1 \cdot 0.3 \cdot 2.6 \cdot 10^{-10}} = 1{,}280\ m \qquad (5)$$

For the system with a fracture spacing *(2B)* of 1 m, an effective hydraulic conductivity *(K_{eff})* of 1 x 10^{-5} m/s, a hydraulic gradient *(J)* of 0.001, a total porosity *(n)* of 0.3 and an effective diffusion coefficient *(D_{eff})* of 2.6 x 10^{-10} m^2/s, it will require a transport distance of approximately 1.3 km before equilibrium has been reached. At this transport distance, the equilibrium distance has been reached and the effective porosity equals the matrix porosity for distances equal to or larger than Lt = 1,280 m. The estimation of Lt is highly sensitive to the value of K_{eff}, as it can vary substantially (see Chapter 4 on literature). If a value of K_{eff} = 1 x 10^{-4} m/s is used instead, a distance of 12.8 km is found before the effective porosity becomes constant. As the parameters for different rock types are different, travel distances to reach equilibrium will depend on rock type.

3.5 DP – Dual porosity model

When dealing with clay, chalk or marl (a mixture of clay and chalk), the hydraulic conductivity (permeability) of the matrix is normally low enough to ensure that the migration of solutes is controlled by diffusion (see Chapter 4 for exceptions). In the fractures, the advective flow will primarily take place. In that case, it is valid to describe the fractured aquifer as a dual-porosity media, where advective flow is restricted to the fractures, and the only transport mechanism accounted for in the matrix is diffusion.

3.6 Dual-porosity vs. dual-permeability approach

If equilibrium between matrix and fractures (see above) cannot be assumed for the problem of interest, a dual continuum description can be used instead, since there is no requirement for equilibrium between the two domains for a dual continuum model. Hence, either a dual-porosity approach, where advective transport is assumed only to take place in the fractures or the dual-permeability approach, where advective transport may take place in both the fracture and the matrix domain, can be applied. The requirement for using the dual-porosity method and hereby ignoring the advective flow in the matrix is that transport in the matrix is dominated by diffusion. To evaluate that, the Peclet number for the matrix can be used (Barker, 1993):

$$P_c = \frac{L_d K_m J}{n_m D_{eff}} \tag{6}$$

where L_d is the diffusion distance [m], K_m is the hydraulic conductivity of the matrix [m/s], J is the hydraulic gradient [1], n_m is the porosity of the matrix, and D_{eff} is the effective diffusion coefficient of the matrix [m2/s]. If Pc < 1 the transport is dominated by diffusion, while for Pc > 1 the transport is increasingly influenced by advection. Pc is primarily a function of Km which for unfractured chalk varies in the range from 1x10^{-9} – 1x10^{-7} m/s. Using best estimates (conf. e.g., Bonnesen et al., 2009) for each parameter in Eq. (6) results in Pc = 1m * 1x10^{-8} m/s* 1x10^{-3}/(0.35 * 3x10^{-10} m^2/s) ≈ 0.1. Hence, this implies that transport in normal carbonate aquifers under standard conditions is dominated by diffusion. The presented work and recommendations derived from it are therefore based on the assumption that on the scale of

BNBO, transport in the matrix is dominated by diffusion, and thus, transport in fractured carbonate aquifers in Denmark can be described by the dual-porosity model. The parameters needed for the dual-porosity model includes the effective hydraulic conductivity (same as for EPM), the matrix (n_m) and fracture (n_f) porosities (see differential equation presented in Appendix A), and the mass transfer coefficient, β. Analytical expressions for both porosities and mass transfer coefficient for different fracture configurations are found in Appendix A.

3.7 Well testing of fractured aquifers

The oil industry has developed an interesting method for analyzing the response of pumping tests in fractured aquifers (Nielsen, 2007) that is relevant in connection with contaminant transport. Based on the early response (first few minutes) from the pumping test the properties of the fracture system can be analyzed using a dual-porosity model of the reservoir. The classical manuscript of Warren and Root (1963) describes how the fracture storage, S_f, and the fracture hydraulic conductivity, K_f, can be estimated. If the pumping test is carried out in a phreatic aquifer, S_f equals the specific yield, S_y, of the fractures.

"Specific yield, also known as the drainable porosity, is a ratio, less than or equal to the effective porosity" (Dingman 2008). It is here assumed that the referred effective porosity equals the fracture porosity of a fracture system. Further "Specific yield can be close to effective porosity, but there are several subtle things which make this value more complicated than it seems. Some water always remains in the formation, even after drainage; it clings to the grains of sand and clay in the formation. Also, the value of specific yield may not be fully realized for a very long time, due to complications caused by unsaturated flow." The capillary forces of the fracture system are, however, expected to be relatively small which facilitates fast drainage of the fracture openings. However, estimates of the specific yield of the fracture system obtained from pumping tests may not be directly applicable as the fracture porosity in dual-porosity flow and transport modelling, but based on the definition of the two parameters one would expect that a relation between them could be formulated. Interpretations of fracture properties based on well testing are therefore considered to be of potentially high value to flow and transport studies. Unfortunately, only a few data have been available to the present study, see Chapter 4, but a reinterpretation of existing pump tests in phreatic fractured formations using dual-porosity concepts could be a promising path to obtain information about the fracture system that is otherwise inaccessible.

4. Flow and transport parameters in Danish carbonate rock types: a literature review

4.1 Background and purpose

The existing literature on non-reactive solute transport in fractured carbonate rocks such as chalk, limestone and marl in Denmark was reviewed to investigate differences in flow parameters in different types of carbonate rock aquifers. The carbonate rock types will from now on be mentioned as ‘chalk and limestone’ or just chalk. The aim is to obtain the best knowledge-based estimate of the porosity, which should be used in BNBO calculations in fractured carbonate rocks. The literature review is based on Danish studies of fractured chalk and limestone and international published data on carbonate aquifers given in textbooks. Student projects from Danish universities and research institutions were a valuable source of information on chalk and limestone porosity and hydraulic conductivity. Moreover, relevant technical reports from consultants and authorities that were available were reviewed and available data were compiled in a table overview.

A webinar was held on 10 February 2021 with consultants, stakeholders and authorities to identify potential non-public available data, as well as other information about porosity and groundwater flow in fractured chalk and limestone that can be included in the present work. Finally, a video meeting was held with Kurt Ambo Nielsen (consultant), where experiences with a dual-porosity interpretation of pump tests in fractured chalk and limestone were discussed (Nielsen, 2007). The rather scarce hydraulic flow parameter coverage on specific carbonate rock types in Jylland was confirmed by interviewing relevant persons at the universities in Aarhus (Steen Christensen) and Aalborg (Jacob Birk Jensen, now WatsonC).

4.2 Danish flow and transport parameter values

This section provides an overview of data available on relevant parameters for the different carbonate rock types in Denmark. The focus is on collecting the following parameter values: effective porosity (n_{eff}), matrix porosity (n_m) and fracture porosity (n_f), hydraulic conductivity (K), and the mass transfer coefficient (β) between the matrix domain and fractures for non-reactive solutes.

Table 4.1 gives an overview of available parameters in literature from the various Danish fractured carbonate aquifer types. Upper Cretaceous chalk, Danian and Selandien limestone and marl aquifers are the most common in Denmark. Appendix B lists 34 field and laboratory studies on data from 19 locations in Denmark. The review of the available literature shows that chalk and limestone sites from Eastern Denmark dominate the collected data (Figure 4.1). Different porosity types (effective, matrix or fracture porosity) in the category ‘K and porosity values’ in Figure 4.1 has not been distinguished. The same applies to the K values where there are not distinguished between (matrix dominated hydraulic conductivity or fracture dominated hydraulic conductivity). Only a very sparse data set was available from studies of porosity and hydraulic conductivity at Funen and Jutland chalk and limestone study sites.

The Danish carbonate rock type names presented in this chapter are: ‘Skrivekridt’ (Upper Cretaceous chalk), ‘Slamkalk’ (Danian calcilutite – not shown in Table 4.1), ‘Bryozokalk’ (Danian bryozoan limestone), ‘Kalksandskalk’ (Danian calcarenite), ‘Grønsandskalk’ (Selandian Lellinge Greensand) and ‘Kerteminde mergel’ (Selandian marl deposit).

Table 4.1. Parameters of porosity, hydraulic conductivity and mass transfer coefficient in various Upper Cretaceous, Danian and Selandian chalk, limestone and marl aquifers in Denmark

Carbonate rock type	Geologic Age	Test method	n_{eff}	n_m	n_f	K_m	Kh_{eff}	Kv_{eff}	β
Kerteminde mergel	S	PT, CT, M				√	√	√	
Grønsandskalk	S	PT					√		
Bryozokalk	D	PT, TT, CT, PAT, M		√	√	√	√	√	√
Kalksandskalk	D	PT, CT		√			√		
Skrivekridt	UC	PT, CT, TT, M	√	√	√	√	√	√	√

Geologic Age: Upper Cretaceous (UP), Danian (D), Selandian (S)
Test method: pump test (PT), cone test (CT), tracer test (TT), packer test in well (PAT), modelling (M)

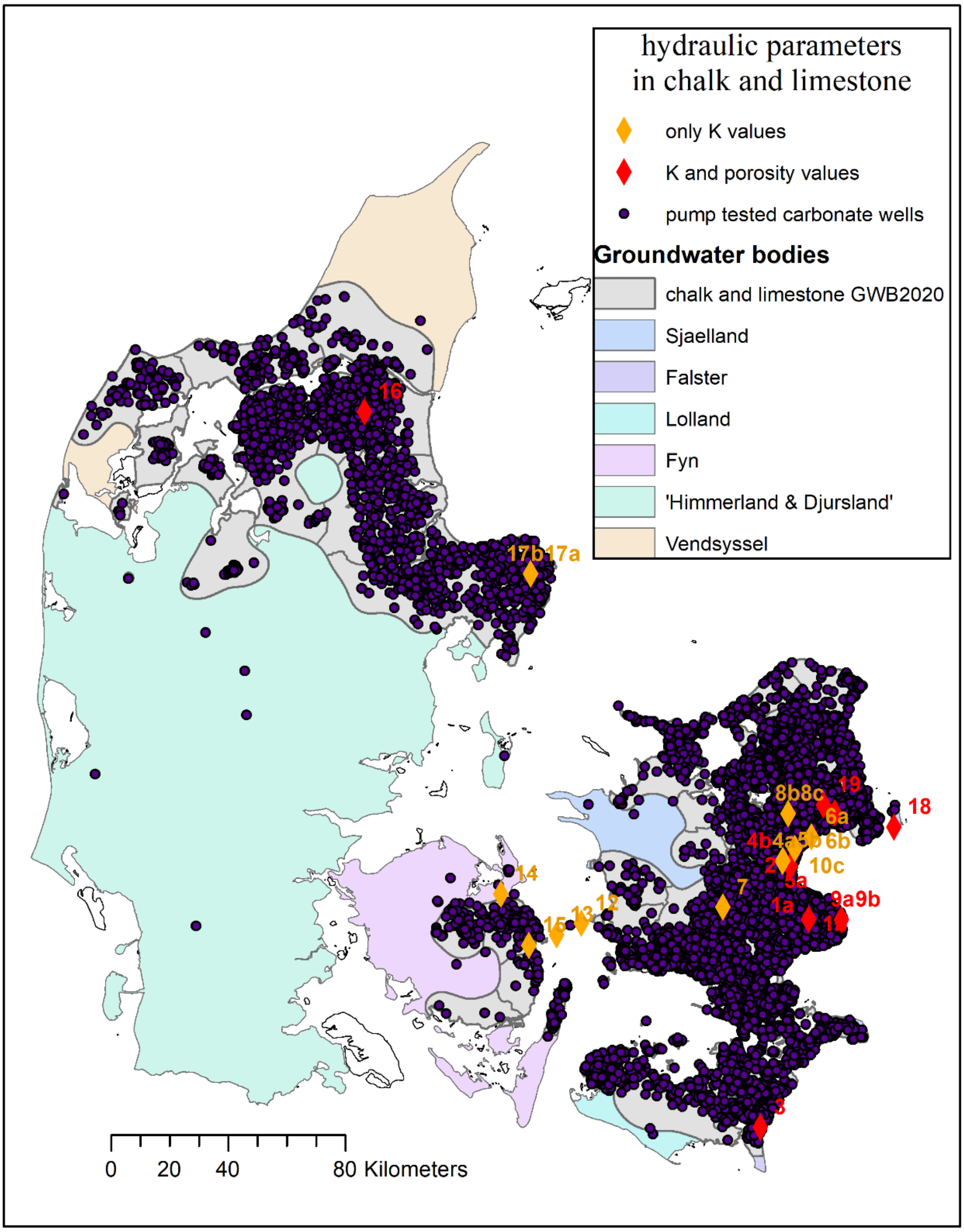


Figure 4.1. Chalk and limestone locations in Denmark that provide (a) field and laboratory data on porosity and hydraulic conductivity (red diamond), (b) solely hydraulic conductivity data (light brown diamond) and (c) hydraulic conductivity data derived from pumping tests in open and screened chalk wells (black dots) with transmissivity data reported to the JUPITER database (in total 9437 pumping tests). Location IDs refers to Appendix B. The grey polygon represents the extension of chalk and limestone groundwater bodies (Troldborg 2020).

In Parts of Vendsyssel, Southern Jutland, Fyn and Sjælland chalk and limestone rocks do not provide conditions for groundwater abstractions (no extended groundwater bodies has been delineated in those areas). This explains the ‘Himmerland & Djursland’ term. There are a few chalk and limestone groundwater bodies in central Jutland, South of Limfjorden also.

Various aquifer test methods were used to determine the hydraulic properties of the chalk and limestone aquifers. Hydraulic conductivity is either determined in the field using pumping tests (PT); packer tests in boreholes (PAT), or tracer tests (TT). In the laboratory, various experiments with chalk and limestone plugs (CT) were used. Porosity data were backed out from tracer testing (TT) and efforts on modelling (M) using different conceptual assumptions (cf. Chapter 2).

It is well known from the literature that the different test methods represent different aquifer volume scales. A consistent increase in K values with scale was reported in unconsolidated sand, volcanic rocks and carbonate rocks by Schulze-Makuch et al. (1999). Schulze-Makuch and Cherkauer (1998) analyzed hydraulic conductivity concerning scale during individual aquifer tests in porous, heterogeneous carbonate rocks in southeastern Wisconsin, USA. Results from this study indicate that hydraulic conductivity generally increases in carbonate rocks during an individual test as the volume of aquifer impacted increases, and the rate of this increase is the same as the rate of increase determined by using different measurement methods (Figure 4.2).

The data collected in the present literature review represent very different volumes of the aquifer tested. Plug or core typically represent test volumes of 10^{-5} to 10^{-4} m^3, which predominantly represent the non-fractured part of the aquifer (i.e. matrix domain). At the other end of the aquifer, the volume scale is the model volume domain, which can vary considerably in scale between 10^4 to 10^{10} m^3. The field method that comes closest to the model volume scale is pumping tests (10^3 to 10^5 m^3). In comparison, a typical BNBO catchment is assessed to have a size aquifer volume of more than 10^3 m^3.

A data set of transmissivity data solely obtained from pumping tests (approximately 9500 pumping tests) in fractured chalk and limestone wells was collected from the public available drilling and groundwater database named JUPITER at GEUS. It is assumed by using data from a single aquifer test method used across Denmark that it is possible to assess regional differences in hydraulic conductivity in the carbonate rock type aquifers. The compiled pumping test data are presented at the national and regional level in sections 4.7 and 4.8. by estimating a transmissivity value and dividing with the open length (sometimes screen part) of the investigated borehole.

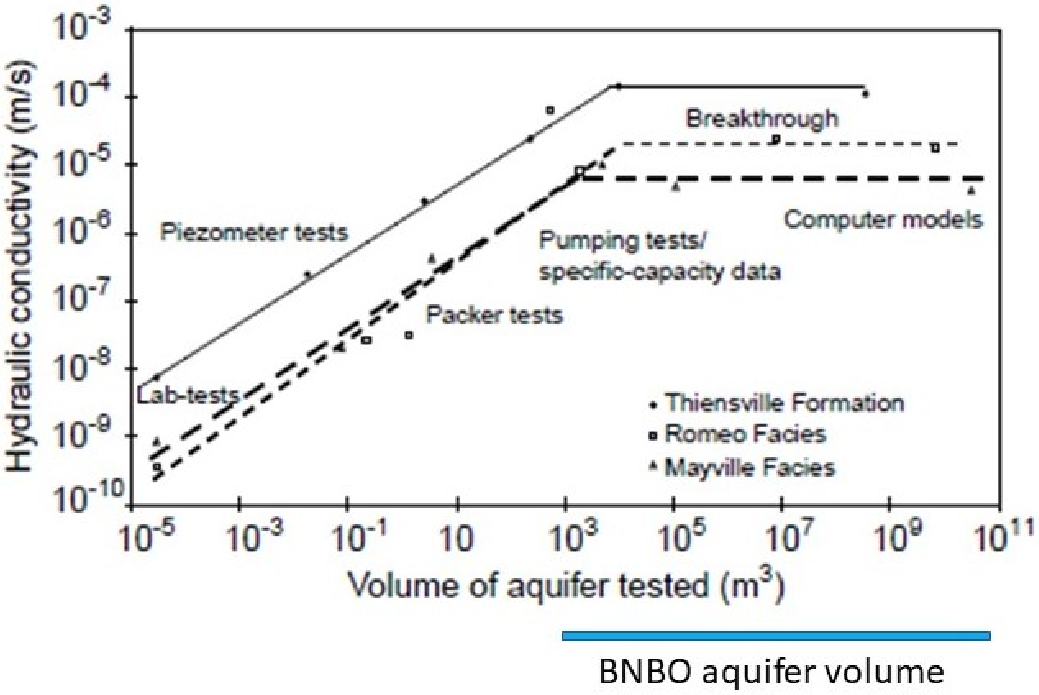


Figure 4.2. Relationship between estimated hydraulic conductivity and spatial scale in heterogeneous, porous carbonate rock (Schulze-Makuch and Cherkauer, 1998). The expected BNBO aquifer volume is shown at the bottom (blue bar).

4.3 Porosity

The literature review has for the most part provided information on the matrix porosity in the relevant carbonate rock types. Only very limited information is available on fracture porosity in Danish fractured chalk and limestone.

In Figure 4.3 data on porosity from Kalksandskalk (KK), Bryozokalk (BK) and Skrivekridt (SK) are shown. The matrix porosity (n_m) varies somewhat between the three aquifer types: 10-40% in KK; 5-45% in BK and 20-50% in SK. Fracture porosity (n_f) is estimated to range between 0.02-1.6% in BK and a single study shows 4 % fracture porosity in SK (Table 4.2). No fracture porosity data is available from Kalksandskalk in the reviewed literature. All the fracture porosity numbers given above are estimated based on the modelling of tracer test results from the experimental field sites in Ølsemagle, Marielyst and Karlstrup. For comparison, international textbook examples show that carbonate aquifer data from Canada, USA, Mexico and England on the matrix porosity varies between 2.4 and 30% and the fracture porosity is in the lower range of 0.01-0.1% (Ford and Williams, 2007). Freeze and Cherry (1979) indicate that the porosity (matrix) falls in the range of 0-20% in limestone (dolomite) and 5-50% in karst limestone. The matrix porosity values of the Danish chalk and limestone aquifers shown in table 4.2 are relatively high in comparison with carbonate aquifer values elsewhere.

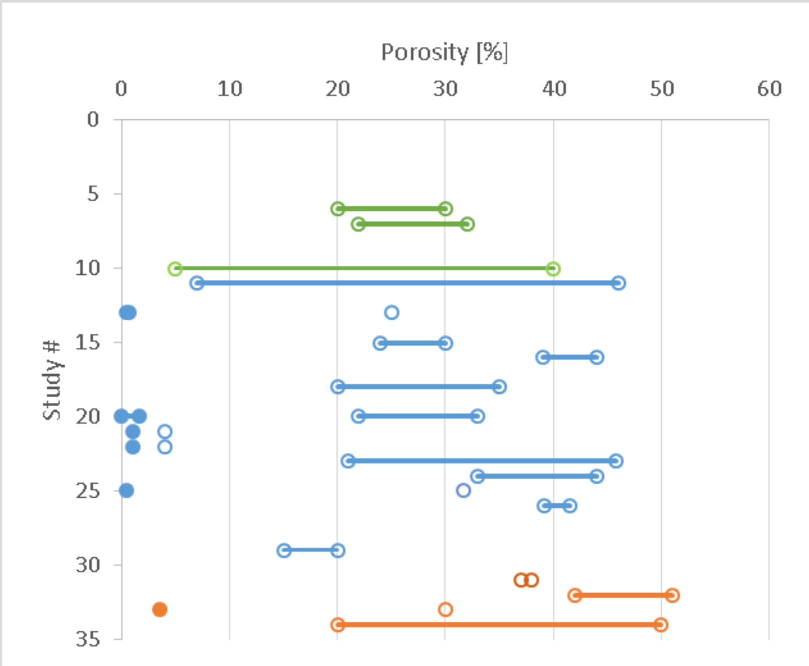


Figure 4.3. Matrix porosity (open circles) and fracture porosity (filled circles) in Kalksandskalk (green), Bryozokalk (blue) and Skrivekridt (orange).

Table 4.2. Statistics on fracture, matrix and effective porosity from field and laboratory studies divided into carbonate rock types

Parameter	Carbonate rock type	Min (%)	Average (%)	Max (%)	Number of studies
n_m	KK	5	24,7	40	3
	BK	4	26.2	45.8	13
	SK	20	37.3	51	4
n_f	BK	0.016	0.82	1.6	5
	SK		3.6		1
n_{eff}	SK	0.015	0.32	0.86	2

4.4 Hydraulic conductivity

The hydraulic conductivity of the matrix is determined directly by field and laboratory tests, or indirectly by modelling. Effective hydraulic conductivity (K_{eff}) is directly obtained from pumping tests or indirectly determined by modelling of tracer test results obtained in the field or laboratory. Figure 4.4 shows the reported values of matrix and fracture hydraulic conductivities in the field and laboratory studies. Statistics on the matrix and fracture hydraulic conductivities (min, average and max values) are given in Figure 4.5. The distinction between matrix-dominated and fracture-dominated hydraulic conductivity is a continuum and not a sharp value. The threshold is differently used among petroleum geologists and water resources managers/scientists. In petroleum geology, a value 2 x 10^{-7} m/s (approximately 20 millidarcy) is used as the threshold where values above 2 x 10^{-7} m/s are impacted by fracture flow in chalk and limestone in the North Sea. In water resources management, the limit will be somewhat higher for hydraulic conductivity (> 10^{-6} m/s) based on thoroughly expert experience on parameter selection for groundwater modelling in Denmark by GEUS. If the threshold value of $1x10^{-6}$ m/s is used in Figures 4.4 and 4.5, most of the K values below $1x10^{-6}$ m/s will be matrix dominated K values as reported in the literature studies.

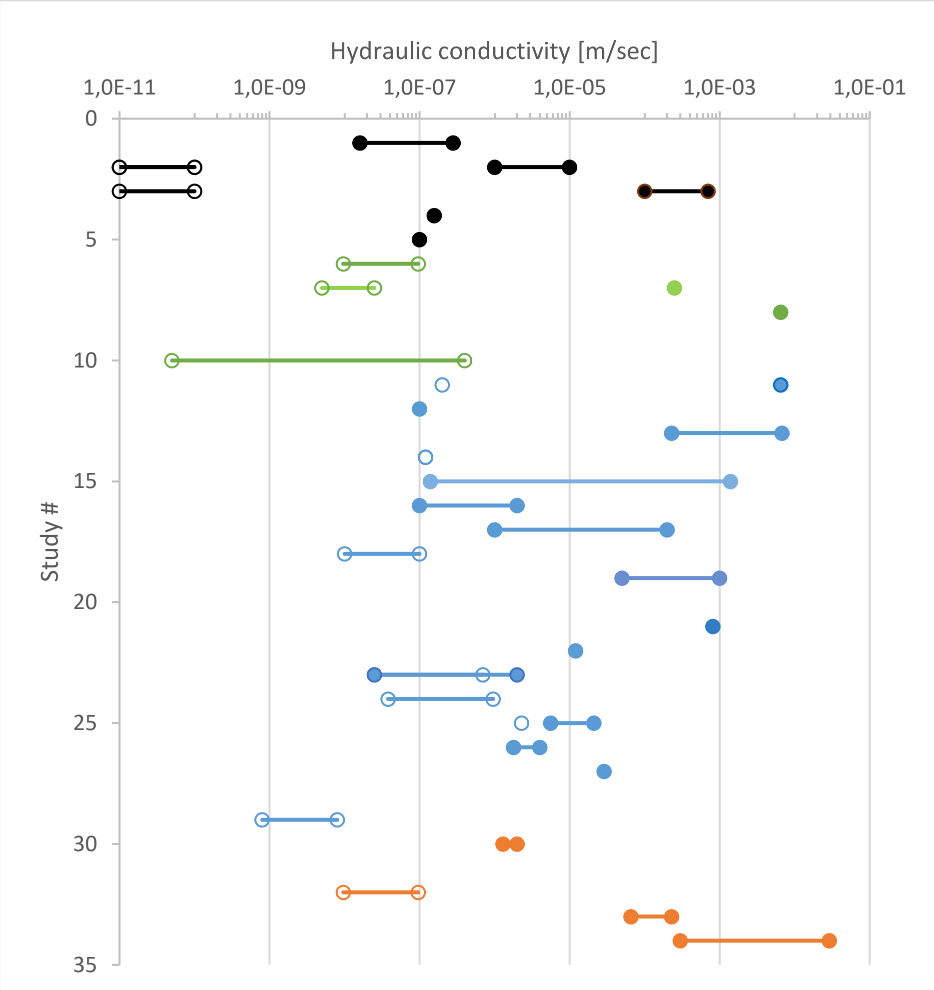


Figure 4.4. Effective and matrix hydraulic conductivity determined in different carbonate rock types with different hydraulic tests. All the hydraulic conductivities shown are measured values. KM: Kerteminde mergel (black); KK: Kalksandskalk (green); BK: Bryozokalk (blue); SK: Skrivekridt (orange). Open circles are matrix and solid circles are reported as effective data.

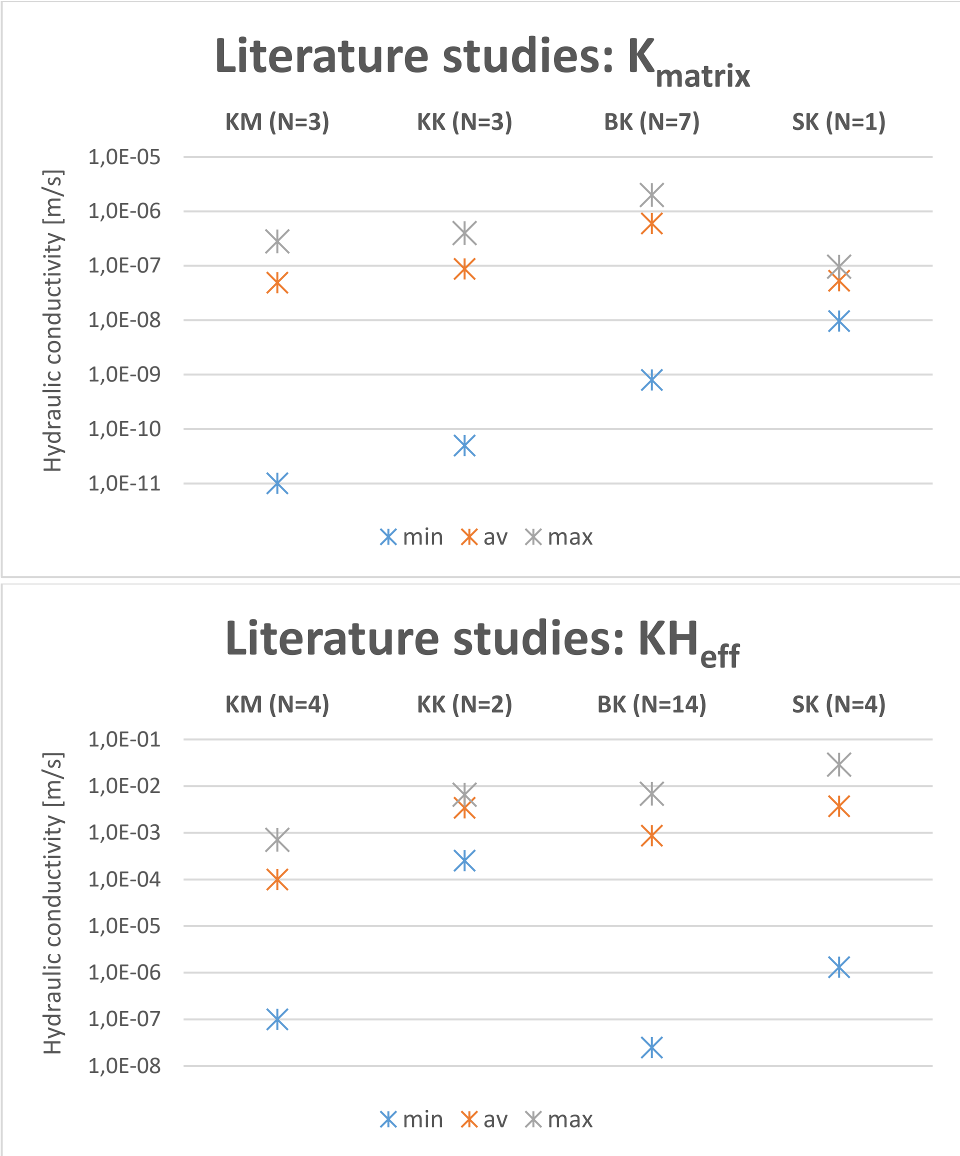


Figure 4.5. Statistics on matrix dominated (K_m) (upper) and fracture dominated (lower) effective hydraulic conductivity (K_{eff}) at field and laboratory studies divided into carbonate rock types. N = number of studies.

In 2014 GEO and GEUS compiled an extensive data set of hydraulic properties determined on chalk and limestone plugs from the Copenhagen area (Galsgaard et al., 2014). The plugs were collected by GEO in connection with the Metro, Øresunds bridge and motorway constructions, pollution studies and other research projects in chalk and limestone southwest of Copenhagen. The systematic data collection of plug data, representing the same aquifer test volume, provides a good representation of matrix properties for Bryozokalk and Kalksandskalk in the Sjælland region. The hydraulic conditions in Bryozokalk, Kalksandskalk and Faxekalk show a significant positive correlation between porosity and hydraulic conductivity (Figure 4.5). Data from the Faxekalk rock type can be ignored since Faxekalk hydraulic properties is not relevant for the BNBO topic and are not used as groundwater aquifer in Denmark. There seem to be two populations of data in Figure 4.6. The first group with low K values in the interval 10^{-11} to 10^{-8} m/s and a porosity range of 5 to 20%, likely represent matrix-dominated chalk and limestone samples (plugs) without the influence of fracture flow. Typically, the matrix data can be described with a power function relation. The other population of data represent slightly higher K values in the range of 10^{-8} to 10^{-6} m/s and porosity values between 20 and 45%. It should be noted that the relevant hydraulic conductivity for fractured chalk and limestone rocks types used for water supply and BNBO catchment calculations is one to two decades higher than the upper end of the laboratory determined K values at 10^{-6} m/s based on plug-test derived results (figure 4.6).

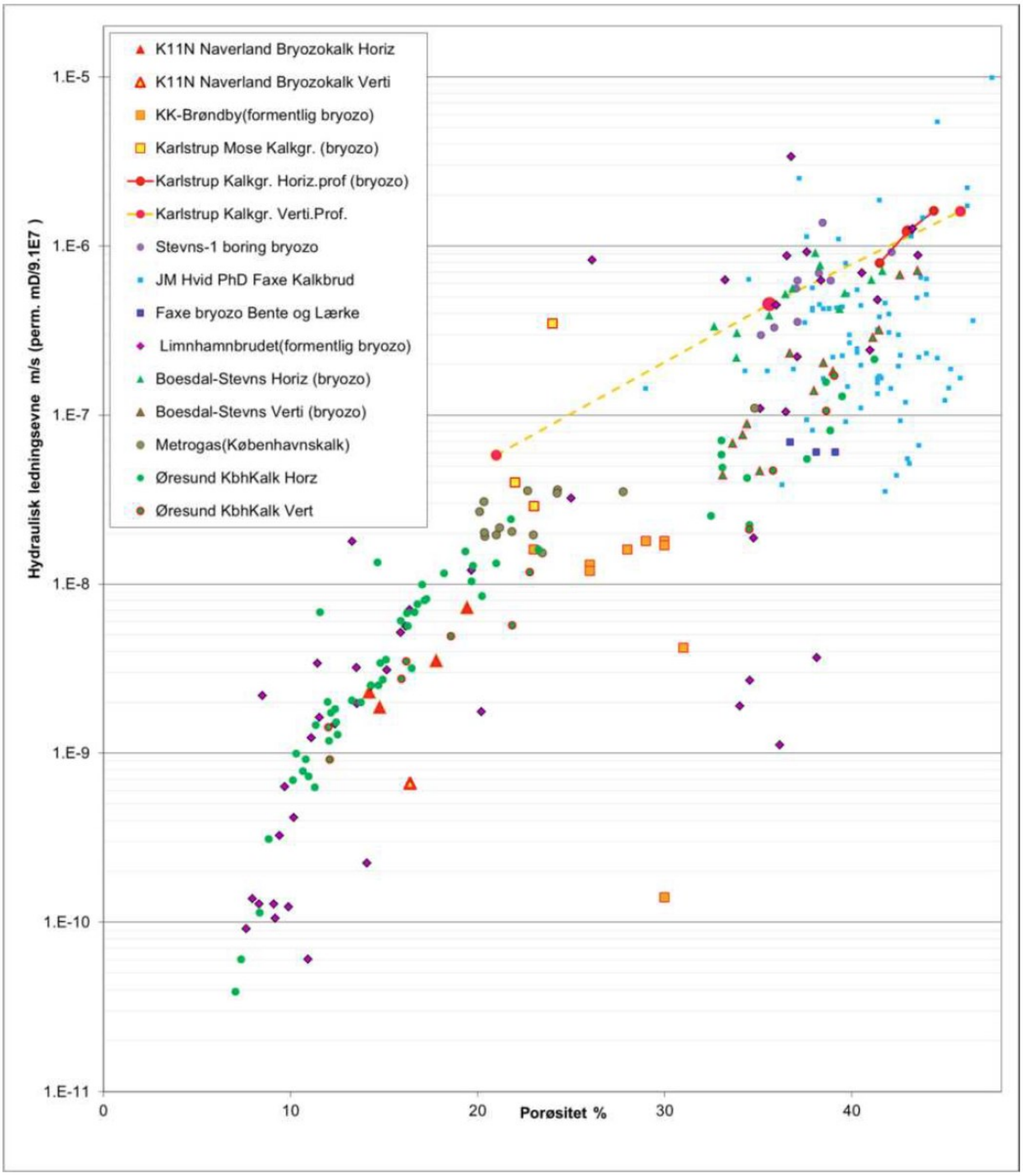


Figure 4.6. Porosity and hydraulic conductivity of matrix determined on lime plugs taken in Bryozokalk, Kalksandskalk and Faxekalk from several studies in the Copenhagen region (Galsgaard et al., 2014). The dotted line in yellow and solid line in red made for the GEO survey must be ignored.

4.5 Mass transfer coefficients

The mass transfer coefficient (β) can only be determined indirectly using the modelling of tracer test results. The literature review clarified that there is only limited data from Denmark on the mass transfer coefficient. In Bryozokalk there are field locations in Hellested at Stevns and in Karlstrup that provide the β value determined between $2x10^{-7}$ to 0.008 d^{-1} and an average β value of 3.9×10^{-3} d^{-1}. In Skrivekridt there are three field locations in Sigerslev at Stevns, Marielyst at Falster and in Mjels chalk quarry south of Limfjorden with information on the β value with a range of 1.7×10^{-5} to 0.001 d^{-1} and an average β value of 3.1×10^{-3} d^{-1}. The statistics of the model-derived β value based on field tracer tests in Bryozokalk and Skrivekridt are given in Figure 4.7. These numbers were used in the conceptual modelling.

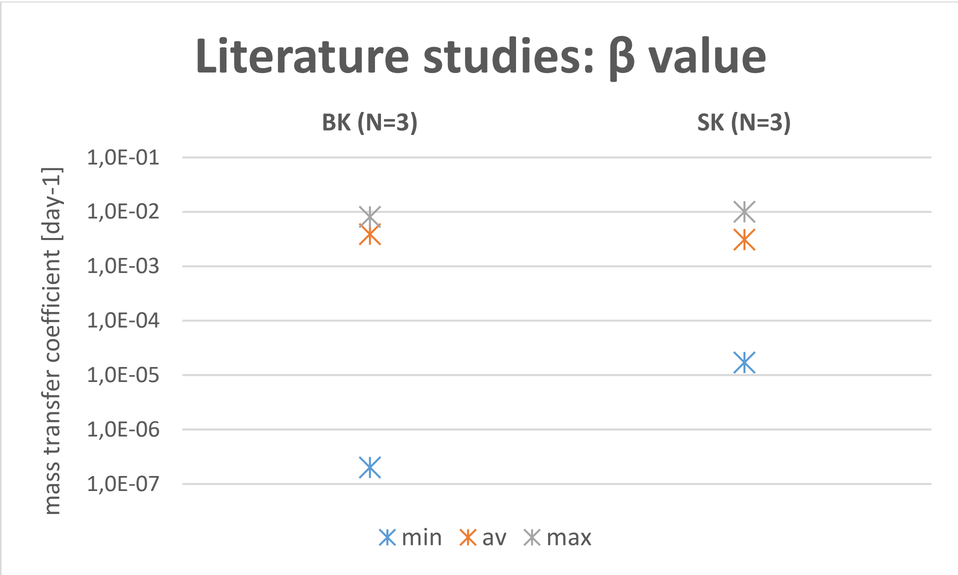


Figure 4.7. Statistics on the mass transfer coefficient β value determined in Bryozokalk and Skrivekridt. N = number of field tracer studies.

4.6 Hydraulic conductivity of chalk and limestone on a national level

The mean hydraulic conductivity (all mean values are calculated as arithmetical mean) of the different carbonate aquifer rock types on a national level is calculated based on pumping test data available in the JUPITER database. A total of 9107 pumping tests in open or screened chalk and limestone boreholes provide transmissivity data from past time to the year 2019.

The calculated transmissivity from JUPITER data (in the unit m^2/s) is converted to a hydraulic conductivity in the unit m/s by dividing the T value by the length of the screen (depth to filter bottom subtracted depth to filter top in meters). In a few cases, the chalk and limestone boreholes are screened across several carbonate rock type lithologies. In those cases, the same T value is used for each of the lithologies.

Mean K values shown with 68% confidence intervals (± one standard deviation) for the data set at the national level show no significant difference in the intervals between the measured hydraulic conductivities for the different types of limestone, as shown in Figure 4.8. Mean K values for each type of limestone at the national level show reasonably small differences between 7.9 x 10^{-5} to 3.2 x 10^{-4} m/s. Histograms and normal distributions were calculated for all carbonate rock types. Pumping test data from all carbonate rock types show a high degree of log-normal distribution as expected, see Appendix D.

Outliers were removed from the data set resulting in a total of 8930 used pumping tests, i.e., extremely high hydraulic conductivity in chalk and limestone wells defined as K values above 1 x 10^{-2} m/s, as well as K values lower than 1 x 10^{-6} m/s. Overall, high-end outliers make up 2 % (~ 193 pumping tests) and low-value outliers make up 3.8% (~ 363 pumping tests). Outliers are further elaborated in section 4.8.

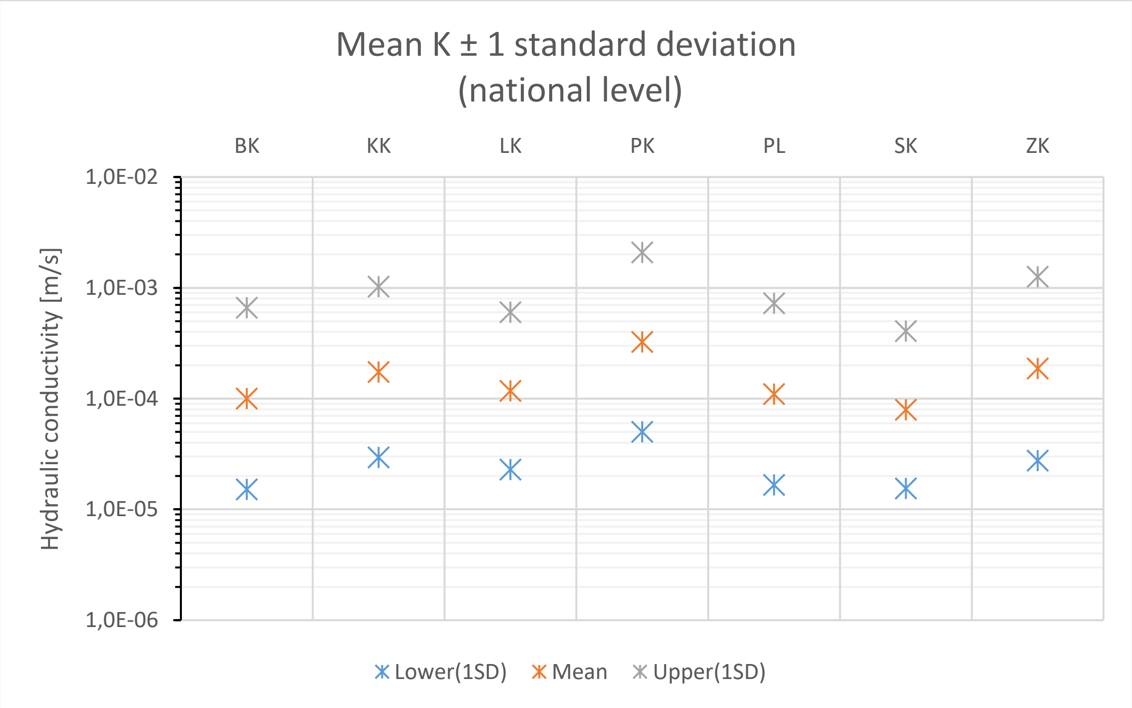


Figure 4.8. Mean K and 68% confidence intervals (± one standard deviation) were obtained from pump tests (exclusive outliers, see text) in screened or open chalk wells (in total 8930 pump tests across Denmark). The mean K is given for all chalk and limestone types. Bryozokalk (BK), kalksandskalk (KK), Slamkalk (LK), Grønsandskalk (PK), Kerteminde Mergel (PL), Skrivekridt (SK), Chalk with flint of uncertain geologic time (ZK).

4.7 Regional differences in the hydraulic properties of the chalk and limestone

The regional differences in the hydraulic properties of the chalk and limestone aquifers were calculated for the geographic regions in Denmark where the chalk and limestone boreholes occur (figure 4.1). The regions are Vendsyssel, 'Himmerland & Djursland', Fyn, Sjælland, Lolland and Falster. In this report, the area south of the Limfjord is called 'Himmerland and Djursland' (that also includes the areas Kronjylland, Mors and Salling). The number of pump tests carried out in chalk and limestone boreholes in the different regions are given in Appendix C1. Mean K values are calculated for the individual carbonate rock types and regions, where minimum, average and maximum values of hydraulic conductivity is given where more than 20 pumping tests were performed within a certain rock type in a region. Figure 4.9 summarize the calculated mean K values in all regions and relevant carbonate rock types. Skrivekridt can be observed across Denmark (except for Fyn) as an aquifer. The variation of K values in the Skrivekridt is relatively small, 0.46 to 1.55 x 10^{-4} m/s. The K value is highest in central and northern Jutland and lowest on Sjælland. Bryozokalk has the same mean K value range as Skrivekridt. However, K values are twice as high in Bryozokalk as in Skrivekridt on Sjælland. Slamkalk is not delineated as a carbonate aquifer type, however, this carbonate rock is quite common, especially on Sjælland and Himmerland & Djursland and represent more than 400 pumping tests. The mean K value of Slamkalk corresponds to what is observed in Skrivekridt. Kalksandskalken (KK) occurs only in the 'Himmerland & Djursland' region and in the northern Sjælland. The K values in the two parts of the country are almost the same. The Grønsandskalk (PK) is an important carbonate aquifer on both Sjælland and Fyn. The mean K value in the Grønsandskalk on Sjælland is highest in all regions and carbonate rock types in Denmark. The Kerteminde mergel (PL) has K values in the same order of magnitude as Skrivekridt and Bryozokalk on Sjælland and Fyn. Appendices C1 and C2 show the hydraulic conductivity values and ± one standard deviation that forms the basis of the graphical representation in Figures 4.9.

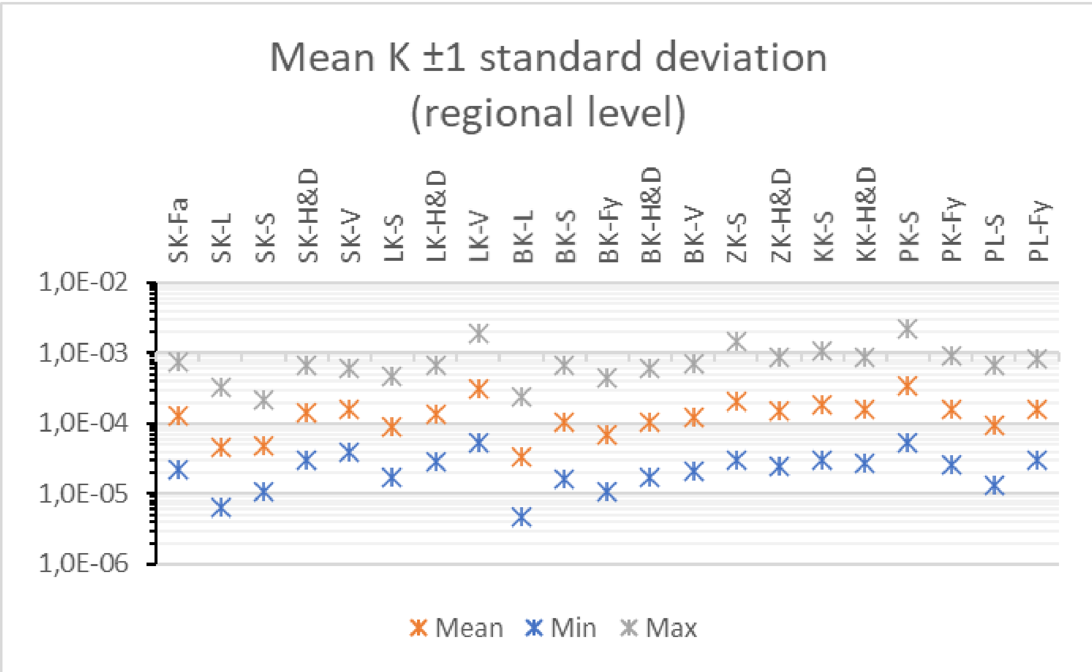


Figure 4.9. Mean K and 68% confidence interval (one standard deviation) were obtained from pumping tests in screened and open chalk/limestone wells (in total 8660 tests without outlier values). Data are geographical distributed on the following regions: Falster (Fa); Lolland (L), Sjælland (S), Fyn (F); Himmerland & Djursland (H&D); Vendsyssel (V). The mean K values + one standard deviation is given for all carbonate rock types (SK, LK, BK, ZK, KK, PK, PL).

Median (50 % percentile), 25 % and 75 % percentiles values for the 6 rock types across Denmark are also calculated and summarized in Table 4.4 in the summary section (4.9).

4.8 Extreme hydraulic conductivities

The extremely high K values are assumed to represent hydraulic conditions in the chalk and limestone with pronounced fracture systems or fault zones. Additional occurrence of locally widespread areas with "karst" dominated conditions can be developed. The very low K values probably represent the major volume of chalk and limestone without fractures/faults. The low K values likely correspond to matrix-dominated hydraulic conditions.

The extreme K data set is deducted from two populations of extraordinary low and high K values (in total 8930 pumping tests), The populations are defined by K_{eff} values above 1 x 10^{-2} m/s (extreme high K) and K_{eff} values lower than $1x10^{-6}$ m/s (matrix dominated). The extreme high-end K values make up 2 % (a total of 193 pumping tests) and extreme low K values make up 3.8% (a total of 363 pumping tests), see Table 4.3. The extremely high K values are assumed to represent hydraulic conditions in the chalk and limestone with pronounced fracture systems or fault zones. Additional occurrence of locally widespread areas with 'karst' dominated conditions can be developed. The very low K values probably represent the volume of chalk and limestone without fractures/faults. The low K values likely correspond to matrix-dominated hydraulic conditions. The karst topic is further discussed in Section 6.2.

Tabel 4.3. Number of wells in the normal fractured chalk, matrix dominated chalk and the 'karst' dominated chalk populations

Carbonate rock types	Normal fractured chalk K < 1 x 10^{-2} to K > $1x10^{-6}$ m/s	Matrix dominated chalk K < $1x10^{-6}$m/s	'karst' dominated chalk K > $1x10^{-2}$ m/s
Kerteminde mergel (pl)	256	1	6
Grønsandskalk (pk)	832	14	23
Københavnskalk (kk)	2078	85	31
Bryozokalk (bk)	2454	120	58
Kalk med flint (zk)	632	35	25
Skrivekridt (sk)	2218	34	16
Slamkalk (lk)	460	22	7
Total	8930	363	193

Chalk wells with matrix and 'karst' dominated K values is shown in Figure 4.10. There is apparently a predominance of matrix dominated results in North Sjælland and areas south of Copenhagen. Only a few low K results are found in central Jutland. Matrix dominated wells do not show a significant correlation to any particular carbonate rock types. Regarding the population of 'karst' dominated wells it appears to be a link between the location of high K values and a lineament in the middle of Sjælland and an east-west stretch across the central

Jylland. The distribution of 'karst' dominated areas by the extreme high K values and pieces of evidence of karst features in and near terrain surfaces will be further discussed in Section 6.2.

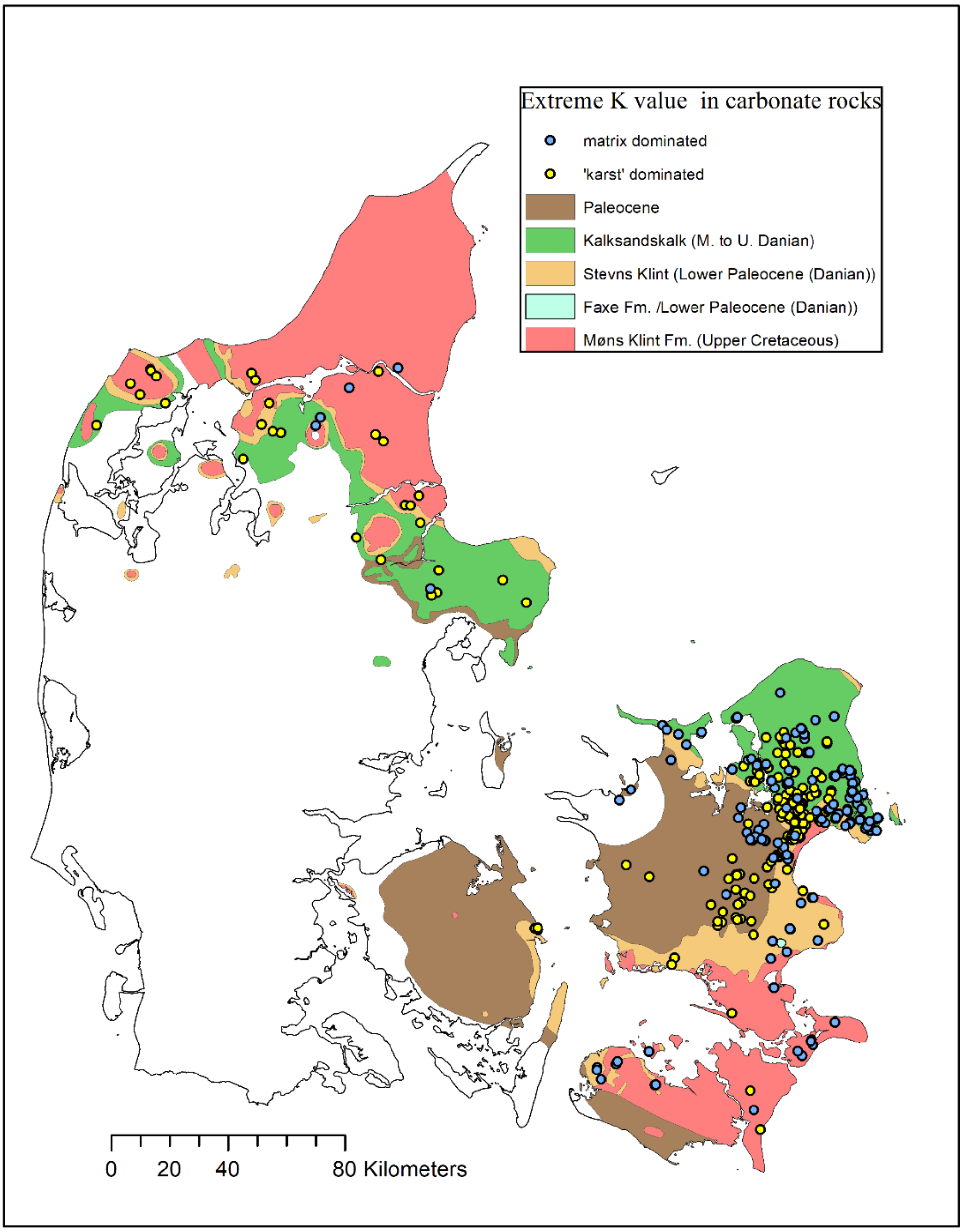


Figure 4.10. Matrix and 'karst' dominated pump test results in chalk and limestone wells related to the chalk and limestone rock types in Upper Cretaceous to Selandian deposits.

An analysis of the pump test data was made to see if there is a connection between K_{eff} and aquifer test volume that the individual pump tests represent. In total 4676 pump tests provided information about the duration and capacity of the pump test in the JUPITER database, thus the aquifer volume could be calculated for each of these pump tests. Figure 4.11 shows the K_{eff} and estimated aquifer test volume of each pump test distributed on the matrix dominated chalk (60 wells), 'karst' dominated chalk (44 wells) and the rest of the pump tests in the normal fractured chalk. Hydraulic conductivities show a spread of 8-9 decades. Aquifer volume varies within 6 orders of magnitude with matrix dominated chalk of 10^{-1} to 10^{3} m^3, normal fractured chalk of 10^{-1} to 10^4 m^3, and the 'karst' dominated chalk of 10^1 to 10^3 m^3. The analysis indicates that there are 1 to 2 orders of magnitudes difference in aquifer volume between pump tests carried out in matrix dominated chalk and 'karst' dominated chalk. There are no correlation between K_{eff} and aquifer volume in the three populations. In addition, the pump test data from JUPITER show much high variability in both K_{eff} and aquifer volume than reported by Schulze-Makuch and Cherkauer (1998).

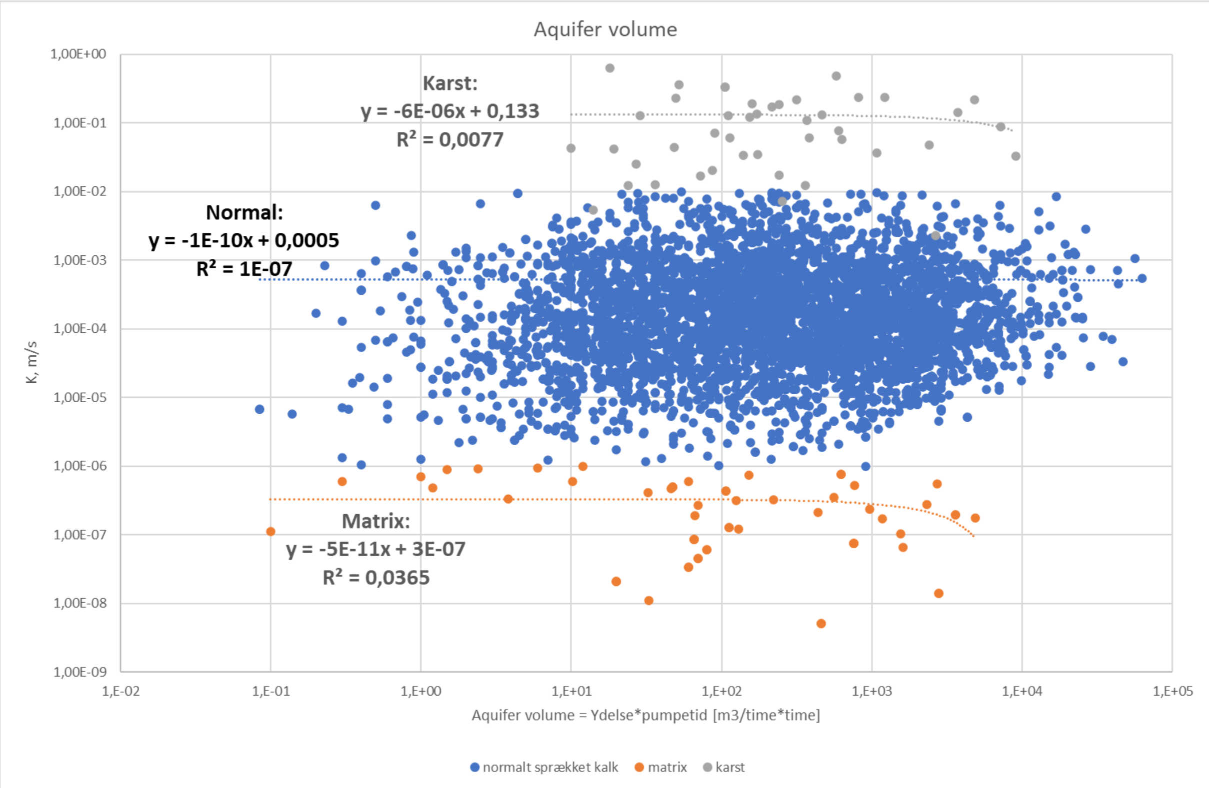


Figure 4.11. Plot of hydraulic conductivity and calculated aquifer volume based on 4676 pump test results in the Jupiter database.

4.9 Summary

The existing literature on non-reactive solute transport in fractured carbonate rock types such as chalk, limestone and marl in Denmark was reviewed to investigate regional differences in flow and transport parameters in the carbonate aquifers. The review is based on 34 studies at 19 locations with a dominance of studies in the eastern part of Denmark. In addition, data extraction was made from the JUPITER database to compile hydraulic conductivity data collected in the field on a spatial scale relevant to an assessment of BNBO. The pumping test data was divided into three populations representing matrix dominated chalk, normal fractured chalk, and extremely high K values of 'karst' dominated chalk. Pumping test data indicate that the flow in the carbonate aquifers of Denmark is dominated by fractures.

The regional differences in the hydraulic properties of the chalk and limestone aquifers were calculated for the regions Vendsyssel, 'Himmerland & Djursland', Fyn, Sjælland, Lolland and Falster. Mean K values in Skrivekridt is relatively small, 0.46 to 1.55 x 10^{-4} m/s. The K value is highest in central and northern Jutland and lowest on Sjælland. Bryozokalk has the same mean K value range as Skrivekridt. However, K values are twice as high in Bryozokalk as in Skrivekridt on Sjælland. Slamkalk is not for now delineated as a carbonate aquifer type in Denmark, however, this carbonate rock is quite common, especially on Sjælland and Himmerland & Djursland. The mean K value of Slamkalk corresponds to what is observed in Skrivekridt. Kalksandskalken (KK) occurs only in the 'Himmerland & Djursland' region and in the northern Sjælland. The K values in the two parts of the country are almost the same. The Grønsandskalk (PK) is an important carbonate aquifer on both Sjælland and Fyn. The mean K value of the Grønsandskalk on Sjælland is the highest of all regions and carbonate rock types in Denmark. The Kerteminde mergel (PL) has K values in the same order of magnitude as Skrivekridt and Bryozokalk on Sjælland and Fyn. Table 4.4 summarizes the calculated median, 25 and 75 % percentiles of hydraulic conductivity for the six carbonate rock types observed in Danish aquifers.

Table 4.4 Median, 25 % and 75 % percentiles of hydraulic conductivity of Danish carbonate aquifers

Rock type	Median (50 %)	25 % percentile	75 % percentile
All	**1.34×10^{-4} m/s**	**3.60×10^{-5} m/s**	**5.11×10^{-4} m/s**
Kerteminde mergel	1.29×10^{-4} m/s	3.20×10^{-5} m/s	4.48×10^{-4} m/s
Grønsandskalk	3.48×10^{-4} m/s	9.18×10^{-5} m/s	1.37×10^{-3} m/s
Kalksandskalk	1.78×10^{-4} m/s	5.60×10^{-5} m/s	6.75×10^{-4} m/s
Slamkalk	1.17×10^{-4} m/s	3.80×10^{-5} m/s	3.70×10^{-4} m/s
Bryozokalk	9.55×10^{-4} m/s	2.70×10^{-5} m/s	3.76×10^{-4} m/s
Skrivekridt	8.00×10^{-5} m/s	2.60×10^{-5} m/s	2.43×10^{-4} m/s

5. Conceptual solute transport modelling

The conceptual solute transport modelling is performed to analyze the impact of different flow and transport parameters on estimating solute transport in fractured porous media within the spatial and temporal frame of a BNBO. The conceptual solute transport modelling is done in three steps: 1) analyzing the sensitivity of relevant parameters for the solute transport, 2) estimating transport distances for several relevant Danish chalk and limestone aquifers with parameters found in the literature review based on a dual-porosity solute transport model. 3) Testing the possibility of using an equivalent domain model to reach transport distances found in 2).

5.1 Conceptual model setup and assumptions

The conceptual modelling of BNBO has been performed with MODFLOW to simulate laminar groundwater flow and MT3D to simulate non-reactive (conservative) solute transport in dual-porosity and equivalent single porosity model conceptualizations. MODFLOW is the United States Geological Survey's modular hydrologic model. MT3D is a finite-difference groundwater mass transport modelling software, often used with MODFLOW. Figure 5.1.1 illustrate the different elements of the conceptual models. The length and withs of the models vary according to parametrization, e.g. simulations with high hydraulic conductivities require long travel distances. Different model sizes were used because larger model domains are more computationally demanding than small models with the same cell size (vertical and horizontal discretization). All models are resolved using a 10 m x 10 m grid in the horizontal plane and a constant 2-meter vertical discretization. The models simulate groundwater flow in a confined aquifer with an 0.001 m (one per mille) gradient determined by specified head boundary conditions to the left (upgradient) and right (downgradient). In the downgradient part of the model domain, an abstraction well is defined with the MODFLOW well package with a total abstraction between 10,000 and 1,000,000 m^3/yr. The spill (simulated pollution) is always simulated in the upper numerical grid layer in the same row (the centre row) as the abstraction well. A homogeneous hydraulic conductivity field is assumed, e.g., the values are the same for the entire simulated numerical grid.

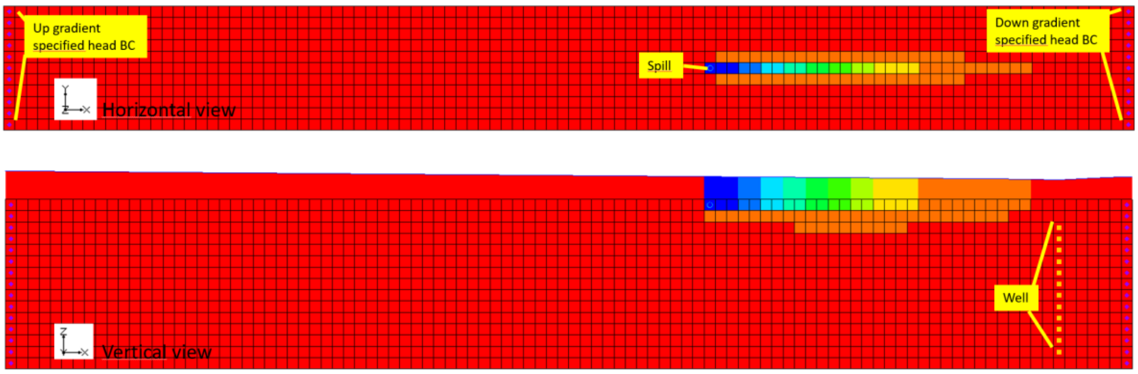


Figure 5.1.1 Conceptual model in horizontal (X-Y) and vertical (X-Z) plane.

The spill is simulated as a continuous spill where a given concentration of 1 mg/L (milligram per litre) is injected and in practice kept constant throughout the full simulation period, in the injection cell. The spill is simulated as a conservative tracer, e.g. no degradation or sorption of the solute is simulated. Dilution only occurs as a result of advective transport, dispersion and diffusion, and as a result of the exchange between fractures and matrix. Breakthrough of pollutant, first arrival, is defined as the time where the concentration at the abstraction well do reach a limit value of 0.1 µg/L (microgram per litre). Thus, the first arrival is defined as 1/10,000 of the spill concentration. Homogeneity of the chalk aquifer is assumed in the conceptual models.

5.2 Estimation of recommended parameters

The literature review analyzed the existing literature for parameter values typical for carbonate rocks within Danish freshwater aquifers. Regional variation of parameter values can only be supported if sufficient data is available. Therefore, it is only reasonable to work with regional values of hydraulic conductivity. Regarding porosity for fracture and matrix, mass transfer coefficient and dispersivity, data are not available to an extent that can justify regionally distributed values. For some rock types, no parameter values are available (also see chapter 4) and here we recommend that values observed for other available Danish carbonate rock types are used. The following sections describe the analyzed parameters and report the recommended values. The recommended values are mean if otherwise is not mentioned.

5.2.1 Porosity

For the porosity of the matrix, n_m, a relatively large number of observations are available from three carbonate rock types in Danish aquifers: Skrivekridt n_m = 38 %, Bryozokalk n_m = 26 %, and København Kalk n_m = 25 %. This is within the ranges reported by 'Vangkilde et al. 2011 (Geovejledning 8). The weighted average of these values is 30 %.

The porosity of the fractures, n_f, have been described to a much lesser extent for the Danish aquifers and therefore a single mean value for Danish carbonate aquifers of n_f = 0.8 %, is recommended. The range of n_f is 0.1 – 1.6 %.

5.2.2 Hydraulic conductivity

Effective hydraulic conductivity (or just hydraulic conductivity) varies by several orders of magnitude between different carbonate rock types (Figure 4.5). Nevertheless, the mean hydraulic conductivity values for the rock types observed in the Danish chalk regions (Falster, Lolland, Sjælland, Fyn, Himmerland & Djursland, and Vendsyssel) with 50 or more samples, are close to each other. The mean values range between 0.33 x 10^{-4} m/s and 3.39 x 10^{-4} m/s (Appendix C2) for the chalk regions (and rock types). One way to minimize the number of different values recommended for different rock types is to define that if the variation between the individual mean values is less than a factor of two, the chalk regions can be defined with one weighted average. For instance, the mean values for the chalk regions for Skrivekridt with 50 or more samples are Falster=1.29, Lolland=0.46, Sjælland=0.49, Himmerland & Djurs=1.41, and Vendsyssel=1.55 (x 10^{-4} m/s). In this case, a weighted average based on a number of observations for Lolland and Sjælland is calculated to be 0.48 x 10^{-4} m/s, and an average value for Falster, Himmerland & Djurs, and Vendsyssel is calculated to be 1.41 x 10^{-4} m/s. This analysis results in 9 different values for the 6 Danish rock types within the 6 Danish chalk regions (geo-provinces) of Sjælland, Lolland, Falster, Fyn, Djurs Himmerland and Vendsyssel. Further details on this simple approach can be seen in Appendix E. This simple analysis does not offer an obvious conclusion on whether it is reasonable to use different values of hydraulic conductivity for the different rock types or chalk regions. Therefore, a more statistical correct approach was applied.

To statistically test if the mean values between the chalk regions and rock types are significantly different, a t-test was used to see (test) if the null hypothesis was true or false (testing if the mean values of two populations are equal/the same). T-tests were performed between all individual chalk regions for the 6 rock types with 50 or more observations but also between the 6 rock types, individually. The results for these t-tests can be studied in detail in Appendix E. The tests revealed that only a few chalk regions for each of the six individual rock types have statistically similar mean values (Skrivekridt: Sjælland-Lolland, Vendsyssel-Himmerland/Djurs, Bryozokalk: Sjælland-Himmerland/Djurs, Himmerland/Djurs-Fyn, København kalk: Sjælland-Himmerland/Djurs). The t-test was also performed between the six rock types where all observations across the chalk regions were combined in the same population (e.g. for all observations of SK, BK, LK, KK, PK and PL). Here, only Kerteminde Mergel - Bryozokalk, and Kerteminde Mergel - Slamkalk have statistically the same mean values (Appendix E). Again, the statistical tests/analysis do not offer an obvious division of chalk units into groups (because some do, and some do not show statistically different mean values).

Because the above analysis does not indicate or show an obvious way to group the chalk aquifers into geographical chalk regions, it is recommended only to divide the Danish chalk aquifers into the six lithological units they are reported by in JUPITER. This acknowledges the geological development of the Danish chalk, but also the large degree of similarity between the rock types and chalk regions regarding hydraulic conductivity (see figure 4.8 and figure 4.9). These different values can be used for guiding the hydrological modelling of chalk aquifers in general. For analyzing the impact of the established range of hydraulic conductivity on solute transport relevant for BNBO, it is important to test the range of values estimated for the Danish carbonate rock types and geological regions. The mean of all carbonate rock samples (n=8300) is 1.35 x 10^{-4} m/s with a 25th and 75th percentile of 0.36 x 10^{-4} m/s and 5.11 x 10^{-4} m/s, respectively. The two percentiles are thus very close to the upper and lower observed mean values for the hydraulic conductivities seen for the different rock types distributed in the geological regions also. Because the 25th and 75th percentile values correspond very well to the estimated range of mean values of the individual chalk types (between 0.33 x 10^{-4} m/s and 3.39 x 10^{-4} m/s), the 25th and 75th percentile values are used to analyze the effects on the transports distance in the conceptual BNBO set up together with the mean value. Furthermore, the mean value of 1.35 x 10^{-4} m/s is very close to the median value (50th percentile) of 1.34 x 10^{-4} m/s for the entire dataset (n=8300). Another argument for using the 25th and 75th percentile (0.36 x 10^{-4} to 5.11 x 10^{-4} m/s) of the entire dataset for further numerical analysis, is that they also correlate very well with the median values for the six rock types (0.80 x 10^{-4} to 3.48 x 10^{-4} m/s, table 4.4). More precisely, the range of median values for the six rock types is well included in the range between the 25th and 75th percentile. This means that by using the 25th and 75th percentiles as end members for the recommended values of hydraulic conductivity for Danish chalk aquifers, the variability between the six overall types of chalk is well represented.

5.2.3 Mass transfer coefficient and Dispersivity

The mass transfer coefficient for Danish carbonate aquifers is investigated in Skrivekridt and Bryozokalk with a mean value of $\beta = 3.5 \times 10^{-3}$ 1/d. The chosen mean value of the mass transfer coefficient is in reasonable agreement with the few but useful studies reported in Bryozokalk and Skrivekridt studies mentioned in Section 4.6.

Dispersion in terms of longitudinal dispersivity, α_L, is given the value of 1 m. Dispersion is a function of the heterogeneity of the aquifer. In a fractured carbonate aquifer, the most important heterogeneity is characterized by the distance between fractures (so-called spacing), horizontally and vertically. Assuming a spacing in the order of 1 – 10 m (can be observed at outcrops, e.g., Stevns Klint) it is estimated that the horizontal dispersivity is in the order of 0.1 m to 1 m.

5.3 Modelling sensitivity of parameters

Before the simulation of solute transport with the recommended parameter values, a sensitivity analysis of relevant parameters for solute transport in a dual-porosity domain are performed. The horizontal hydraulic conductivity, matrix porosity, fracture porosity, longitudinal dispersivity and the mass transfer coefficient are tested with parameter ranges found during the initial literature review. Tested values are shown in Table 5.3.

Table 5.3 Range of parameter values found from the literature review. The values highlighted in yellow are found to be the most representative for Danish conditions.

Abstraction m^3/år	Kh m/s (m/d)	α_L m	β 1/d	n_f	n_m
1,000,000	6.83×10^{-3} (590)	0.01	4.00E-02	0.00016	0.1
500,000	1.00×10^{-3} (86.4)	0.1	3.30E-03	0.00100	0.2
200,000	5.00×10^{-4} (43.2)	1	8.64E-04	0.01000	0.3
50,000	1.00×10^{-4} (8.64)	10	1.00E-05	0.03600	0.4
10,000	5.00×10^{-5} (4.32)				0.51

Highlighted values are kept constant when the other parameters are tested in the one-way sensitivity analysis. The impact of abstraction rates was also tested because advective flow increases as a result of abstraction, especially close to the abstraction well as illustrated in figure 5.3.1

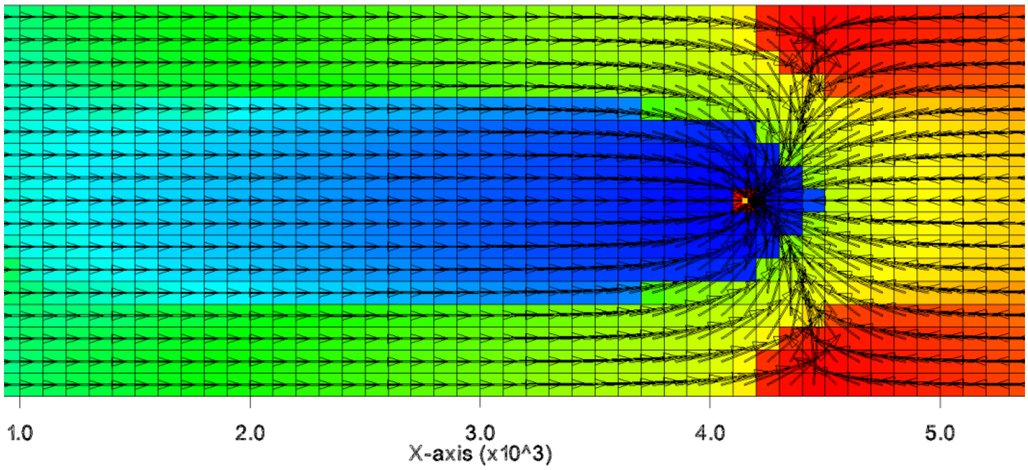


Figure 5.3.1 Conceptual velocity map of flow with flow vectors. Velocity increases from 0.01 m/d (red) to 0.2 m/d (blue) and size and direction of flow vectors (arrows) indicate flow velocity and direction.

The sensitivity of the parameters is tested by estimating the change in travel distance (from spill to well) when a parameter is changed. To find the location of the spill that corresponds to one year of travel time to the well, the location of the spill entry point is adjusted (in the uppermost layer and in the same row as the abstraction well), either closer or further away from the well, to find the distance where the first arrival equals 365 days. The distance varies as a result of different parameter combinations (table 5.3). The distance is constrained by the 10 m discretization, which is the horizontal cell size of the numerical grid and is considered as the horizontal distance between spill point and well. The spill point is estimated iteratively, using several model runs, typically between four and ten, for a given parameter set. For instance, in a situation where the horizontal distance between spill point and well is 210 m, and the first arrival is observed at the well on day 340. Hence, the estimated one-year transport distance is (210m/340d) x 365 d/yr = 224 m/yr. This process is repeated for each set of parameters listed in table 5.3 and result in a sensitivity matrix for abstraction, hydraulic conductivity, matrix and fracture porosities, longitudinal dispersivity and the mass transfer coefficient. Figure 5.3.2. and 5.3.3 illustrate the relative sensitivities of the tested parameters. In figure 5.3.2, the one-way sensitivity tornado diagram, negative values (x-axis) are present because 0 distance (m travel/yr) indicate the starting point of the parameter sensitivity "search", the simulated ranges with the parameters marked in yellow in the above table 5.3. The Tornado diagram (Figure 5.3.2) is strongly asymmetrical, especially for hydraulic conductivity and the mass transfer coefficient because travel distance increase exponentially with increasing values (decrease for the mass transfer coefficient) and because the "starting point" (0m) is much close to the minimum simulated than the maximum simulated distances. Especially for hydraulic conductivity, a high increase in the simulated distance is seen for the highest tested value (compare with figure 5.3.3 for hydraulic conductivity).

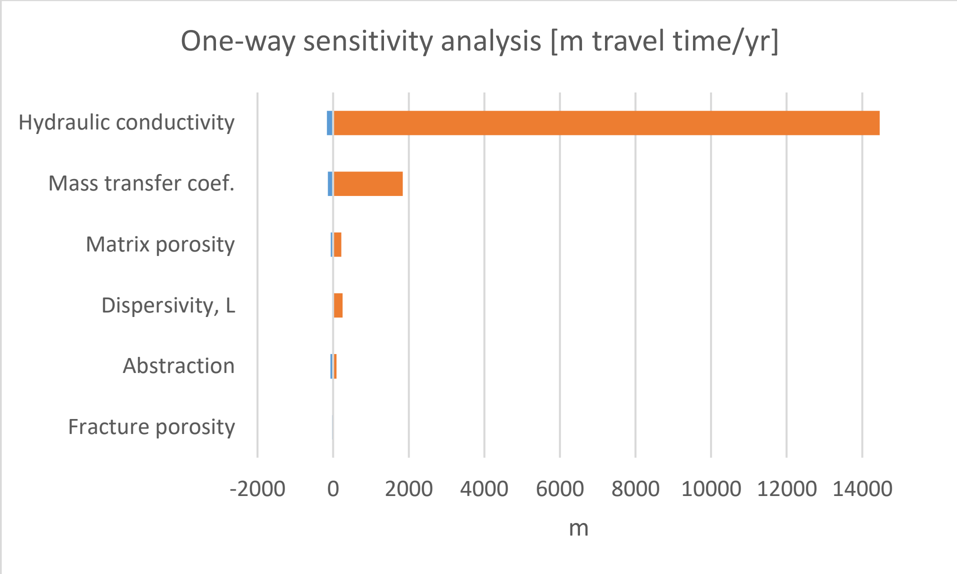
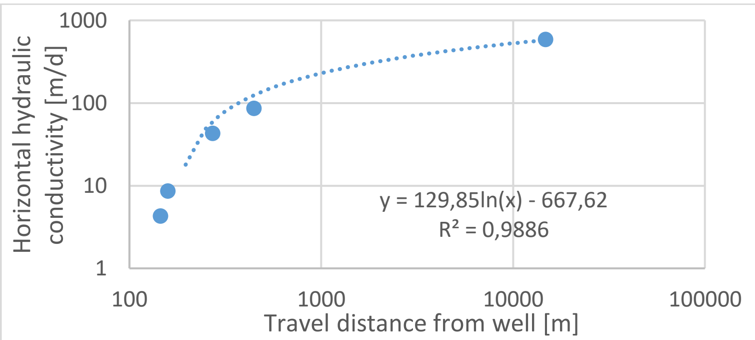


Figure 5.3.2 Overview (tornado diagram) of parameter sensitivities for the prediction of one-year travel distances in the dual-porosity domain conceptual BNBO model. A detailed figure of the impact of parameter values on travel distances can be found in Appendix F. X-axis: 0 m indicate the starting point of the sensitivity analysis (parameters for starting point marked with yellow in table 5.3).

The results of the one-way sensitivity analysis clearly illustrate that the hydraulic conductivity of the aquifer has the highest impact on the one-year travel distance. Figure 5.3.3 elaborates this result with an illustration of all the simulated distances (x-axis) for each tested parameter value (y-axis). The plot for hydraulic conductivity also illustrates that only the very uppermost tested value results in travel distances above 500 m. This high K-value of 6.83 x 10^{-3} m/s results in a travel distance of 14,457 m. The second-highest value, 1 x 10^{-3} m/s have a travel distance of 447 m/yr which indicate a rapidly increasing travel distance with K-values above 10^{-3} m/s.



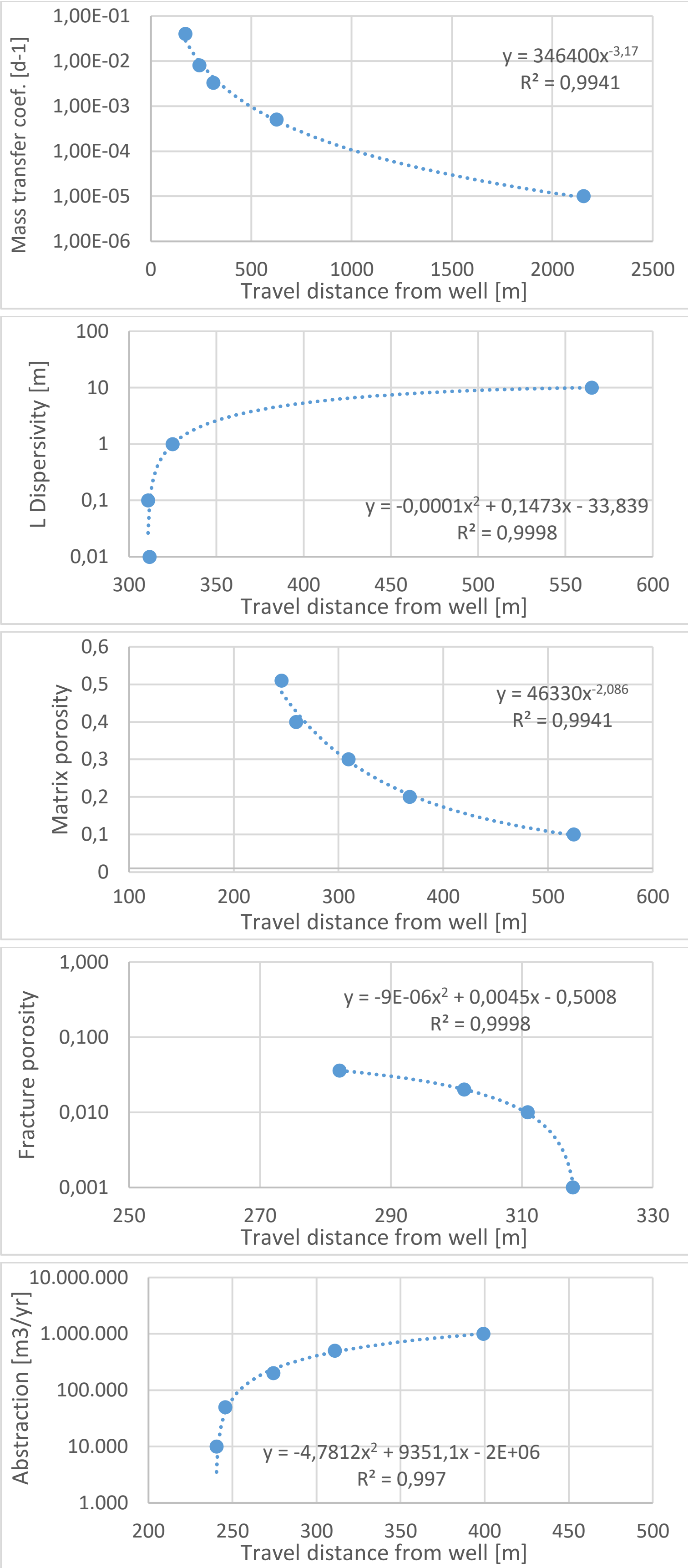


Figure 5.3.3 Simulated one-year travel distances for tested and reasonable parameter ranges found in the literature. Notice the changing x-axis (distance) for the individual parameter (y-axis).

The impact on distance from the mass transfer coefficient is complex. As described in the theory chapter, this parameter determines the rate of exchange of solutes between fracture and matrix. The sensitivity of the parameters is high because, with high values, the solute is quickly removed from the fractures to the matrix and thereby the contaminant plume in the fractures become diluted, thus the first arrival becomes slower and the travel distance shorter. On the other hand, with a very low exchange between matrix and fracture, the fracture concentration is not diluted by solutes diffusing into the matrix and therefore, a high concentration can be maintained in the fracture which leads to a longer travel distance.

The impact of matrix porosity on distance can be understood when considering the matrix porosity as a reservoir for diluting the spill. If the reservoir is large, e.g., the porosity of 0.4 (40 %) or 0.5 (50 %) it has a large potential to dilute the solute concentration in the fracture. Opposite, with a small matrix porosity, the low volume of water in the matrix, has a lower potential to dilute the solute concentration of the fracture. For these processes to occur, a sufficiently large mass transfer coefficient must be specified.

The fracture porosity affects the possible travel distance but in two opposite directions. One process is a result of the advective transport processes where lower fracture porosity results in higher flow velocities and therefore higher travel distances. The other process reduces the travel distance when porosity decreases because the concentration of a solute in a small fracture is more easily lost to the matrix with a small fracture volume. Again, the mass transfer coefficient will affect the exchange between fracture and matrix. The combination of the two processes, working in opposite directions results in the relative and somewhat unexpected small effect of fracture porosity on travel distance.

Based on the sensitivity analysis it can be concluded that all of the parameters can affect the simulated one-year travel distance from spill to abstraction well. Therefore, the review of observed parameters values in section 5.2 becomes important for the evaluation of the one-year travel distance between spill and abstraction.

5.4 Recommended parameters

The analysis and estimation of appropriate parameters found in the scientific literature, reports, thesis and databases are shown by the sensitivity analysis to be very important for simulating solute transport in fractured carbonate rocks. In the following section, the knowledge from the sensitivity analysis will be combined with the parameter values found in the review of typical parameters for Danish carbonate aquifers. The aim is to model the typical parameter values in the conceptual BNBO dual-continuum-models, or double-porosity (DC, DP, defined section 5.1, and figure 5.1.1) and estimate one-year travel distances for these typical parameter values. Secondly, to test if estimated one-year travel distances can be replicated using an equivalent porous medium, EPM (single porosity), model with an effective porosity, in contrast to fracture and matrix porosities as in the DP models. In this way, the results in terms of one-year travel distance from the DP models are considered as the "truth" which the effective porosity of the EP models is calibrated toward. According to the theoretical section, Figure 3.3, the effective porosity is changing continuously from time zero, t=0, where the effective porosity equals the fracture porosity until a certain time and distance after the spill, where the effective porosity equals the porosity of the matrix. Concerning BNBO modelling using EPM models, it is important to know whether the effective porosity reaches the matrix porosity (t-eq.) for the simulated time and distance, or the effective porosity is somewhere in-between fracture and matrix porosity (t-eq. is not reached). This is important to know because if t-eq. is not reached the parametrization of effective porosity only applies under the conditions and with the parameters it was estimated at ($n_f < n_{eff} < n_m$).

Based on the sensitivity analysis and the estimation of recommended parameters, it is very relevant to model the variation of observed hydraulic conductivity on travel distances. The observed variation of hydraulic conductivity of Danish carbonate rocks is described by a mean of 1.35 x 10^{-4} m/s (n=8300), a lower value of 3.60 x 10^{-5} m/s (the 25 percentile) and an upper value of 5.11 x 10^{-4} m/s (the 75th percentile). As described in section 5.2 these values represent the different Danish carbonate rock types in the different regions. An abstraction of 500.000 m^3/yr is used in the BNBO models and a gradient of 0.001 is specified in the aquifer.

Figure 5.4.1 shows the simulation of BNBO distance (one year) with the mean hydraulic conductivity value of 1.35 x 10^{-4} m/s with the dual continuum model.

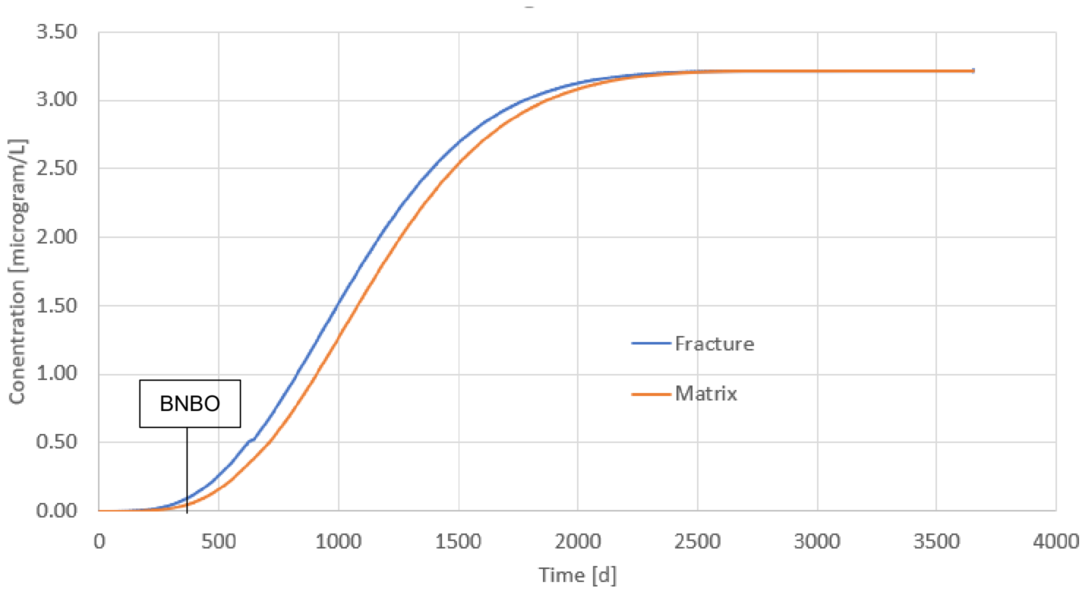


Figure 5.4.1 Breakthrough curve (DP model) at abstraction well simulated until equilibrium conditions between fracture concentration and matrix concentration occurs approximately after 7 years. The total simulation time is 10 yr. n_f=0.8 %, n_m=0.3 %, β=3.5 x 10^{-3} 1/d α_L=1 m. BNBO 365 d timeframe and first arrival is marked with a black box and line.

With a first arrival (conc.= 0.1 µg/L) at 1 yr (365 days) the distance is 180 m from spill to abstraction well. The fracture concentration is higher than the matrix concentration until equilibrium is reached after approximately 7 yrs. The fracture concentration at the abstraction well reaches the first arrival concentrations before the matrix concentrated, as expected. Figure 5.4.2 zooms into the relevant one-year time horizon for the BNBO assessment. Here, the breakthrough curves from the DP model are shown together with the EP model, where the effective porosity was estimated to a value of 13 % to match the first arrival at the DP model with a spill 180 m away from the abstraction well. The breakthrough curves from the EPM model with effective porosity of 12 and 14 % are also shown to illustrate how the timing of the first arrival (conc. = 0.1) changed by tens of days just by changing the effective porosity by 1 %.

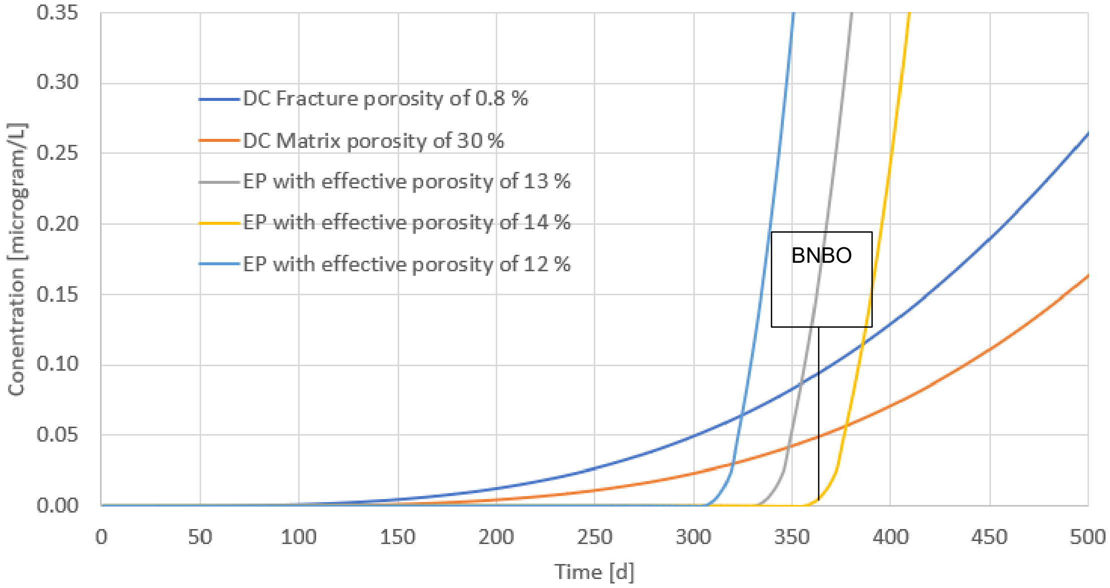


Figure 5.4.2 First arrival at the abstraction well with a concentration of 0.1 µg/L for DP (DC) and EP models (with simulation effective porosity 12-14 %).

The figure illustrates how the first arrival occurs differently with only a slight change in effective porosity. The figure also shows that if a more exact match of the EP to the DP model should be reached, the effective porosity is between 13 and 14 %. Because this estimation of an EP, effective porosity value is only an approximation to the results found in the correct DP model, it is reasonable to estimate the effective porosity as a whole number (integer). Figure 5.4.2 also illustrates the fracture concentration develop (increase) before the concentration in the matrix.

In the same way as an effective porosity of 13 % is found in the EPM to match the DP model first arrival with a distance of 180 meters for hydraulic conductivity of 1.35 x 10^{-4} m/s, effective porosities for the 25th and 75th percentiles values of hydraulic conductivities is also found to match the first arrival in the DP model, in the EPM model. As noted in section 5.2, the 25th and 75th percentiles with values of 3.6 x 10^{-5} m/s, and 5.1 x 10^{-4} m/s, respectively, are near the average values of the carbonate rock types in the regions with the lowest and highest average. The lowest is the Bryozokalk on Lolland with a value of 3.3 x 10^{-5} m/s, and the highest Grønsand on Sjælland with a value of 3.4 x 10^{-4} m/s.

In the DP model, the 25 percentile values of K = 3.6 x 10^{-5} m/s gives a one-year travel distance of 150 m. This is matched with an effective porosity of 17 % in the EPM model. The first arrival curves for the two models can be found in Figure 5.4.3.

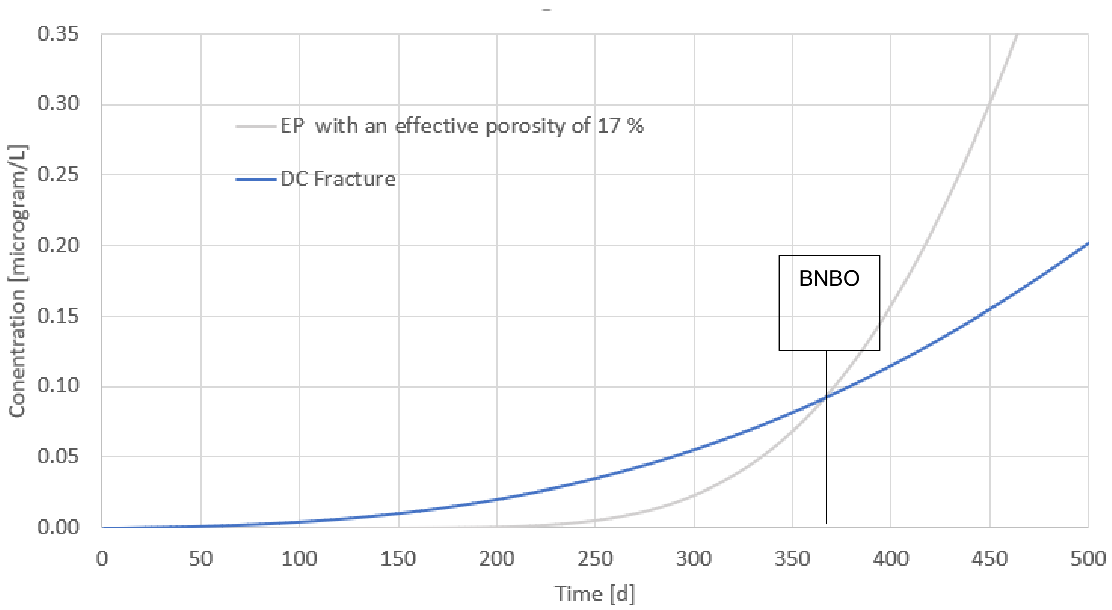


Figure 5.4.3 First arrival simulated in DC (DP) and EP models with 1 yr travel distance of 150 m. Hydraulic conductivity is 3.6 x 10^{-5} m/s in the models.

In the DP model, the 75th percentile equal to K = 5.1 x 10^{-4} m/s yields a one-year travel distance of 310 m. This is matched with an effective porosity of 11 % in the EPM model. The first arrival curves for the two models can be found in Figure 5.4.4.

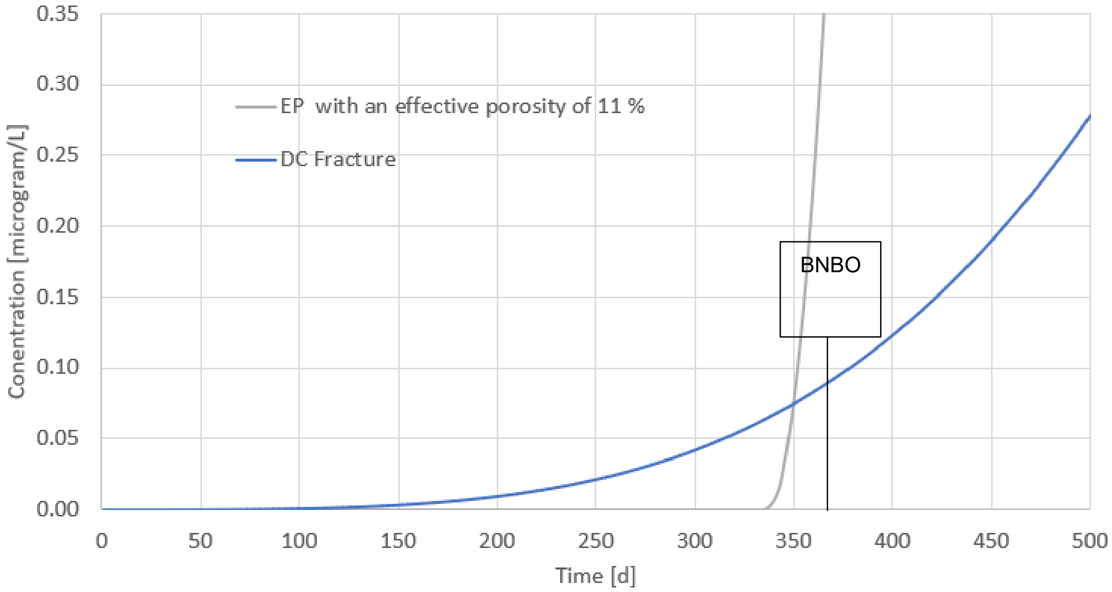


Figure 5.4.4 First arrival simulated in DC (DP) and EP models with 1 yr travel distance of 310 m. Hydraulic conductivity is 5.11 x 10^{-4} m/s in the models.

Comparing the estimated three effective porosities between 11 % and 17 % in Figures 5.4.2, 5.4.3 and 5.4.4 in terms of the development of first arrival concentrations shows that the effective porosity estimate is only reasonable where the breakthrough curves overlap/crosses each other. Furthermore, the shape of the breakthrough curve of the more correct DP models is very different with a slowly increasing concentration at the abstraction well, whereas the EPM model shows a much sharper breakthrough. This has implications for the model results. For instance, in the current model setup, the first arrival is defined as when a concentration of 0.1 µg/L reaches the well. If the first arrival was defined as twice or half this concentration, the time of the first arrival in the EPM model would only be a few days different, whereas, in the DP model the timing would be different by several tens of days.

5.5 Uncertainty estimates of modelling BNBO

The sensitivity analysis, section 5.3, revealed high sensitivity for the hydraulic conductivity of the simulated chalk aquifer, figure 5.3.2. and 5.3.3. An extensive analysis of hydraulic conductivity for Danish chalk aquifers was therefore performed and used to estimate 3 values of effective porosities. The analysis was, for instance, based on more than 9000 observations of K-values in JUPITER, and resulted in a categorizing of the Danish chalk aquifers into a low, a medium (most of the aquifers, table 8.1) and a high value of hydraulic conductivity. The estimation of effective porosity in the EP model was done for these three values and describe the change in effective porosity as a result of different hydraulic conductivities. The sensitivity analyses also showed that besides the hydraulic conductivity, the second most sensitive parameter, by far, is the mass transfer coefficient, β, figure 5.3.2. The remaining tested parameters in the sensitivity analysis had less impact on the simulated one-year travel distance. In the context of an uncertainty evaluation, it is therefore relevant to further investigate the impact on travel distances of the DP models and responding effective porosities in the EP model. Because limited data are available on β it is decided to test values one order of magnitude higher (β=3.5 x 10^{-2} 1/d) and lower (β=3.5 x 10^{-4} 1/d) than the mean value used and recommended (β=3.5 x 10^{-3} 1/d).

The DP model with β=3.5 x 10^{-2} 1/d had a one-year travel distance of 120 m. This is less than the model with the recommended model with β=3.5 x 10^{-3} 1/d which is also expected based on the experience from the sensitivity analysis of the parameter, where travel distance decrease with increasing mass transfer coefficient because the concentration in the fractures are diluted more and therefore the breakthrough is later (or the one-year travel times decreases). Figure 5.5.1 shows the breakthrough curves with the first breakthrough at 1 yr for the dual-porosity and equivalent-porosity models.

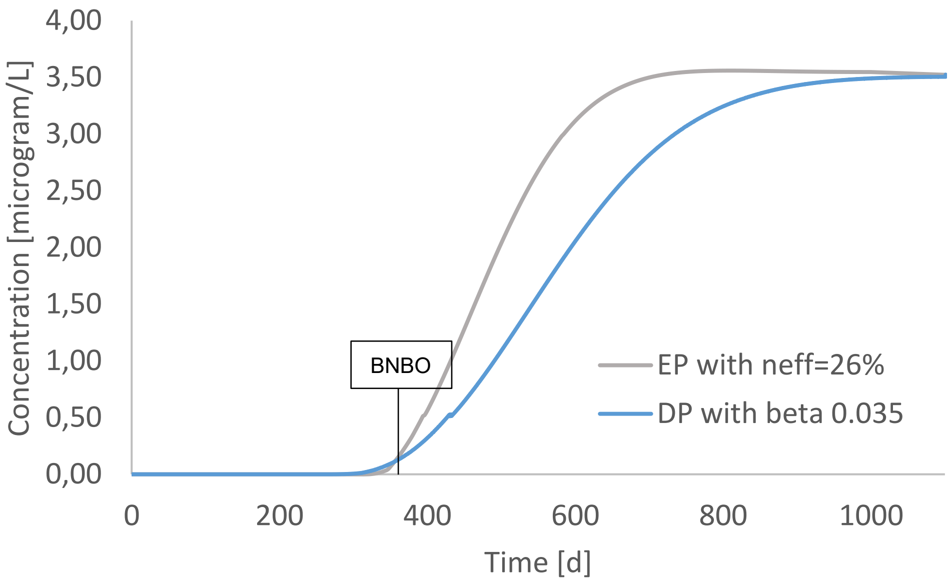


Figure 5.5.1 Breakthrough curves with EP and DP models with an estimated effective porosity of 26 % in the EP model having similar timing (1 yr) as the DP model with parameters: K=1.35 x 10^{-4} m/s, β=3.5 x 10^{-2} 1/d, (DP: nm=30 %,n_f=0.8 %), (EP: n_{eff}=26 %).

The corresponding EP model needs an effective porosity of 26 % close to the matrix porosity of 30 % to simulate the same timing and distance as the DP model with the high mass transfer coefficient (3.5 x 10^{-2} 1/d).

The simulation of the low mass transfer coefficient, resulting in a very slow exchange of solutes between matrix and fractures, enables faster travel and a higher one-year travels distance of 480 m in the fractured dual-porosity chalk domain. To achieve a similar first breakthrough in the EP model, an effective porosity between 3 and 4 % with the first arrival after 324 and 432 days, respectively (figure 5.5.2).

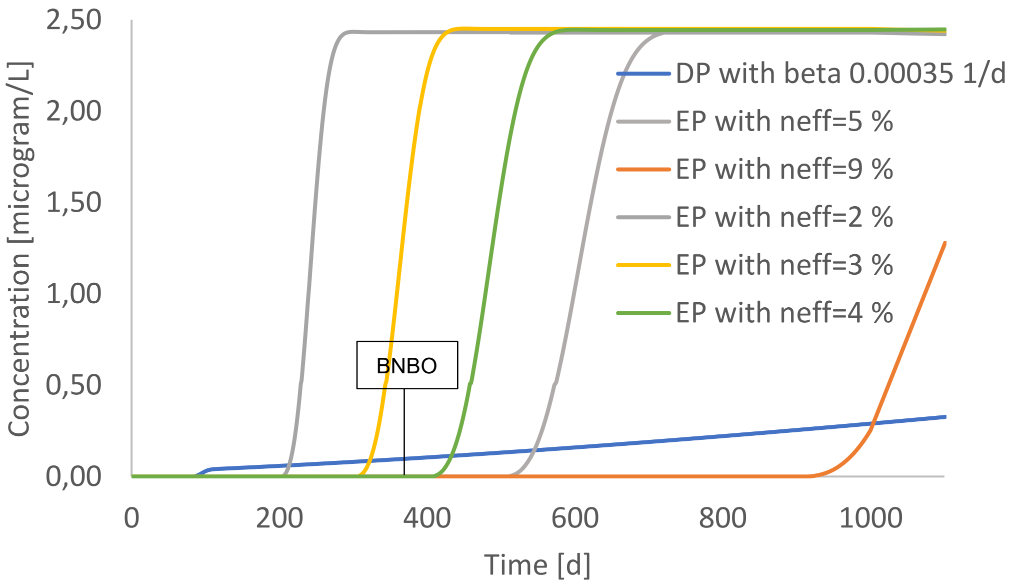


Figure 5.5.2 1 Breakthrough curves with EP and DP models with an estimated effective porosity of 3-4 % in the EP models having similar timing (1 yr) as the DP model with parameters: K=1.35 x 10^{-4} m/s, β=3.5 x 10^{-4} 1/d, (DP: n_m=30 %,n_f=0.8 %), (EP: n_{eff}=9 %, 5 %, 4 %, 3 %, 2 %).

The analysis of the most sensitive parameter next to hydraulic conductivity underlines that the estimation and values of effective porosity are very sensitive to model parametrisation. With a high exchange between matrix and fractures (high β), the front of the pollution plume (first arrival) is diluted because a lot of the solutes escapes to the chalk matrix. The one-year travel distance becomes short. In the opposite situation, with a low exchange (low β), the concentrations in the fractures are only slowly diluted which result in a fast-moving front of the simulated pollution.

5.6 T-equilibrium and implications for longer transport paths (In Danish: Indvindingsområder)

Results from the conceptual BNBO modelling shows that the effective porosity with one year of travel time is somewhere between fracture and matrix porosities with estimated effective porosities of 11, 13, and 17 %, with hydraulic conductivities of 5.11 x 10^{-4}, 1.35 x 10^{-4} and 3.60 x 10^{-5} m/s, respectively. With higher hydraulic conductivity, the effective porosity to match the DP within a one-year travel time is less than in domains with lower hydraulic conductivity. Figure 5.6.1 illustrates results where the EP model (K=1.35 x 10^{-4} m/s) with an effective porosity of 0.3 is the same as the matrix porosity of the DP model. The models show the same breakthrough at approximately 21000 days (58 yr) and the same constant concentration of the models after 31000 days or 85 years.

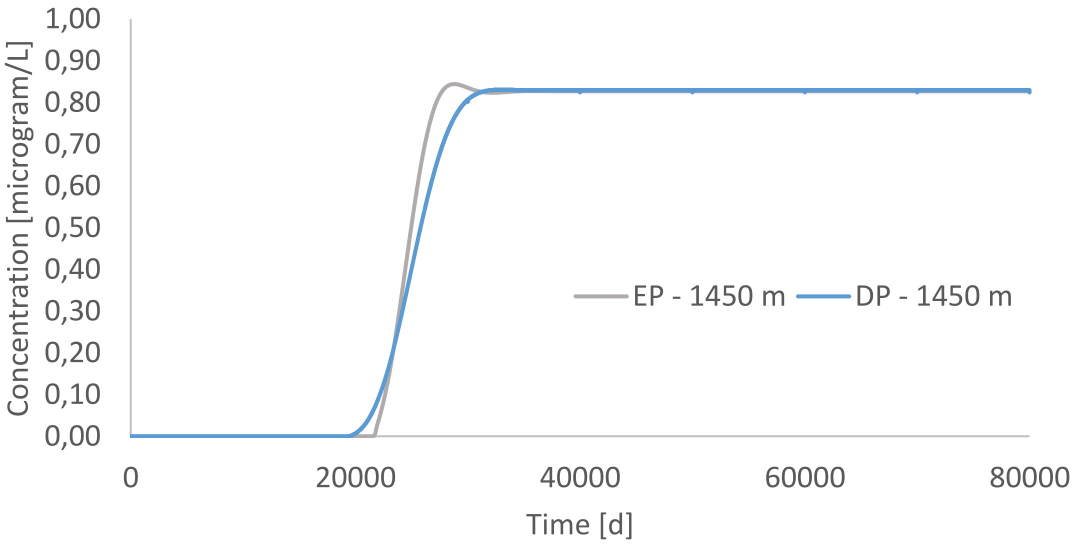


Figure 5.6.1 Breakthrough curves for dual porosity (DP) model (K=1.35 x 10^{-4} m/s, β=3.5 x 10^{-3} 1/d, n_m=30 %,n_f=0.8 %) and equivalent porosity model (EP) with n_{eff}=30 %. Breakthrough is for both models around 21000 days or 58 years. Horizontal distance between spill and abstraction well is 1450 m.

Figure 5.6.1 also illustrate that final equilibrium between models only exists when max. concentrations are reached at the abstraction well 1450 m away from the simulated spill site, after 85 years.

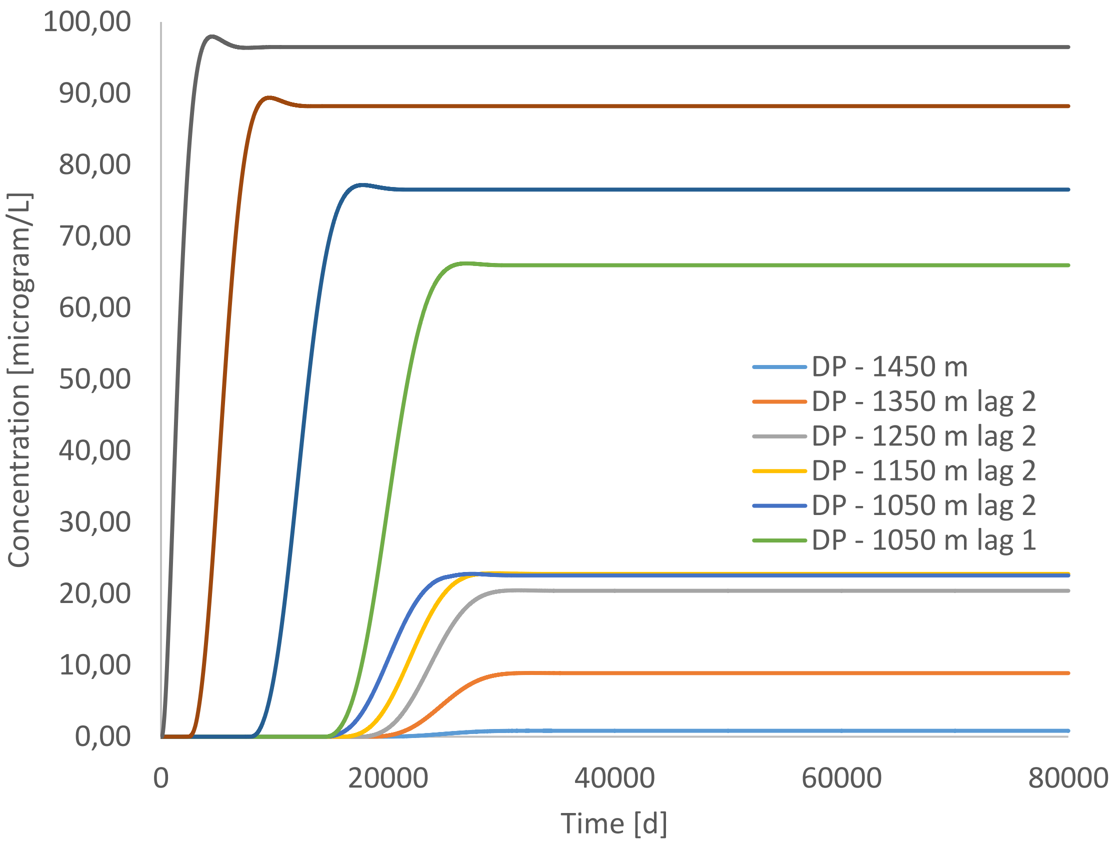


Figure 5.6.2 Breakthrough curves at different distances from the spill simulated with the DP model ($K=1.35 \times 10^{-4}$ m/s, $\beta=3.5 \times 10^{-3}$ 1/d, nm=30 %,n_f=0.8 %, n_{eff}=30 %). DP - 1450 m is the same as shown in figure 5.6.1.

The above figure 5.6.2 show breakthrough curves at different locations between the spill and abstraction well for the DP model also shown in figure 5.6.1. The breakthrough timing and maximum concentrations vary as a result of the distance to the spill.

Figure 5.6.3 investigates the breakthrough after the time/distance where the DP and EP models, with the same matrix or effective porosity, applies but for models with $K=5.11 \times 10^{-4}$ m/s. Because of the increased distance from the spill (a 1000 m longer distance between the spill and well than in figure 5.6.1) the first breakthrough occurs after 115 years and the maximum concentration is reached after 142 years.

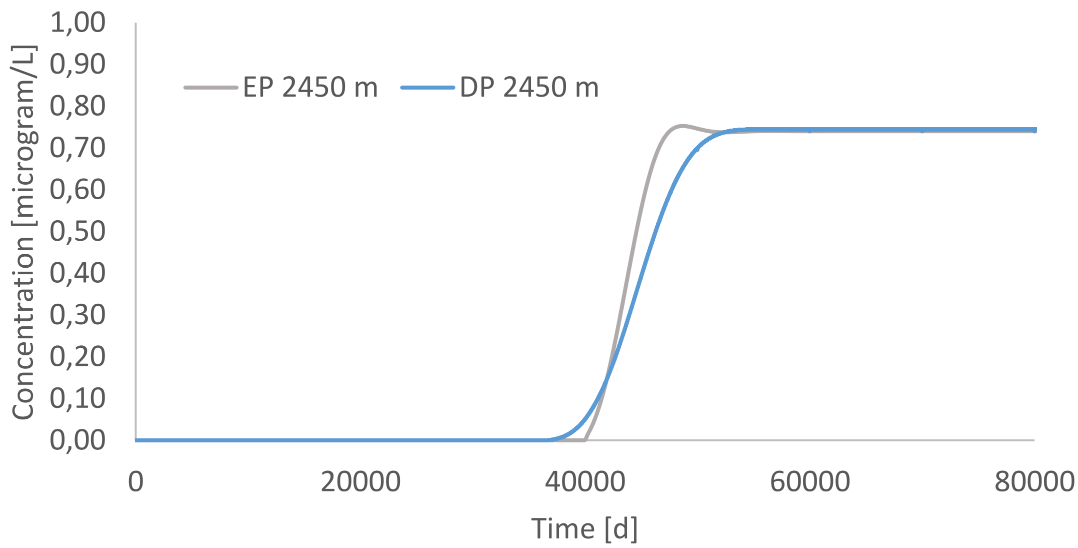


Figure 5.6.3 Breakthrough curves for dual-porosity (DP) model (K=5.11 x 10^{-4} m/s, β=3.5 x 10^{-3} 1/d) with n_f=0.8 % and nm=30 % and equivalent porosity model (EP) with n_{eff}=30 %. Breakthrough is for both models around 42000 days or 115 years and maximum concentration is reached after 52000 days or 142 years. The horizontal distance between spill and abstraction well is 2450 m.

The simulations show that with a substantially longer travel time than relevant in the framework of BNBO (with a one-year perspective) the EP and DP models become alike and T-equilibrium has been reached (after at least 58 years). Nevertheless, this estimation of T-equilibrium only applies for the exact parametrization it is investigated at (K=1.35 x 10^{-4} m/s, β=3.5 x 10^{-3} 1/d, nm=30 %,n_f=0.8 %, n_{eff}=30 %). When parametrization slows the solute transport for instance, with a lower hydraulic conductivity than the above examples, the T-eq distance becomes less the 1450 m.

The above results have implications for solute transport within the temporal and spatial scale of a well-capture zone or catchment. Often, parts of the well-capture zone lie beyond a temporal scale of 60 years and a spatial scale of 1.5 km. On the other hand, average groundwater ages of the abstracted well-water are often younger than 60 years. Especially, when assessing groundwater pollution relevant for solute transport studies, average groundwater ages in the abstraction well is less than 60 yr (e.g. at Bolbro well-field, Odense, where wells with younger groundwater (5-30 yr) show elevate pesticide concentrations (diphenyl cloridazon) and wells in the well-field with older groundwater ages (>50 yr) do not elevate pesticide concentrations.

5.7 Perspectives and recommendations from modelling

The sensitivity of the model parameters revealed hydraulic conductivity as the single most important parameter when estimating a one-year travel distance from a spill site to an abstracting well. It is also evident that increasing hydraulic conductivity will result in a decrease in the effective porosity in an EP model to reach the same one-year travel distance as the DP model. The effective porosity moves toward the fracture porosity when hydraulic conductivity increases and toward matrix porosity when K values decrease. The estimated effective porosities of 11 % (75 % percentile of K-values), 13 % (mean of K-values), and 17 % (25 % percentile of K-values) are all within the part of sensitivity of the parameter, where travel times do not change significantly (from 145 – 272 m, Figure 5.3.3). It is also evident from Figure 5.3.3 that when hydraulic conductivity increases above 10^{-3} m/s (86 m/d), the travel distance increases from less than 500 m to more than 14 km with a hydraulic conductivity of 6.8 x 10^{-3} m/s (590 m/d). Based on the modelling results of the changing effective porosity (from 11 to 17 %) with changing hydraulic conductivities (from 3.60 x 10^{-5} to 5.11 x 10^{-4} m/s) and on the sensitivity analysis showing a rapid increase of one-year travel distance above 10^{-3} m/s, it is not recommended to use the found effective porosities with a known hydraulic conductivity above 10^{-3} m/s. Also, based on the rapidly increasing one-year travel distances with a hydraulic conductivity higher than 10^{-3} m/s, and a high possibility of macro-fracture (enlarged fractures, or channel-flow) above this value, simulation of solute transport in a Darcy-based calculation model is not recommended. The basic assumption for modelling groundwater flow and solute transport based on the flow solution is laminar flow consistency. (Theory chapter 3). If turbulent (not laminar) flow occurs, the physically-based groundwater models (e.g. MIKE SHE, MODFLOW) is not a representation of either groundwater flow nor solute transport process and can therefore not be used to estimate one-year transport distances or BNBO-delineations.

Indication of macro-fractures or channel-flow can be a very high hydraulic conductivity (> 10^{-3} m/s) at the abstraction well, or at specific horizontal intervals of the abstraction well in focus. Most estimates on hydraulic conductivities of abstraction wells are based on average values for the entire open vertical interval of the well, typically 10-30 m in Danish chalk abstraction wells. This means that the hydraulic conductivity is much higher in certain intervals of the abstraction well if groundwater flows are focused in macro fractures (which is often seen in Danish chalk aquifers).

In summary of the above considerations, groundwater models based on the Darcy assumptions cannot be used to calculate BNBO areas if turbulent flows occur. Indication of turbulent flow can be highly focused flow in macro-fractures either directly observed or indicated as high hydraulic conductivities. Furthermore, analysis of modelled 1 yr travel distance (BNBO) shows that with hydraulic conductivities of 10^{-3} m/s and higher, travel distances increase to several kilometres (with K=6.83 x 10^{-3} m/s the 1 yr travel distance is more than 14 km). This will lead to a very elongated and thin area of BNBO. Because of the model's imperfect knowledge of the location of the discrete macro fracture(s), the elongated BNBO will most likely not be placed correct (modelled to have a wrong geographic location).

The estimated effective porosities depend on the exact hydraulic conductivity they are estimated together with. Therefore, the estimated effective porosities should only be applied with these exact hydraulic conductivities when estimating BNBO – areas. In practice, an EP model setup for estimating BNBO should be given the hydraulic conductivity associated with effective porosity, e.g. n_{eff} = 11 % with a K=5.11 x 10^{-4} m/s, n_{eff} = 13 % with a K=1.35 x 10^{-4} m/s, and n_{eff} = 17 % with a K=3.60 x 10^{-5} m/s.

It is recommended that choosing one of the 3 effective porosities with associated K, can be done in two ways:

1) There is no knowledge of macro-fractures or available information on K-values; in this case, the parameters should be assigned according to the chalk type at the intake of the well. The map of the Danish chalk and limestone (carbonate rocks) aquifers, chapter 6, and borehole descriptions in JUPITER can assist this choice. Based on the different analyses of K-values (e.g. table 4.4) Grønsandskalk (PK) should be assigned parameters from the 75th percentile group (n_{eff} = 11 % with a K=5.11 x 10^{-4} m/s), Bryozokalk (BK), Kalksandskalk (KK), Kerteminde Mergel (PL) and Slamkalk (LK) should be assigned parameters from the mean group (n_{eff} = 13 % with a K=1.35 x 10^{-4} m/s), and Skrivekridt (SK) should be assigned parameters from the 25th percentile group (n_{eff} = 17 % with a K=3.60 x 10^{-5} m/s).
2) There is trustworthy knowledge about K-values (K<10^{-3} m/s) and no indication of macro-fractures: in this case, the BNBO estimation model should be assigned the n_{eff} and K-value from the one group (75th percentile, mean, or 25th percentile groups) closets to the site-specific K-value. The site-specific and known K-values should not be used directly in the model but be used to select parameters from one of the 3 parameter groups. If there is more than one known and trustworthy K-value for a model with more than one abstraction well, an average of the known K-values can be used to identify one of the 3 parameter groups. Trustworthy K-values are from hydraulic tests that are well described and documented (e.g. in consultant reports at the given abstraction well).

6. Map of Danish chalk and limestone aquifers

6.1 Method and criteria

This section describes how the lateral extension of the aquifer units consisting of the six chalk and limestone rock types Skrivekridt, Bryozokalk, Kalksandskalk (calcarenit), Slamkalk (calcilutit), Grønsandskalk and Kerteminde Mergel has been delineated on the basis of JUPITER data.

The method used is based on the following selection criteria:

- The lithology with the different types of lime must constitute more than 20% of the intake depth in a chalk and limestone borehole before it is included in the data material
- A hydraulic conductivity must be calculated for each borehole on basis of a T value reported to the JUPITER database by dividing with the screened (open) interval of the well
- Only limestone wells located within the most recent location of chalk and limestone groundwater bodies in Denmark also named GWB2020 (Troldborg, 2020) are included in the present study's delineations of the chalk and limestone rock units

The generic map of Danish chalk and limestone aquifers is shown in figure 6.1 and maps for the individual carbonate rock types are given in figures 6.2-6.7. The following comments are linked to the map:

- A draft version of the map of Danish chalk and limestone aquifers were reviewed by GEUS colleagues experienced in chalk geology. Review comments gave rise to changes in the distribution of two of the chalk and limestone rock types. Examples of this are the distribution of Kerteminde Mergel in Jylland is not included in the shapefile for this part of the country (see Appendix 10.7). It is well known that the rock description of Kerteminde Mergel has caused problems in many cases. Despite quite a few boreholes with Kerteminde Mergel lithology reported in the JUPITER database, especially in the Himmerland area there is no evidence for the large distribution as data indicates. Another example is the distribution of some boreholes with Kalksandskalk lithology in central and southern Sjælland which is not supported by the normal geological view of the distribution of Kalksandskalk in eastern Denmark.
- The distribution of coral chalk in Denmark is quite limited and the rock type is known only from chalk quarries in Faxe and North Jylland (Aggersborg), as well as boreholes in south Sjælland (Næstved) and excavations in the Øresund region. The coral chalk is not considered a groundwater aquifer in Denmark. Therefore, this type of chalk has not received much attention in this study.
- Slamkalk is especially prevalent in central Jylland. It is not widespread in the Pre-Quaternary surface map but is most commonly found in boreholes. The grain size distribution in Slamkalk shows that about half of the rock consists of grain diameters, that are less than 5 μm and the rest in the silt and fine sand fraction. Nevertheless, this chalk rock type shows good hydraulic properties that are comparable to the properties of the other limestone rock types (See Chapter 4).
- There are areas along the margin of the GWB2020 chalk areas where the shapefiles are not drawn all the way to the edge of the GWB2020. This is because no pumping test data has been reported in the JUPITER database from these areas. The lateral extent of the GWB2020 is based in these areas, primarily on the knowledge of chalk and

limestone lithologies in boreholes without transmissivity data and geological data obtained from the latest groundwater mapping by the Danish Environmental Protection Agency.

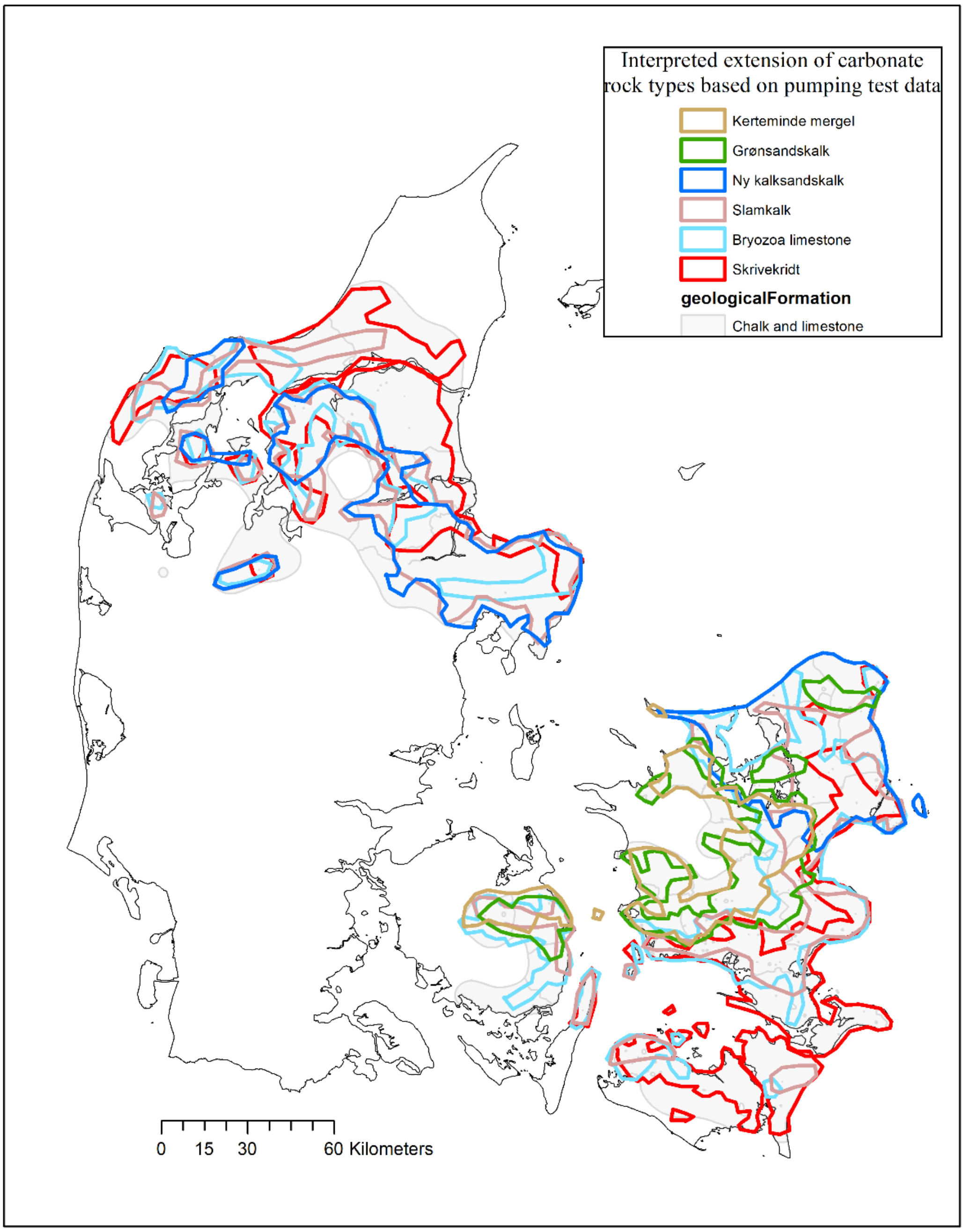


Figure 6.1 Map of the Danish chalk and limestone aquifers on basis of borehole information with transmissivity data (pumping time, capacity and drawdown). The grey polygon indicates the extent of the most recent location of chalk and limestone groundwater bodies in Denmark (GWB2020) (adapted from Troldborg 2020).

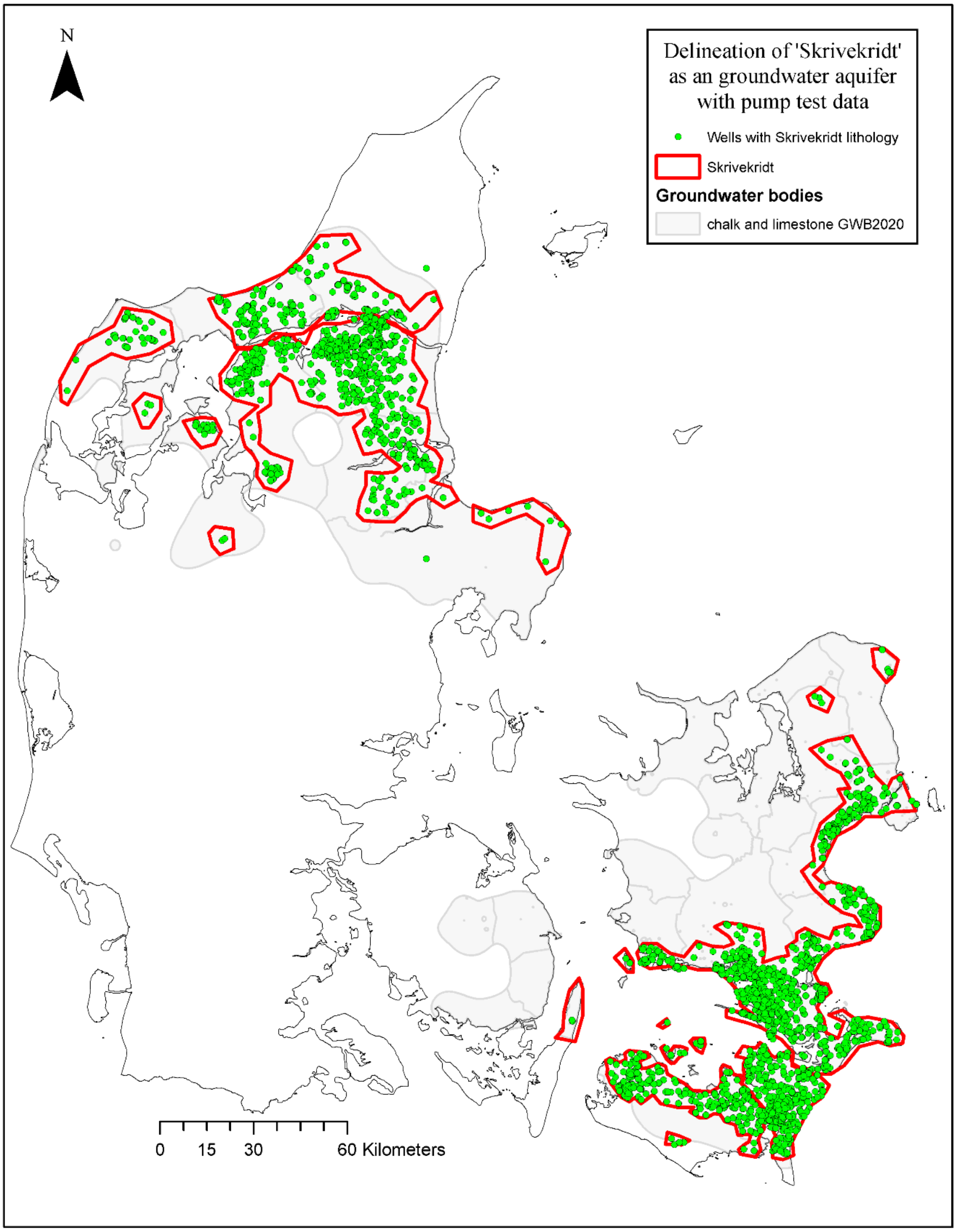


Figure 6.2 Map of the extent of Skrivekridt (red line) at places where pump test data is available (green dots).

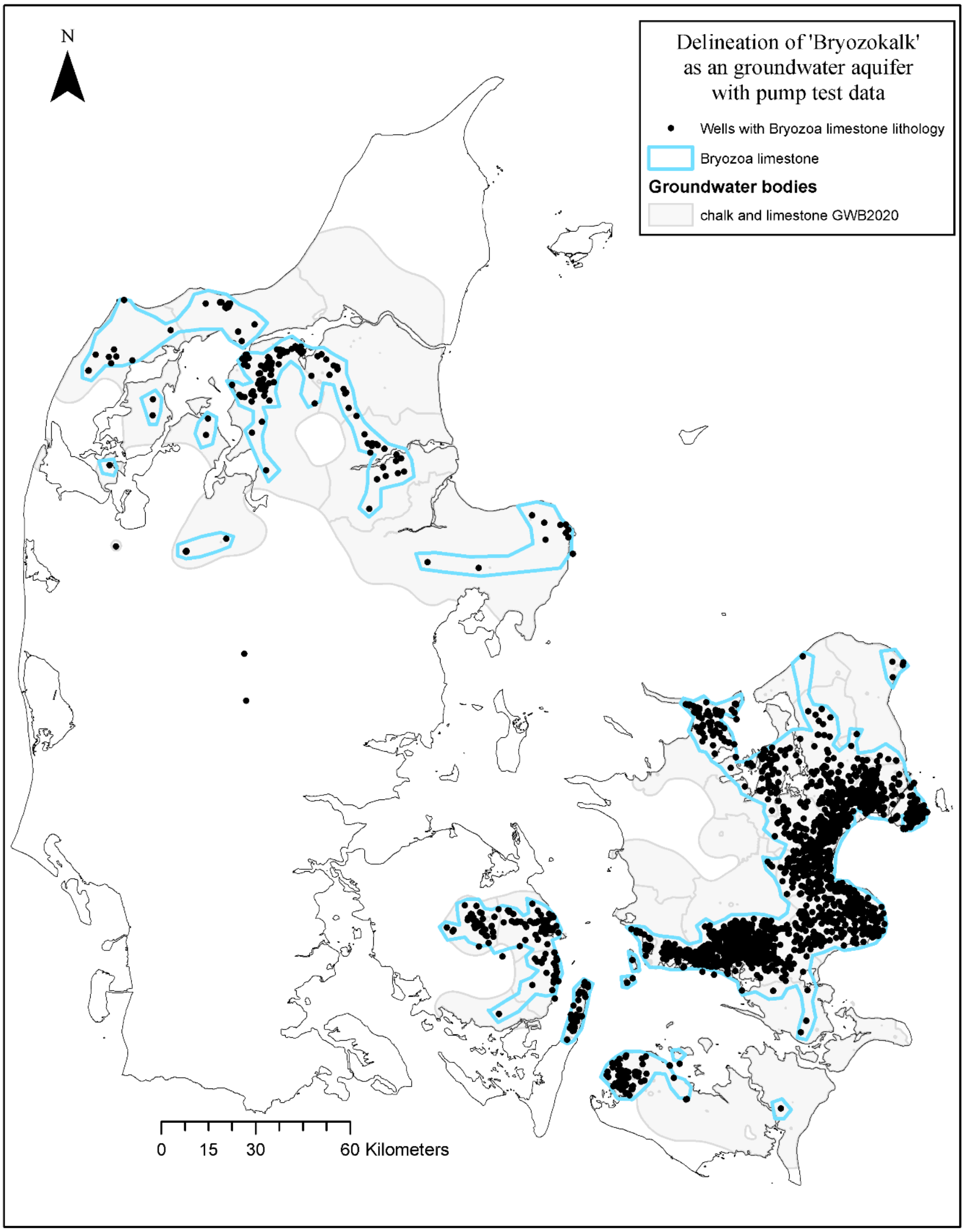


Figure 6.3 Map of the extent of Bryozokalk (light blue line) at places where pump test data is available (black dots).

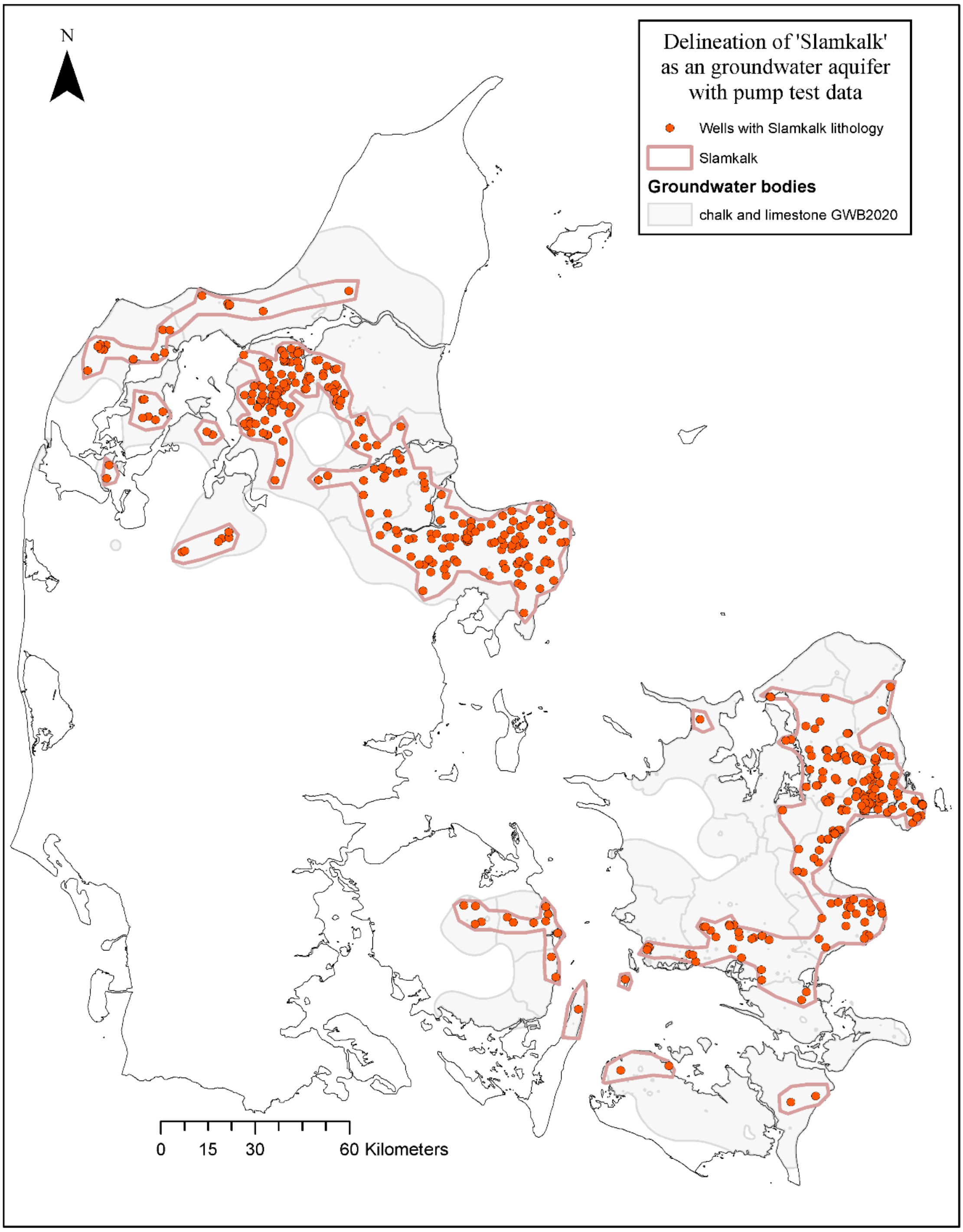


Figure 6.4 Map of the extent of Slamkalk (orange line) at places where pump test data is available (orange dots). Note that the Slamkalk polygon shows the lateral distribution while Slamkalk can occur in more stratigraphic levels in Danian deposits.

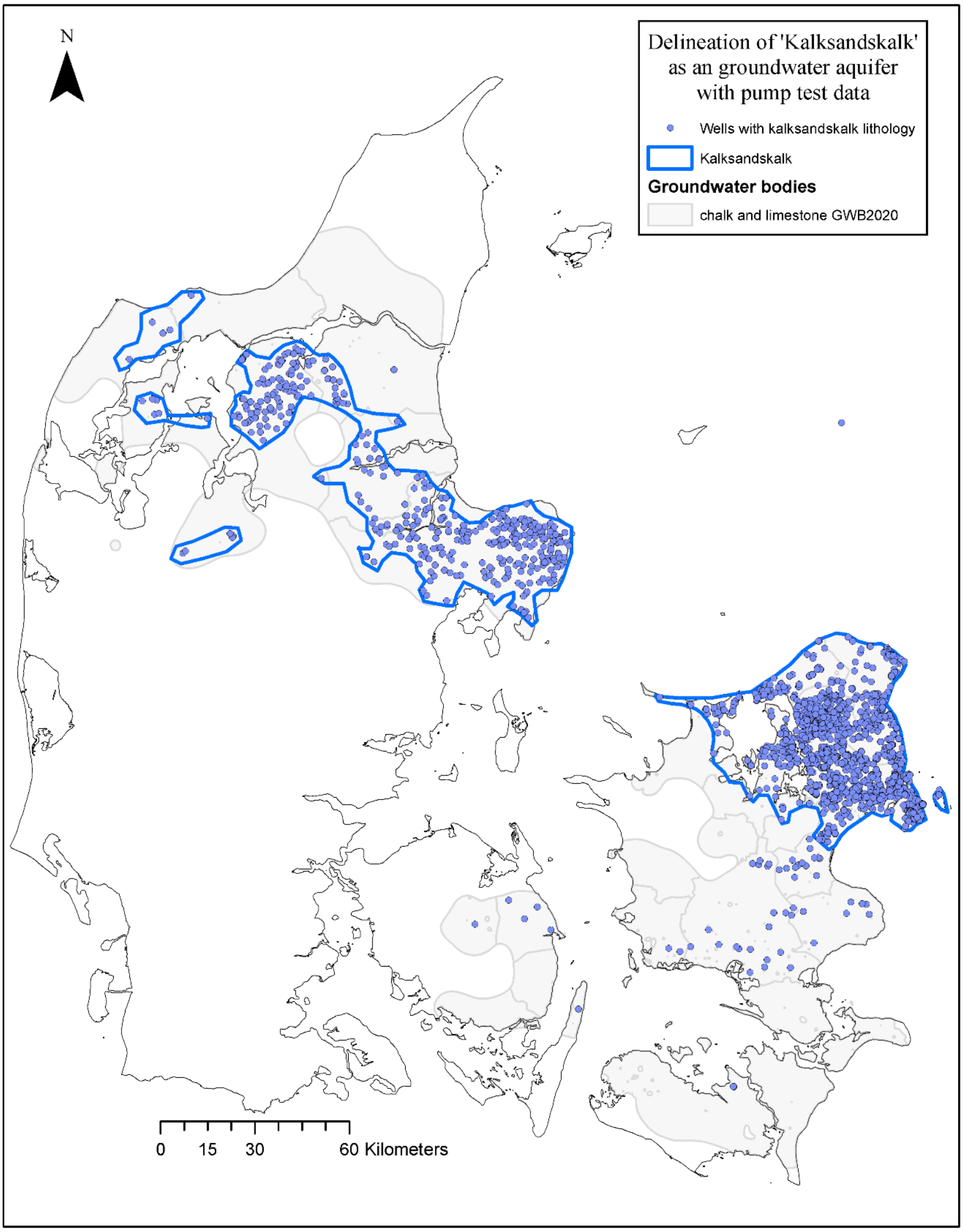


Figure 6.5. Map of the extent of Kalksandskalk (blue line) at places where pump test data is available (blue dots). Note that blue dots in central-south Sjælland and Fyn are considered to be erroneous descriptions of carbonate rock lithology.

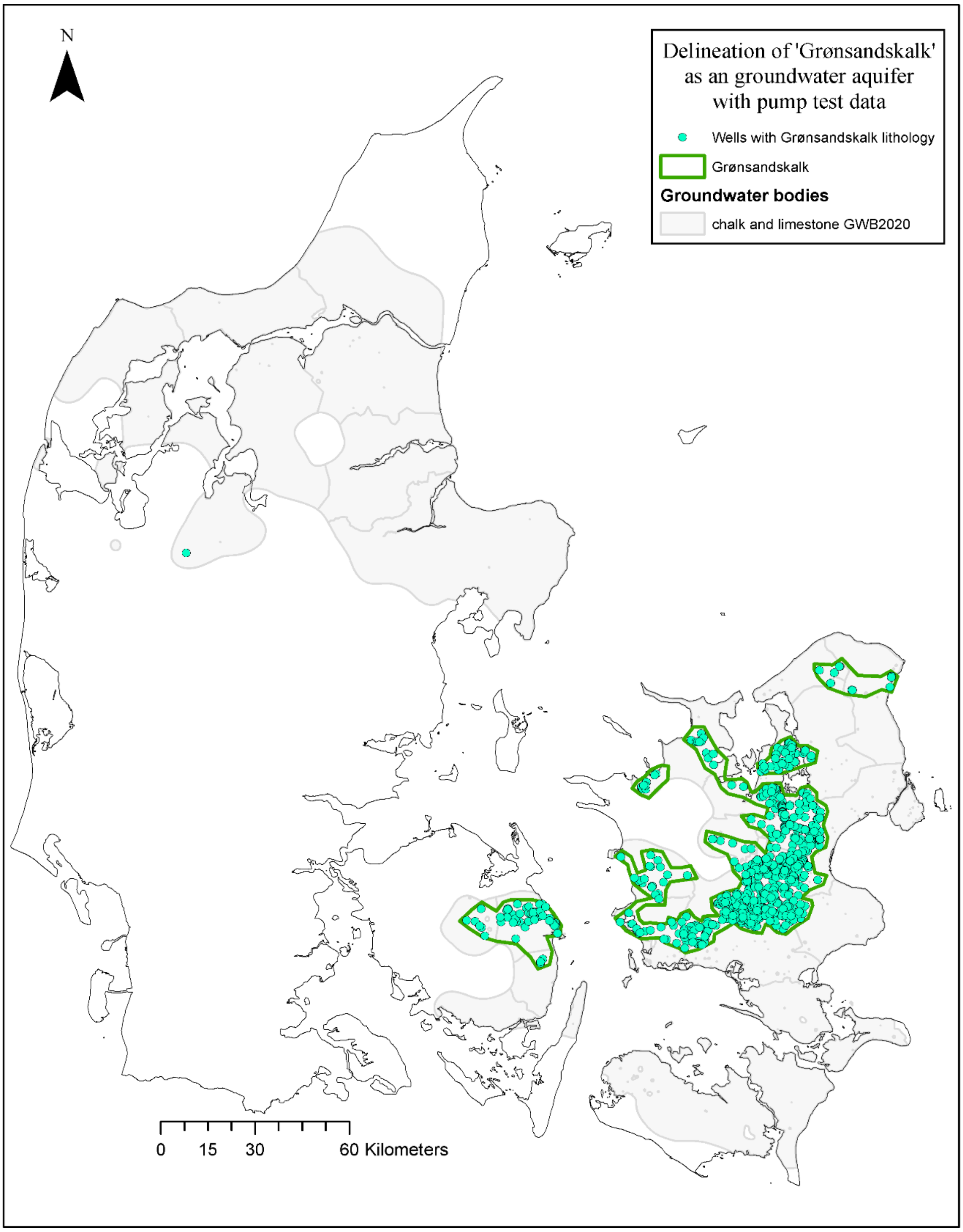


Figure 6.6. Map of the extent of Grønsandskalk (green line) at places where pump test data is available (green dots).

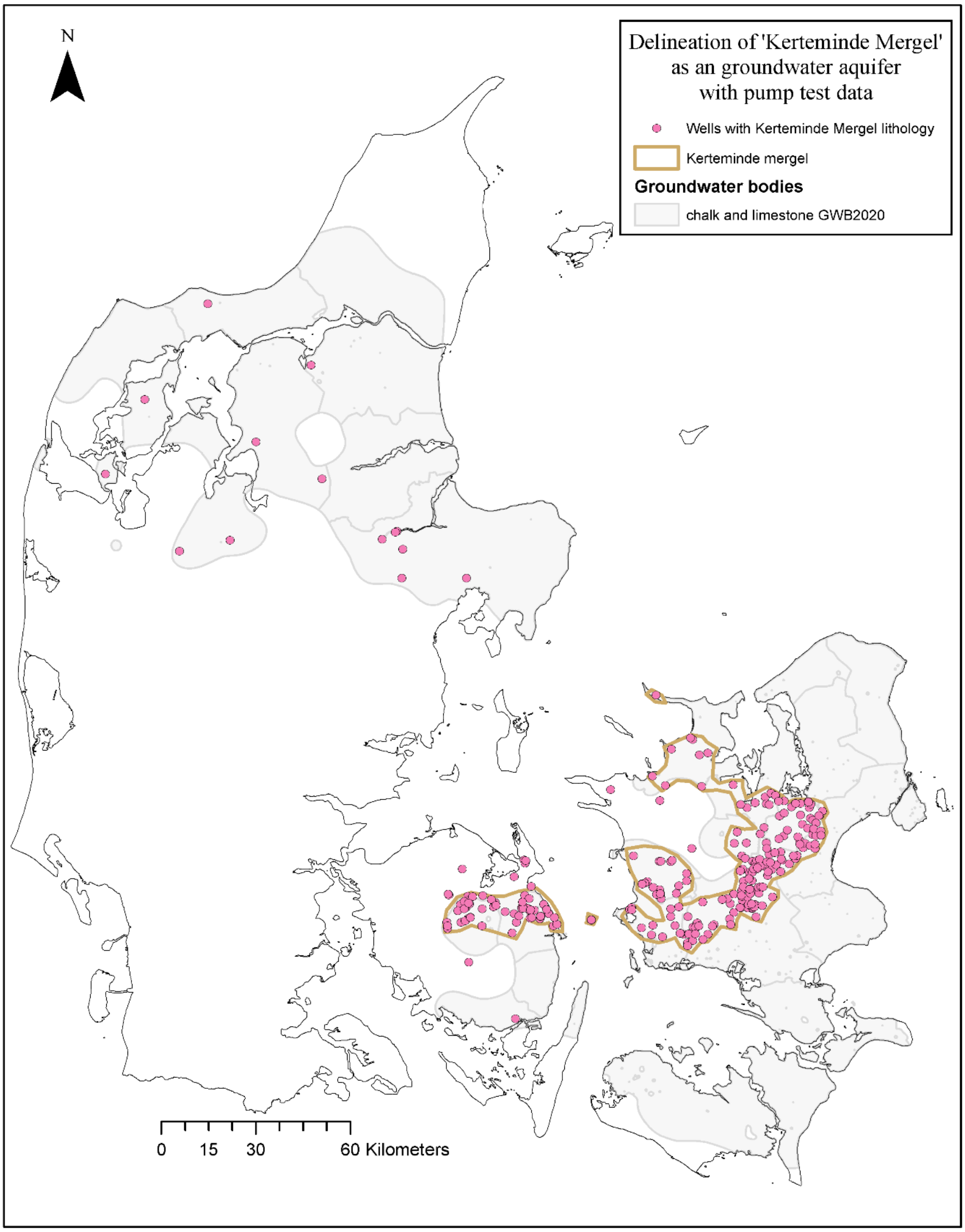


Figure 6.7. Map of the extent of Kerteminde Mergel (brown line) at places where pump test data is available (red dots). Note that boreholes in central and northern Jylland with Kerteminde Mergel lithology are so scattered that it is too uncertain to specify a polygon there.

6.2 Karstification in the Danish chalk and limestone aquifers

Geomorphology and hydrology in karst terrains define the development of characteristic karst features like sinkholes, dolines, karst lakes, karst caves, disappearing streams (Ford and Williams, 2007). Karstic aquifers show some characteristics of dissolution features and physiographic features (Taylor and Greene, 2008) that may favour rapid, turbulent flow from the land surface through subsurface pipe-like voids and conduits that may reach the land surface forming visible springs or less visible wet surfaces near streams. This has implications for groundwater pollution and ecosystem vulnerability in streams (Nilsson and Henriksen, 2021).

Karst hydrogeology has not been studied in Denmark for the last 35-40 years (Bækgaard et al, 1982). However, the latest research from 1982 resulted in an informative hydrogeological map where karstified rocks were outlined, shown simplified in Figure 6.8.

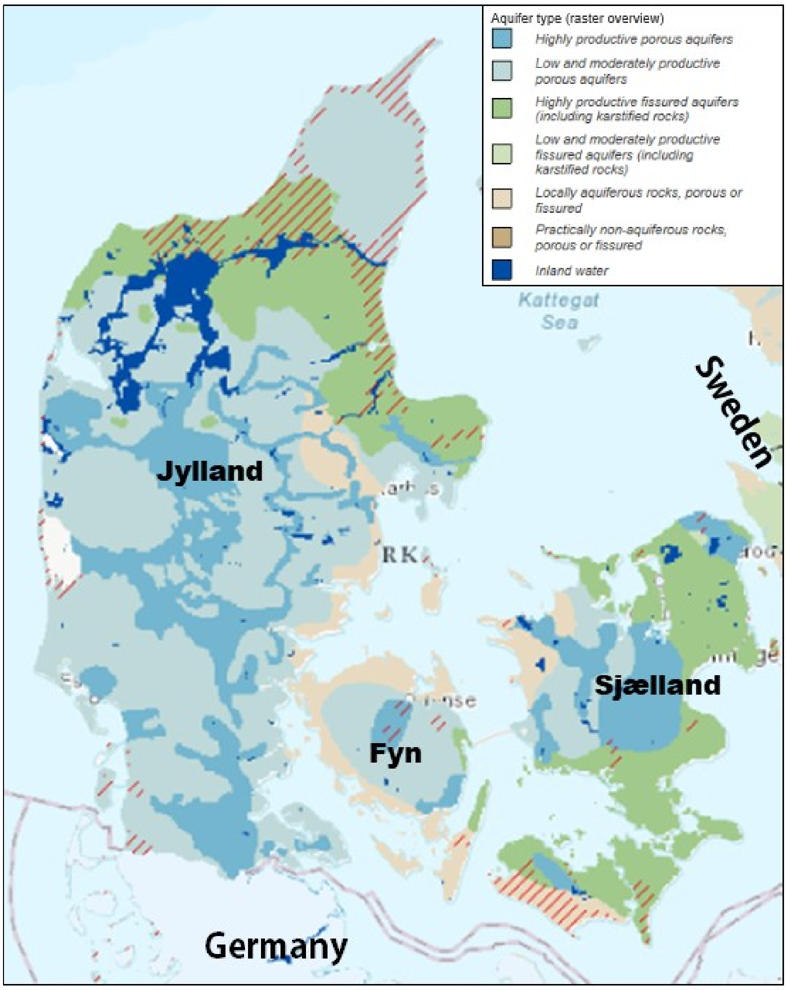


Figure 6.8. Hydrogeological map of Denmark including karstified rocks (BGR, 2015) The map is a screen dump from the German geological survey (see reference for a link to webpage).

Karst landscapes and other karst features in chalk and limestone have been mentioned in the Danish geological literature since the beginning of the 19th century. A thorough literature review by Nilsson and Gravesen (2018) summarizes the findings of karst features and has been supplemented with the most recent findings by citizens that form the basis of the 42 locations shown in Figure 6.9. The karst features can be separated into sinkholes (Danish: jordfaldshuller) that are funnel-shaped (incl. fluviokarst) or vertical-sided dolines (Danish: skorstene), karst-lakes or sinkhole ponds with subsurface outlets, small caves, karst springs and connected losing stream sections to chalk aquifers (here named as disappearing streams). The geographical locations where karst features are found are apparently independent of the underlying carbonate rock type as they occur over both deposits from the

Upper Cretaceous, Danian and Selandian. The locations of karst caves (N=4), karst landscapes (N=3), Sinkholes/Dolines (N=17) and disappearing streams (N=4) occur across the entire country. Karst lakes (N=7) and Karst springs (N=5) is so far only described from localities in the western part of Denmark. There is a reasonably good correlation between the location of the karst features and the thickness of the Quaternary deposits (Nilsson and Gravesen, 2018). The majority of the karst features are located in areas with less than 20-30 meter thickness of Quaternary sediments.

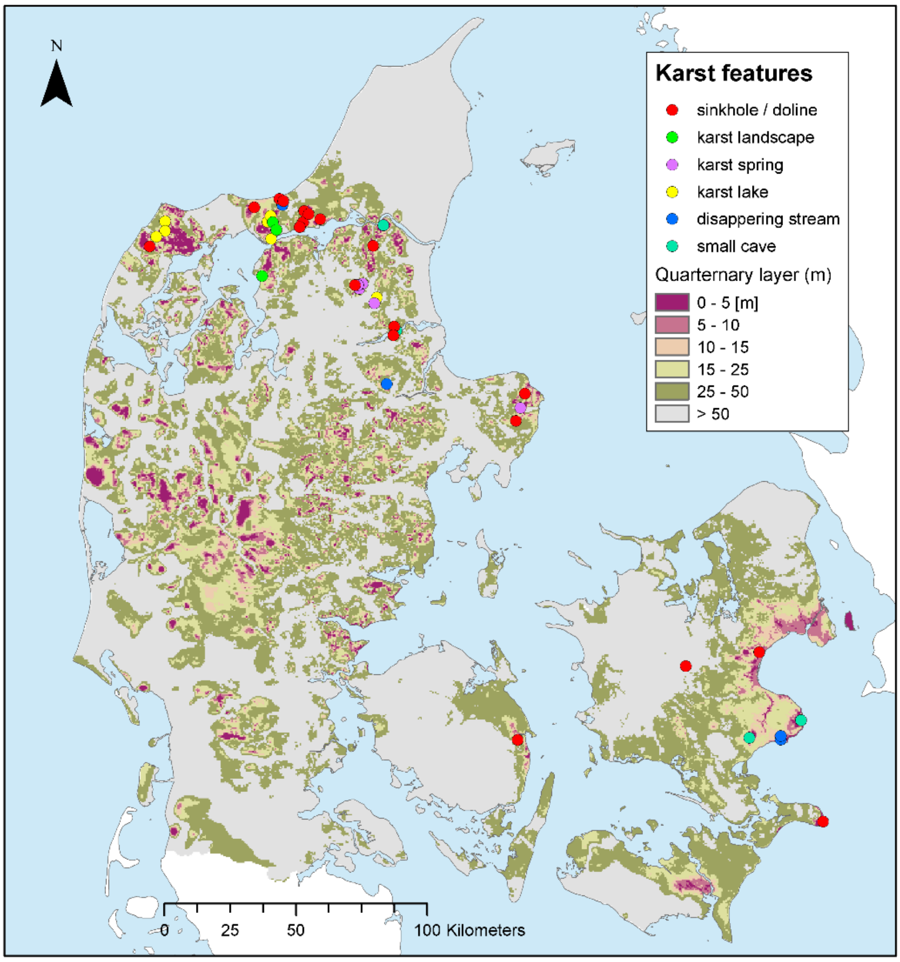


Figure 6.9 Thickness of Quaternary deposits (thickness) and various karst features

In the geographic areas where karst features are registered and high groundwater flow rates are observed from pump tests (Figure 4.10), one must be aware of whether karstic conditions occur in the chalk/limestone aquifers. The distribution will probably be local but can be of great importance for the planning of future water abstraction wells and assessment of pollution risk from the soil surface to the chalk aquifers. Groundwater flow in these areas is very fast and requires modelling assumptions that can describe turbulent flow in the karstified fractures with extraordinary high K values.

7. Test of recommended porosity

The objective of the tests described in the following chapter is to analyze the effect of recommended effective porosities on a real-world case where BNBOs (well protection zones) are to be calculated.

The test is done on one of the hydrological models set up by a consultant during the Danish Groundwater Mapping (Grundvandskortlægningen) and uploaded to the Danish Model database in 2017. The model and wells selected are anonymized and therefore only described in a few details. It is selected based on several criteria, where the most important is that groundwater abstraction occurs in at least one of the known Danish chalk types, also described in JUPITER. Secondly, the model is assessed to produce reliable results during the Danish Groundwater mapping and can therefore be considered a "state of practice" hydrological model. The primary aim of the original model setup and calibration was to estimate the entire capture zones of the abstraction wells. Another advantage of the selected model is that the two included well fields actually represent, in the original calibrated model, hydraulic conductivities in the low end at well field 1 and in the high end at well field 2, compared to what is on average observed for the particular chalk type (Bryozokalk, chapter 4). This is interesting when comparing simulated BNBO (areas) based on the original model parameters of effective porosity (20 %) and hydraulic conductivity, with the same model except for recommended parameters of effective porosity and hydraulic conductivity (Table 1.1 or 8.1).

The applied model is set up in MIKE SHE and covers two well fields, here named Well-field 1 and 2. The well field consists of 8 and 11 individual abstraction wells, respectively.
The analysis is performed on the entire well field instead of on individual wells to achieve a more solid dataset on the average effect of the used parameters to the simulated BNBOs.

Table 7.1 shows results for several different scenarios (different parameterizations) where hydraulic conductivity and effective porosity of the chalk aquifer were altered. The first scenario (from the top of the table) is the parameters of the original model. The next three scenarios (Original model conductivity and 10, 1, and 13 % effective porosity) have the same hydraulic conductivity as the original model but different effective porosities. These scenarios are included because 10 % is the currently recommended effective porosity (MST 2020), 1 % is an example that describes when effective porosity is close to fracture porosity, and 13 % is the recommended porosity for Bryozokalk that well fields 1 and 2 are located in. The last 3 scenarios show results where the hydraulic conductivity is associated with the 3 groups of recommended effective porosities (the three most lower scenarios in Table 7.1). Because the actual chalk type of the aquifer is known to be Bryozokalk, the recommended parameters are an effective porosity of 13 % and a hydraulic conductivity of 1.35 x 10^{-4} m/s (see table 1.1 or 8.1). The Area column of Table 7.1 describes the total areas around all the wells and BNBO areas, where travel times for the groundwater entering the abstraction well are less or up to one year. The increase in area in % is calculated as the difference relative to the area calculated with the model using the original parameters for hydraulic conductivity and effective porosity.

Table 7.1 Calculated BNBO areas for Well-field 1 and 2

Hydraulic conductivity	Effective porosity	Well-field	Area in m^2	Increase of area in %
Original model	20 % - (Original)	1	363747	0
		2	562740	0
Original model	10%	1	557180	53
		2	887590	58
Original model	1%	1	3059405	741
		2	4231807	652
Original model	13%	1	454954	25
		2	774739	38
Recommended 5.11×10^{-4} m/s	11%	1	626477	72
		2	851598	51
Recommended 3.60×10^{-5} m/s	17%	1	339959	-7
		2	356351	-37
Recommended 1.35×10^{-4} m/s	13%	1	453073	25
		2	529946	-6

One important consideration when interpreting the results is that the applied model is not designed to simulate the areas closely around the abstractions wells with any specific precision. The model is set up to simulate the entire hydrological catchment where the two well fields are located. An example of this is the calibration of the model. The model is calibrated against observations of hydraulic heads distributed equally across the entire geographical area of the model. This means that no specific focus has been put on simulating the area close to the wells with any particularly high precision. The hydraulic conductivities found in the model are therefore not, in particular, a result of hydrogeological conditions, close to the well (BNBO) but are parameters that fit the observation across the entire model domain. In this case, the found (calibrated) hydraulic parameters can deviate significantly from what would be found in investigations with a more near-well focus. Therefore, the parameters found by previous model calibrations cannot be expected to be similar to near well observations of the same parameter.

The results from the different scenarios clearly show that changing the parameters has a notable impact on the simulation of the BNBO area (defined as the area within which groundwater travels less or up to one year from the well capture zone to entering an abstraction well). Generally, when porosity decreases, the predicted BNBO area increases. This can most clearly be seen from the top 4 scenarios using the original model's defined hydraulic conductivity where only the effective porosity is changed.

The reason that the two well fields do not respond similarly to the original model with an effective porosity of 20 % is that the hydraulic conductivity of the aquifer was spatially distributed and generally significantly higher, more than a factor 10, around well field 2 than at well field 1. Therefore, the BNBO area actually decreases for the well field both with hydraulic conductivities in the low and middle group (the two bottom scenarios in table 7.1), whereas, it only decreases at well field 1 in with the lowest of the recommended hydraulic conductivities.

The “real-world” case described in this chapter shows that the proposed effective porosities and associated hydraulic conductivities result in modelled BNBO areas similar to predictions with the original model parameters (between 72 % larger and 25 % smaller than simulated with the original model parameters). The latest recommendations (MST 2020) using an effective porosity of 10 % result in 53 and 56 % increase in simulated BNBO areas compared to the original model predictions.

8. Conclusion

The Danish chalk aquifers consist of fractures that are surrounded by a matrix. The literature and data show low hydraulic conductivities for the matrix below 10^{-6} m/s. To support groundwater abstraction, e.g., to drinking water, industry, and agriculture, groundwater flow occurs in the fractures of the chalk, with solute transport controlled by fracture-matrix diffusive interaction. The Danish borehole database, JUPITER, was analyzed for boreholes screened in one of the Danish carbonate (chalk) rock types, and for transmissivity values from hydraulic pump tests. The location of the boreholes with the different chalk types were used to develop a map of the areal distribution of the Danish chalk (Skrivekridt, Bryozokalk, Kalksandskalk [København Kalk], Slamkalk, Grønsandskalk, and Kerteminde mergel). The transmissivity values (n>9100) were used to calculate hydraulic conductivities for the different chalk types and regions across Denmark. The mean value (arithmetic) of hydraulic conductivity for the different chalk types and regions only varied between 0.33 and 3.39 x 10^{-4} m/s and the median values were between 0.80 and 3.48 x 10^{-4} m/s. Statistically, it was tested, if the different types of chalk and regions were significantly different from each other when compared. The results of these tests were inconclusive because some tests showed no difference between the means, although the majority of tests showed a statistical difference between the mean hydraulic conductivities.

Based on the available data for the porosity of the Danish carbonate rocks it is recommended to use a value for fracture porosity of 0.8 % for simulating solute transport with a double porosity model within the framework of near zone wellhead protection zones (BNBO). The typical observed range in fracture porosity is between 0.1 and 1.6 %. Observations of matrix porosities for Skrivekridt, Bryozokalk and Kalksandskalk have average values of 38, 26, and 25 %. Based on the number of observations, a weighted average of 30 % is found for the matrix porosity for Danish chalk aquifers.

The modelling study clearly showed that hydraulic conductivity is the single most sensitive parameter for modelling correct BNBO zone delineation, e.g., based on an administrative defined one-year travel time distances. Based on the review of hydraulic conductivities, 4 out of 6 Danish chalk aquifer types are found to belong to a group with intermediate hydraulic conductivities of 1.35 x 10^{-4} m/s (the mean hydraulic conductivity and 50^{th} percentile of all Danish chalk aquifers based on 8300 observations). The four chalk types belonging to this group are Bryozokalk, Kalksandskalk, Slamkalk and Kerteminde mergel. The chalk type Skrivekridt has a slightly lower hydraulic conductivity of 3.60 x 10^{-5} m/s (corresponding approximately to the 25 % percentile value of all observations). The Grønsandskalk has a slightly higher hydraulic conductivity of 5.11 x 10^{-4} m/s (corresponding approximately to the 75 % percentile value of all observations). The table of recommended parameters for BNBO modelling is therefore grouped into these three categories (main groups), see below Table 8.1.

Within the spatial and temporal scale (one-year) of simulating BNBO, the modelling study clearly showed that t-eq. (t-equilibrium) is not reached. With a hydraulic conductivity of 1.35 x 10^{-4} m/s (the intermediate value), t-eq. has been evaluated to be reached after approximately 1450 m and 85 years. Hence, within the framework of BNBO modelling, the effective porosity varies from fracture porosity (~0.8 %) to matrix porosity (~30 %).

Table 8.1 Recommended parameters for BNBO modelling:

Rock type and region	K	n_f	n_m	n_{eff}	t_{eq}.*	β
Unit	m/s	%	%	%		1/d
Skrivekridt	3.60×10^{-5} (3 m/d)	0.8	30	17	t-eq. not reached, $t\text{-}L_{BNBO} < t_{eq}$	3.5×10^{-3}
Bryozokalk Kalksandskalk Slamkalk Kerteminde mergel	1.35×10^{-4} (12 m/d)	0.8	30	13	t-eq. not reached, $t\text{-}L_{BNBO} < t_{eq}$	3.5×10^{-3}
Grønsand	5.11×10^{-4} (44 m/d)	0.8	30	11	t-eq. not reached, $t\text{-}L_{BNBO} < t_{eq}$	3.5×10^{-3}

**t-L_{BNBO}: time and Length used for BNBO, t-L_{BNBO}<t_{eq} means that t-equilibrium is not reached.*

The effective porosity is highly sensitive to the selected parameterization of the model because the temporal-spatial domain of one-year solute travel in a groundwater abstraction near-zone domain, generally are too short time and distance-wise, to reach solute equilibrium between matrix and fractures. In practice, the recommended effective porosities should only be applied with the same model parameters and solute transport conceptualization by which they were assessed (e.g., K-value, n_f, n_m, β, hydraulic gradient).

Furthermore, it is important to emphasize that the prerequisite for simulation in, respectively, double, and single porous media is the assumption of laminar flow. Laminar flow is typically not present in macro-fractures affected by abstraction, where turbulent flow conditions close to the well exist. For abstraction wells with the indication of macro-fracture flow or channel flow (e.g. with high observed hydraulic conductivities), or direct evidence (e.g. video-logs) of macro-fracture flow, the use of equivalent-porous modelling with an effective hydraulic conductivity is not recommended. Therefore, estimation of BNBO for wells with hydraulic conductivities higher than 10^{-3} m/s (86 m/d) is not recommended. For some areas in Denmark, the karstification of the chalk has been observed. Karstification can indicate flow in macro-fractures (channel flow).

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Appendixes

9.1 Appendix A Theory

In the following, a short description of solute transport in porous and fractured mediums is presented.

Solute transport in a single porosity medium

Two-dimensional, conservative, solute transport in porous media may be described by the advection-dispersion equation:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - \frac{q_i}{n}\frac{\partial c}{\partial x_i} \quad , i,j = 1,2 \tag{A1}$$

where c is the concentration of solute [kg/m^3] and D_{ij} is the dispersion coefficient [m^2/s], which describes the effect of both mechanical dispersion and diffusion

$$\begin{aligned} D_{11} &= (\alpha_L - \alpha_T)\frac{v_1^2}{|v|} + \alpha_T|v| + D_{eff} \\ D_{22} &= (\alpha_L - \alpha_T)\frac{v_2^2}{|v|} + \alpha_T|v| + D_{eff} \\ D_{12} &= D_{21} = (\alpha_L - \alpha_T)\frac{v_1 v_2}{|v|} \\ |v| &= \sqrt{v_x^2 + v_z^2} \end{aligned} \tag{A2}$$

where α_L and α_T are the longitudinal and the transverse dispersivities [m], respectively, and v_i is the pore water velocity given by

$$v_i = \frac{q_i}{n} \tag{A3}$$

D_{eff} is the effective diffusion coefficient that can be described as (ref.)

$$D_{eff} = D_d \tau^2 \tag{A4}$$

where D_d is the free solution diffusion coefficient [m^2/s] and τ is the tortuosity of the sediment. The tortuosity is often approximated as $\tau^2 \approx n$.

In a two-dimensional model, the fractures are represented as one-dimensional elements. Hence, the equation governing solute transport in the fractures may be described as

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial \ell}\left(D_f \frac{\partial c}{\partial \ell}\right) - q_f \frac{\partial c}{\partial \ell} \tag{A5}$$

where ℓ is the distance along the fracture, D_f is the fracture dispersion coefficient [m^2/s], and q_f is the Darcy flux through the fracture [m/s].

Solute transport in a dual-porosity medium

Two-dimensional, conservative solute transport in a dual-porosity medium is described by a transport equation for each domain. The equation describing transport in the fracture zone is given by (ref.)

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial c}{\partial x_j}\right) - v_i \frac{\partial c}{\partial x_i} - \frac{\beta}{n_f}\left(c - c_m\right) = 0 \quad ; \quad i, j = 1,2 \tag{A6}$$

where c_m is the concentration in the immobile matrix zone [kg/m^3], n_f is the porosity of the mobile fracture zone [1], and β is the mass transfer coefficient between the two domains [s^{-1}]. The mass transfer coefficient controls the exchange of solute between the fracture and the matrix domains, together with the concentration gradient between the two zones. The governing transport equation for the matrix domain is given by (Sudicky, 1998)

$$\frac{\partial c_m}{\partial t} = \frac{\beta}{n_m}\left(c - c_m\right) \tag{A7}$$

where n_m is the matrix porosity [1]. From (11) it is seen that the increase in concentration in the matrix zone is proportional to the difference in concentration between the two zones. It is also noticed that the transport equation for the fractures, Eq. (A6), is reduced to the single porosity description, Eq. (A1) if the mass transfer coefficient is set to zero, and the total porosity, *n*, is used to define the velocity, *v*. It should be noticed that the exchange of solutes between the matrix and the fracture domains will result in an enhanced spreading of solute and this process may be described using a higher dispersivity in an EPM model.

Parameterization

Fractured formations are often conceptualized as a system of either parallel fractures or a systems of orthogonal sets of fractures, see Figure A1.

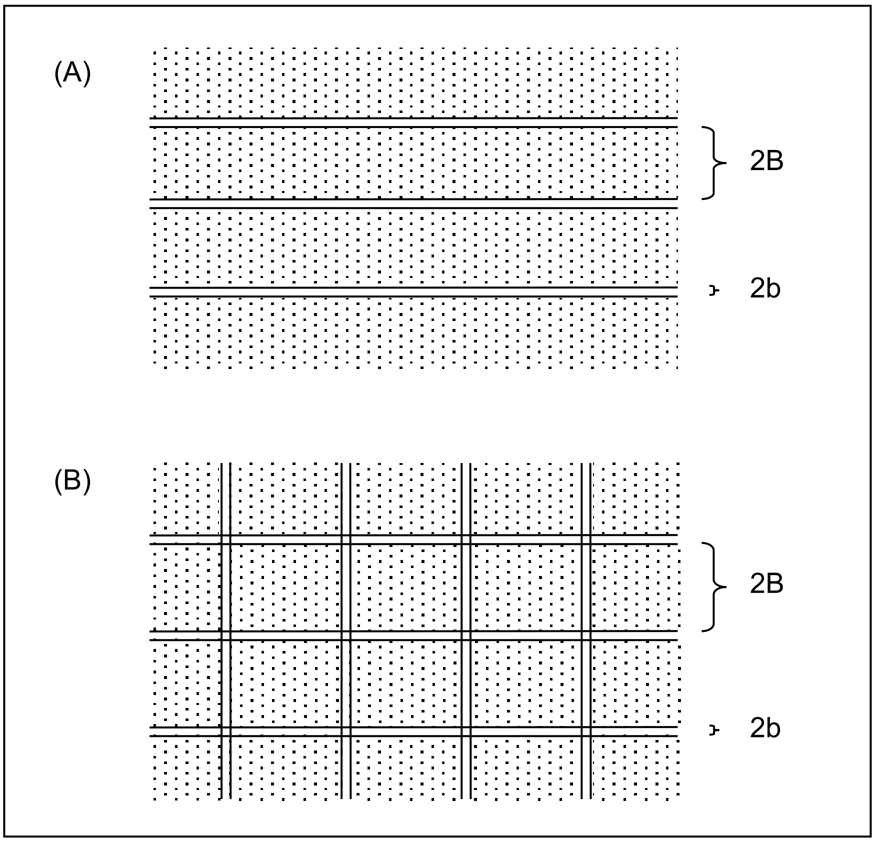


Figure A1. Illustration of a system of (A) parallel fractures and (B) orthogonal fractures. 2b is the aperture of the fractures, while 2B is the spacing between the fractures.

In each case, equivalent continuum parameters (also referred to as bulk parameters) may be derived from information on the fracture system. The bulk hydraulic conductivity for a system of parallel fractures is given by (ref.)

$$K_b = \frac{\rho g (2b)^3}{12\mu(2B)} + K_m \tag{A8}$$

and for a system of orthogonal fracture sets, we get

$$K_b = \frac{\rho g (2b)^3}{6\mu(2B)} + K_m \tag{A9}$$

The fracture porosity corresponds to the fraction of the total volume, where the water can flow freely. In a system of parallel fractures with aperture 2b separated by the spacing 2B, the fracture porosity may be found to

$$n_f = \frac{b}{b+B} \qquad \text{(A10)}$$

while for a system consisting of two orthogonal fracture sets the fracture porosity is

$$n_f = 2\frac{b}{B} \qquad \text{(A11)}$$

Analytical expressions for the mass transfer coefficient may also be derived. For a system of parallel fractures, the mass transfer coefficient is given by (Sudicky, 1990)

$$\beta = \frac{3n_m D_{eff}}{B^2} \qquad \text{(A12)}$$

while for a medium consisting of spheres, around which the water is flowing, a similar expression is found

$$\beta = \frac{15 n_m D_{eff}}{r_0^2} \qquad \text{(A13)}$$

where r_0 is the radius of the spheres, n_m is matrix porosity and D_{eff} is the effective diffusion coefficient. Eq. (A13) may be used for an approximate description of orthogonal fracture sets, where $r_0 = B$. β controls how fast the exchange of solute takes place between the two domains. If β is small, the system will be controlled by the fracture domain, while if β is large, a single porosity system is approximated. In the table below β is quantified for different values of fracture spacing and matrix porosity.

Table A1 Values of the exchange coefficient. 2B: Fracture spacing. r_0 is assumed to equal B.

Parameter	1	2	3	4
n_m (-)	0.3	0.3	0.3	0.1
2B (m)	1	5	0.1	1
D_{eff} (m^2/s)	$2.6 \cdot 10^{-10}$	$2.6 \cdot 10^{-10}$	$2.6 \cdot 10^{-10}$	$2.6 \cdot 10^{-10}$
β (eq. A12) (s^{-1})	9.4E-10	3.7E-11	9.4E-08	3.1E-10
β (eq. A13) (s^{-1})	4.7E-09	1.9E-10	4.7E-07	1.6E-09
β (eq. A12) (d^{-1})	8.1E-05	3.2E-06	8.1E-03	2.7E-05
β (eq. A13) (d^{-1})	4.0E-04	1.6E-05	4.0E-02	1.3E-04

9.2 Appendix B Literature Review

Table B1 Overview of hydrogeological parameters in literature from modelling, lab and field experiments in Danish carbonate rock types applied for groundwater supply. 1x10^{-4}

Carbonate rock type, (study/location)	Location	Porosity			Hydraulic conductivity matrix	Hydraulic conductivity fracture		Mass transfer coefficient	Test method	Reference
		n_m	n_f	n_{eff}	K_m (m/s)	K_h (m/s)	K_v (m/s)	β (d-1)		
KM (1 / 7)	Suså (DGU 216.791)				1.6e-8 – 2.8e-7				CT	Rambøll (2006)
KM (2 / 12)	Øst/central Storebælt				1e-10 - 1e-11	1e-6 - 1e-5			PT	Rambøll (2006)
KM (3 / 13)	Vest Storebælt				1e-10 - 1e-11	1e-4 - 7e-4			PT	Rambøll (2006)
KM (4 / 14)	Kerteminde GV model					1.57e-7	1,57e-8		M	Watertech
KM (5 / 15)	Nyborgmodel					1e-7	1e-8		M	Watertech
KK (6)	???	20-30			9.6e-9 – 9.6e-8				CT	Frykman (2006)
KK (7 / 11)	Hovedstien, Brøndby	22-32			5e-9 – 2e-8	2,5e-4			CT	Frykman (2006); GEO(2014)
KK-crushed (8 / 8c)	Akacievej, Fløng					6.5e-3			PT, TT	Mosthaf et al (2018)
KK (9/ 17a)	Kolindsund					< 1e-3			M	Jensen (2021) speciale
KK (10/18)	Metro/Øresund	5-40			5e-11 – 4e-7				CT	GEO (2014); Knudsen & Klitten (1994)
BK-lower frx (11 / 8a)	Akacievej, Fløng	7-46			2e-7	6.5e-3			PT, TT	Mosthaf et al (2016; 2018)
BK-matrix (12 / 8b)	Akacievej, Fløng					<1e-7			PT, TT	Mosthaf et al (2016: 2018)
BK (13 / 2)	Ølsemagle	25	0.47 - 0.66			6.8e-3 – 2.3e-4			TT	Martinsen and Hunner (2015)
BK (14 / 4a)	Li. Skensved				1.2 e-7	1,9e-5			CT	Milter (2007)
BK (15 / 4b)	Li. Skensved	24; 30				1.4e-7; 1.4e-3			TT, EPM	Milter (2007)
BK (16 / 5a)	Li. Skensved	39-44				1e-7 – 2 e-6			CT	Roskilde (2002)
BK (17 / 5b)	Li. Skensved					1e-6 – 2e-4			PAT, PT	Roskilde (2002)
BK (18 /10d)	Karlstrup	20-35			1e-8 – 1e-7				CT	Jacobsen et al (1993)
BK (19 /10c)	Karlstrup					1e-3 (<10m)			TT	Jacobsen et al (1993)

						5e-5 (>10m)				
BK (20/10a)	Karlstrup	22-33	0.016 - 1.6						PT	Jacobsen (1991)
BK (21/ 10b)	Karlstrup	4	1.1			8.1e-4	8.1e-5	2e-7	TT, DPM	Brettmann et al (1993)
BK (22/ 10b)	Karlstrup	4	1.1			1.2e-5	1.6e-6		TT, DPM	Brettmann et al (1993)
BK (23/ 10e)	Karlstrup	21-45.8			5e-8 – 2e-6	2.5e-8 - 7e-7			CT, PT, M	Larsen et al (2006); GEO(2014)
BK (24 / 9a)	Sigerslev, Stevns	33-44			3.8e-8 – 9.6e-7				CT	Frykman (2001; 2006)
BK (25 / 1a)	Hellested	31.7	0.5		2.3e-6	2.1e-5 (10m) 5.6e-6 (36m)	1.4e-6 (10m) 3.7e-7 (36m)	0.0036	PT,CT, EPM, DPM, DFM	Hansen (2009)
BK (26 / 1b)	Hellested	39,1-41,5				1.8e-6 – 4e-6	7.6e-7 – 1.8e-5	0.008	CT, TT, M, EPM, DPM	Pedersen (2008)
BK (27 / 6b)	Greve					2.9e-5	2.9e-6		Natural tracer, M	Jensen (2014); Thorn (2011)
BK (28/ 17b)	Kolindsund					< 1e-3			M	Jensen (2021) speciale
BK (29/19)	Naverland	15-20			8e-10 - 8e-9				CT	GEO (2014)

Carbonate rock type	Location	Porosity			Hydraulic conductivity matrix	Fracture hydraulic conductivity		Mass transfer coefficient	Test method	Reference
		n_m	n_f	n_{eff}	K_m (m/s)	K_h (m/s)	K_v (m/s)	β (d-1)		
SK (30 / 6a)	Greve					1.3-2e-6	1.3-2e-7		Natural tracer, M	Jensen (2014); Thorn(2011)
SK (31 / 9b)	Sigerslev kalkbrud	37-38		0.34-0.86				0.005-0.01	TT, EPM, DFM, DCM	Bonnesen et al (2005;2009)
SK (32 / 9a)	Sigerslev, Stevns	42-51			9.6xe-9 – 9.6xe-8				CT	Frykman (2001;2006)
SK (33 / 3)	Marielyst	30	3.6			13-1.7e-4 ; 6.6e5 - 2.3e-4		0.00015; 0.0015	TT, PT, M, EPM, DPM	Jensen (2020)

SK (34 / 16)	Mjels kalk-brud	20-50		0.015-0.06		3e-4 – 2.9e-2	2.3e-4 – 3.2e-4	0.000017-0.0017	CT, TT, DPM	Pedersen and Hørlück (2012)

9.3 Appendix C Mean hydraulic conductivities

Appendix C1: Number of pumping tests in open and screened chalk and limestone wells (exclusive outliers) in the various carbonate rock types in the geographic regions.

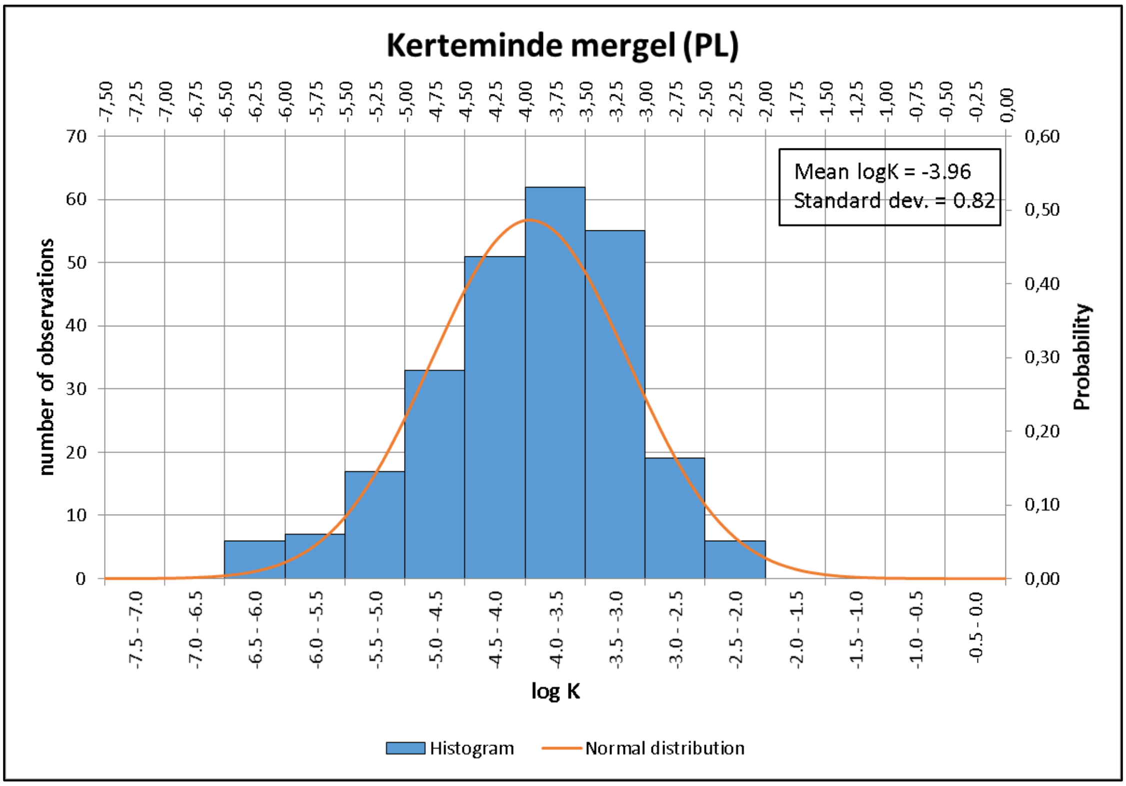
Number of pumping tests in chalk wells (ex. outliers)	Upper Maastrichtian chalk		Danien limestone			Selandien deposits	
	SK	LK	BK	ZK	KK	PK	PL
Falster	243	2	1				
Lolland	218	2	72	6	3		
Sjælland	897	179	2029	414	1640	781	181
Fyn	2	13	183	16	6	50	64
Himmerland & Djursland	614	242	129	177	423	1	9
Vendsyssel	244	22	40	19	6		2
Total på landsplan	2218	460	2454	632	2078	832	256

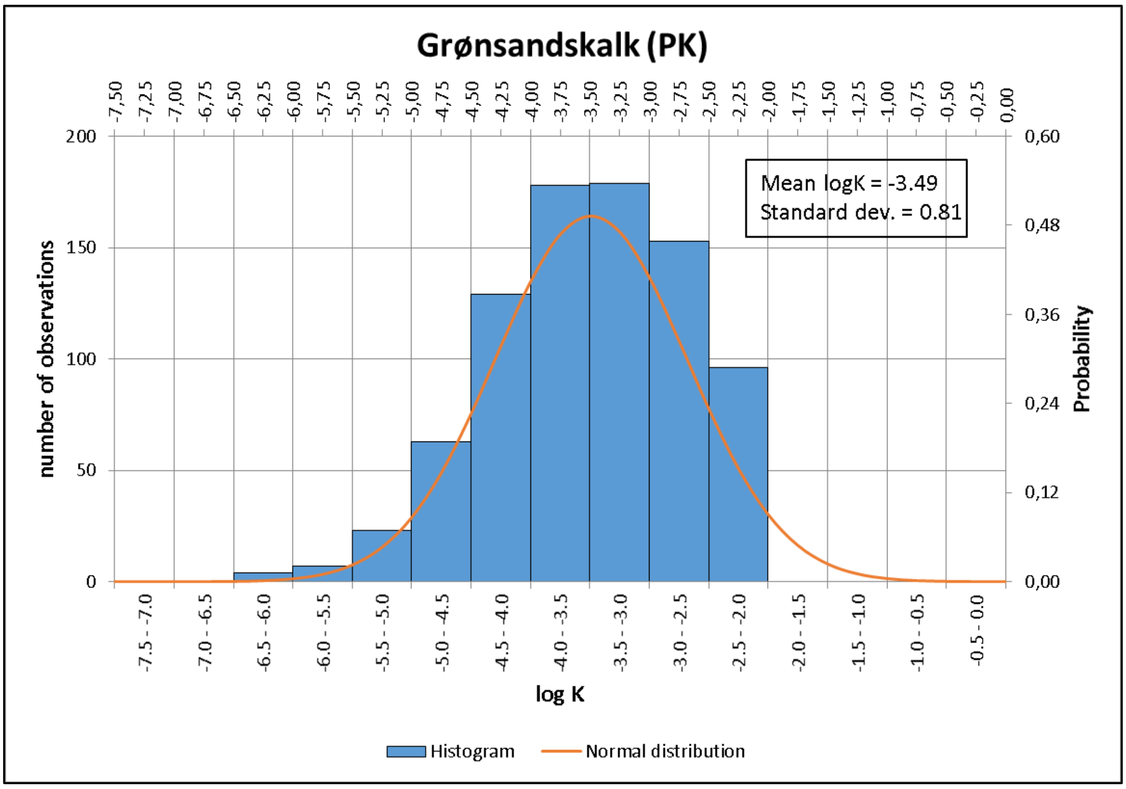
Appendix C2: Average hydraulic conductivity for each limestone type represented in the regions (top). Bottom: number of limestone boreholes with filter setting in the limestone types: Skrivekridt (SK), Skrivekridt with poor sample (LK), Bryozokalk (BK), Bryozokalk with poor sample (ZK), Københavnskalk (KK), Grønsandskalk (PK), Kerteminde mergel (PL). The K values are calculated for the rock types in two groups where there are more than 100 limestone boreholes and between 20-100 boreholes (in italics) with T values in the database JUPITER from pumping tests.

Mean hydraulic conductivity, $K \times 10^{-4}$ [m/s]	Upper Maastrichtian		Danian Chalk			Selandien deposits	
	SK	LK	BK	ZK	KK	PK	PL
Falster	1.29						
Lolland	0.46		0.33				
Sjælland	0.49	0.91	***1.07***	2.09	1.82	3.39	0.96
Fyn			0.69			***1.55***	***1.58***
Himmerland & Djursland	1.41	1.38	1.02	1.48	1.55		
Vendsyssel	1.55	***3.16***	***1.23***				

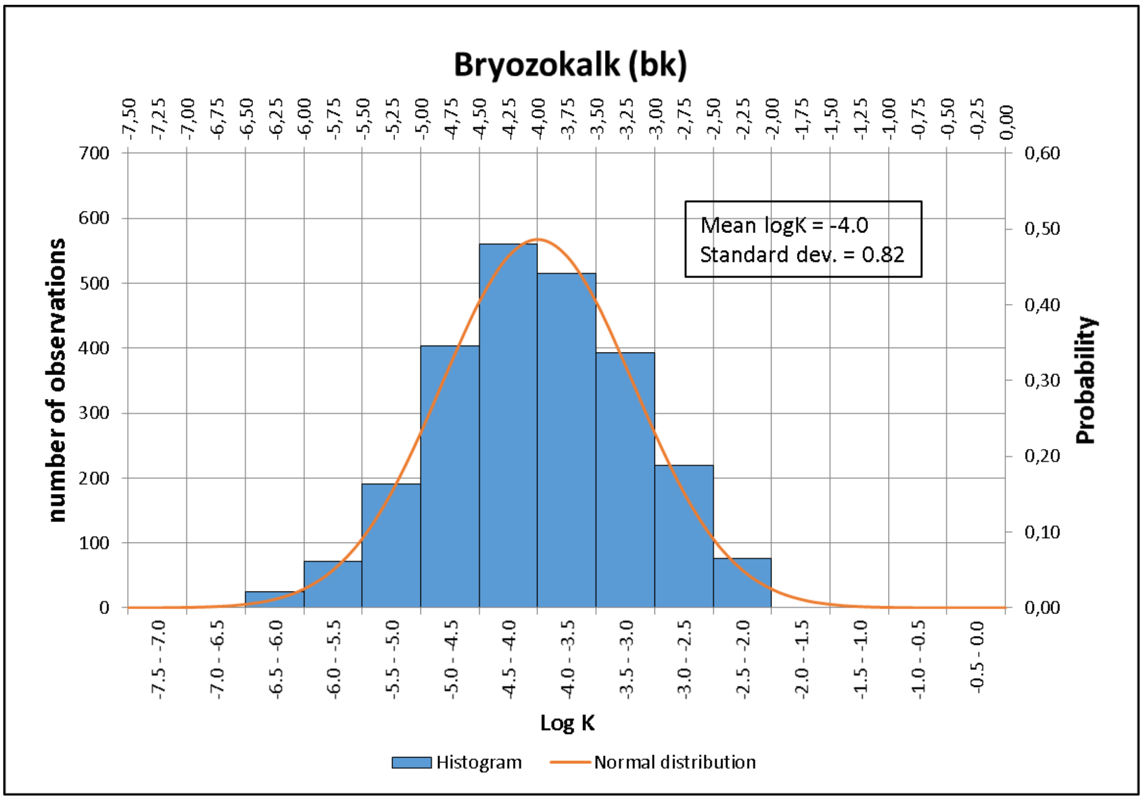
9.4 Appendix D Histograms and normal distributions (mean log K and standard deviation)

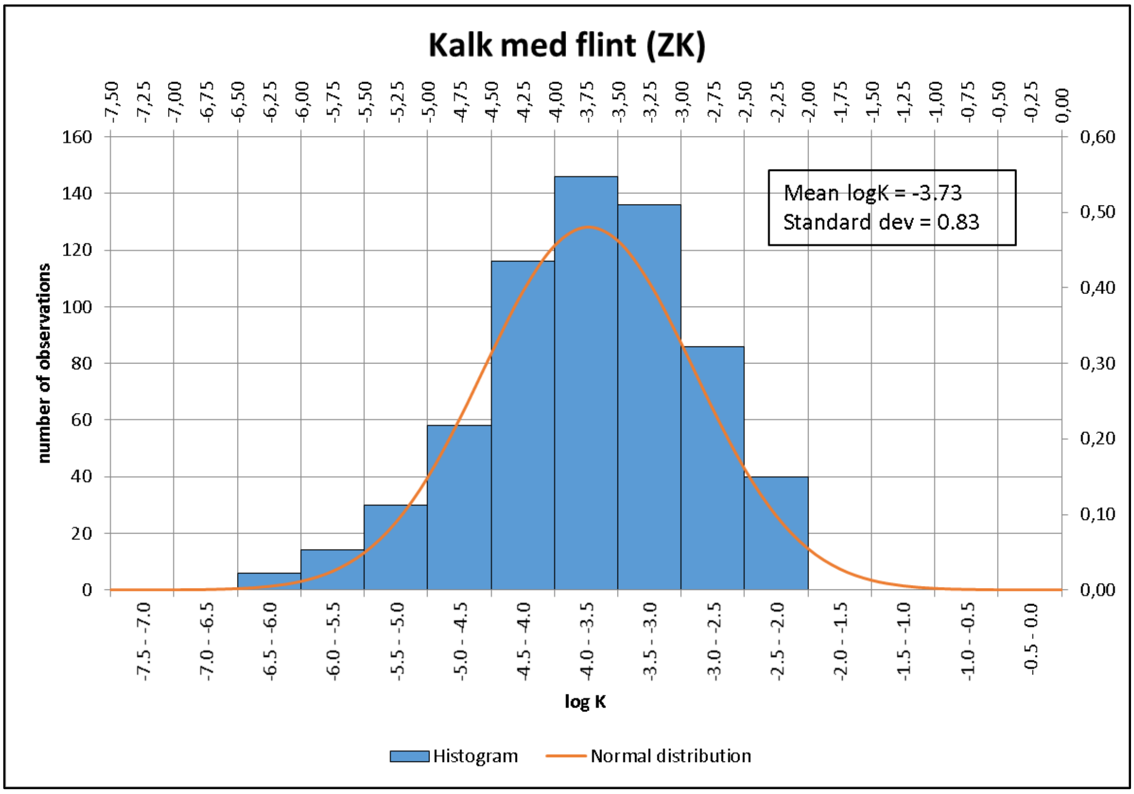
Selandien deposits

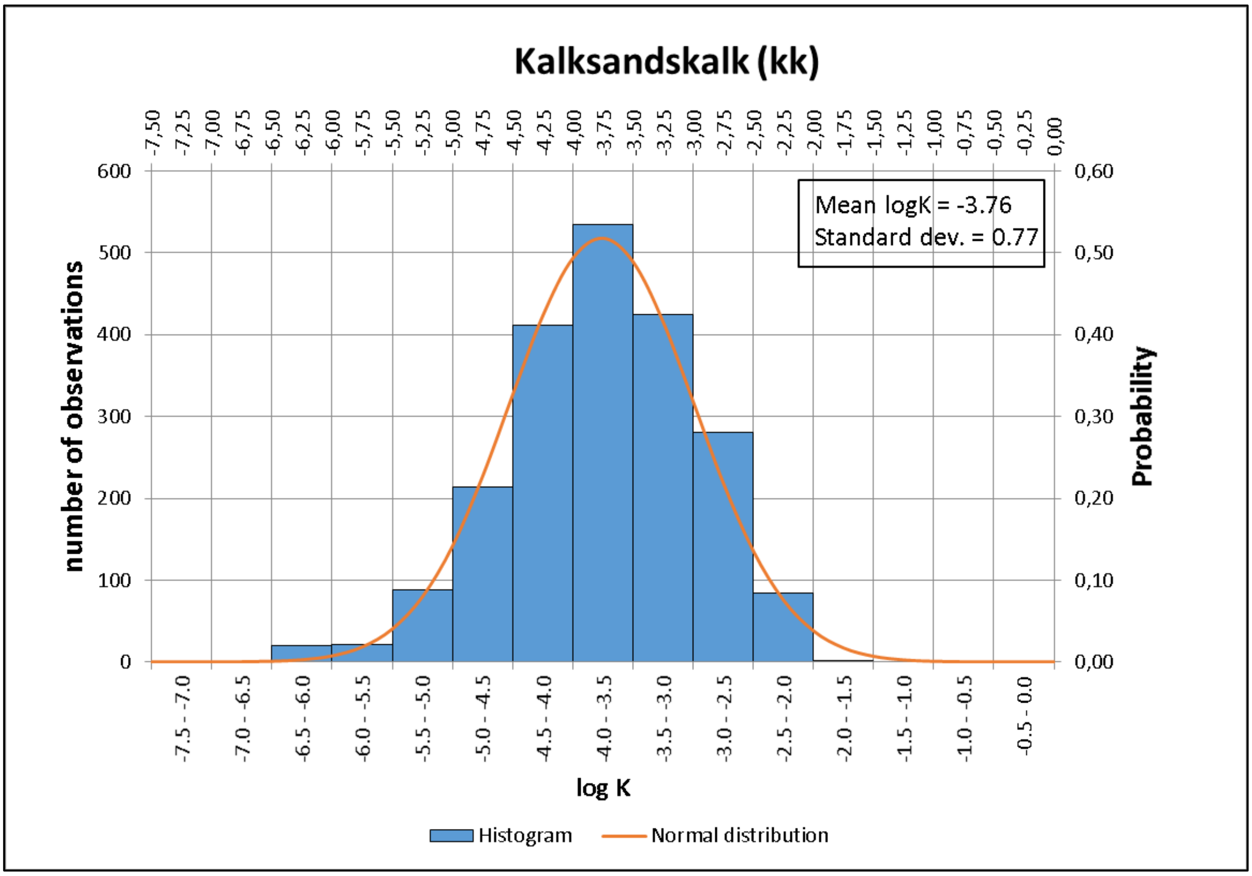




Danien limestone rock types

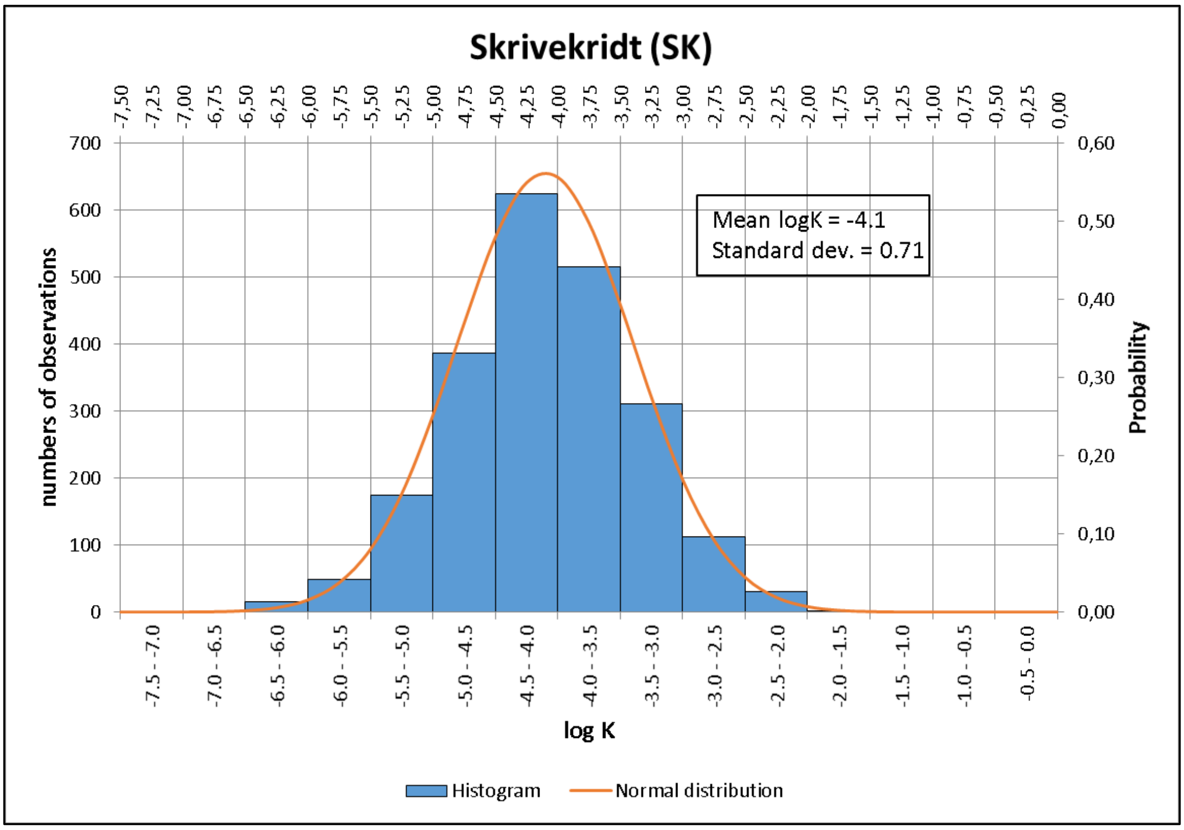


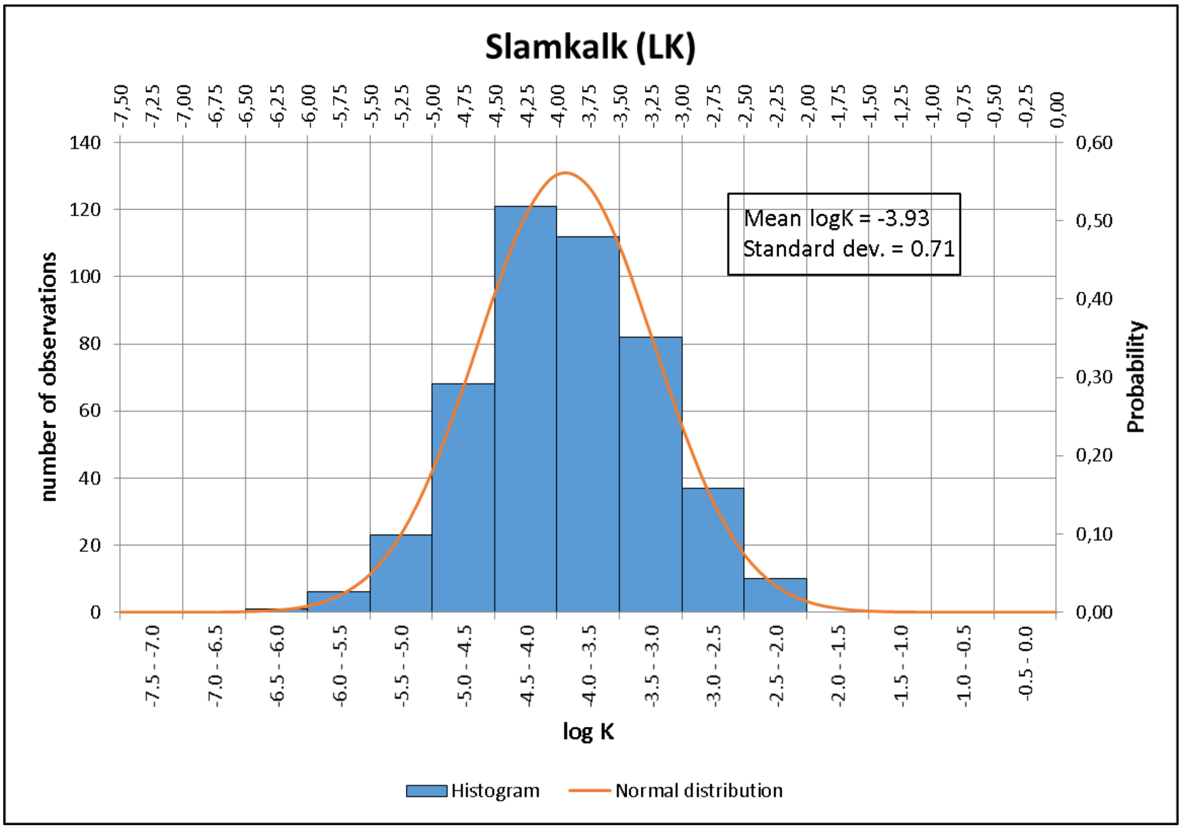




Kalksandskalk (kk)
Mean logK = -3.76
Standard dev. = 0.77
number of observations
Probability
log K
Histogram
Normal distribution

<u>Upper Cretaceous Chalk</u>





9.5 Appendix E Analysis of hydraulic conductivity for the Danish carbonate rock types and geological regions

Mean values for geological regions with less than a factor 2 difference:

Mean hydraulic conductivity, $K \times 10^{-4}$ [m/s]	Upper Maastrichtian		Danian Chalk			Selandien deposits	
	SK	LK	BK	ZK*	KK	PK	PL
Falster	1.41						
Lolland	0.48		0,33				
Sjælland	0.48	1.18	1.04		1.76	3.39	0.96
Fyn			1.04			1.55	0.96
Himmerland & Djursland	1.41	1.18	1.04		1.76		
Vendsyssel	1.41		1.04				

*ZK are poor samples of BK and not included in the analysis because it do not represent a specific carbonate rock formation.

T-tests between geological regions for the 6 Danish carbonate rock types:
The different matrix describes if the null hypothesis is confirmed or rejected, where the null hypothesis is that the mean of the two populations is equal.

Skrivekridt:

	Sjælland	Lolland	Falster	Himmerland & Djurs	Vendsyssel
Sjælland					
Lolland	CONFIRMED				
Falster	REJECTED	REJECTED			
Himmerland & Djurs	REJECTED	REJECTED	REJECTED		
Vendsyssel	REJECTED	REJECTED	REJECTED	CONFIRMED	

Slamkalk:

	Sjælland
Himmerland & Djurs	REJECTED

Bryozokalk:

	Sjælland	Lolland	Fyn	Himmerland & Djurs
Sjælland				

Lolland	REJECTED			
Fyn	REJECTED	REJECTED		
Himmerland & Djurs	CONFIRMED	REJECTED	CONFIRMED	

København kalk:

	Sjælland
Himmerland & Djurs	CONFIRMED

Grønsand:

	Sjælland
Fyn	REJECTED

Kerteminde mergel:

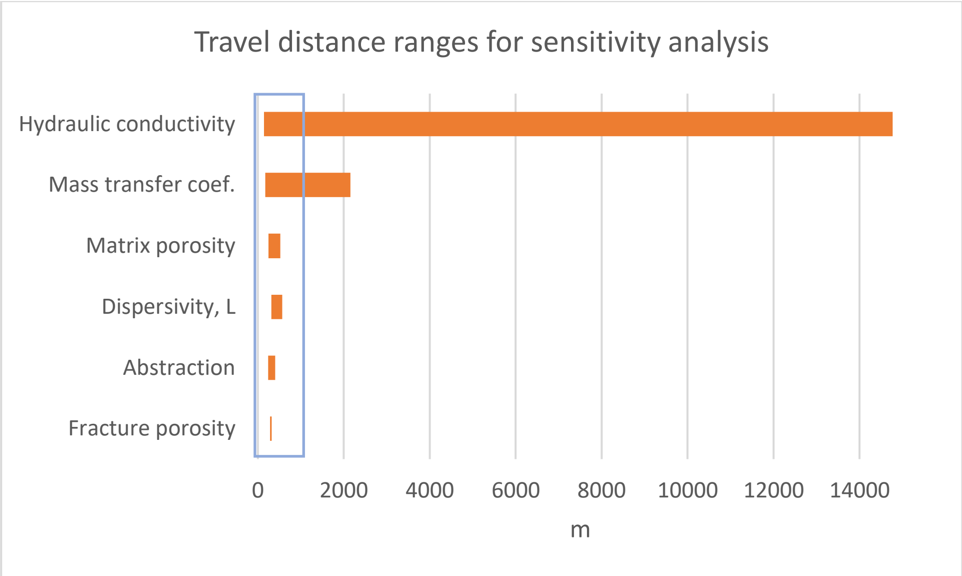
	Sjælland
Fyn	REJECTED

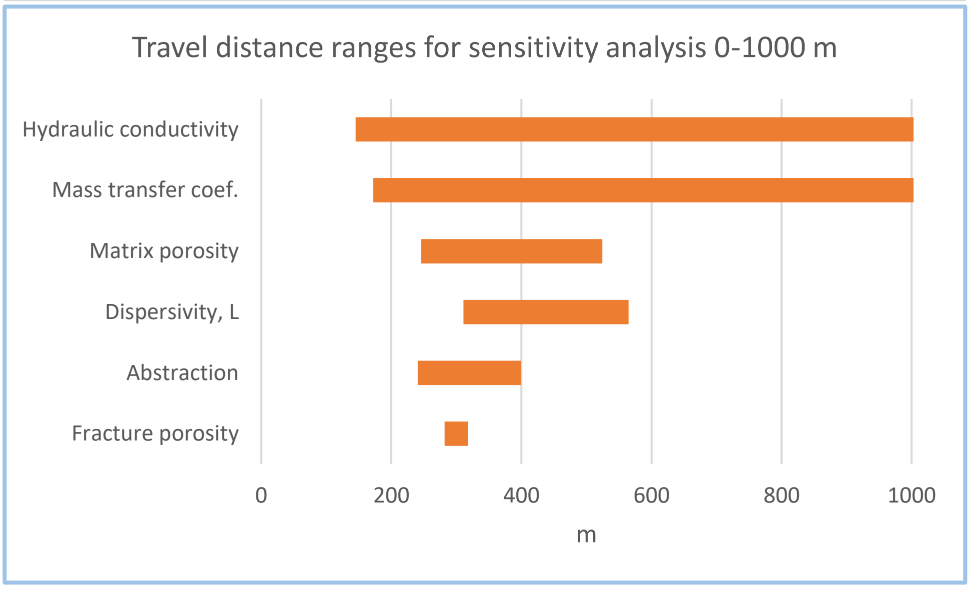
T-tests between the 6 Danish carbonate rock types:

The different matrix describes if the null hypothesis is confirmed or rejected. The analysis is performed between the mean values of each of the rock types with observations from all of the geological regions.

	SK	LK	BK	KK	PK	PL
SK						
LK	REJECTED					
BK	REJECTED	REJECTED				
KK	REJECTED	REJECTED	REJECTED			
PK	REJECTED	REJECTED	REJECTED	REJECTED		
PL	REJECTED	CONFIRMED	CONFIRMED	REJECTED	REJECTED	

9.6 Appendix F Sensitivity analysis





Variation of 1 yr travel distance for the six parameters investigated in the sensitivity analysis. The full range of travel distances found in the one-way sensitivity analysis (top figure) and a zoom on distances between 0 and 1000 meters.