Dispersion: the effects of aquifer heterogeneity
c o n c e p t

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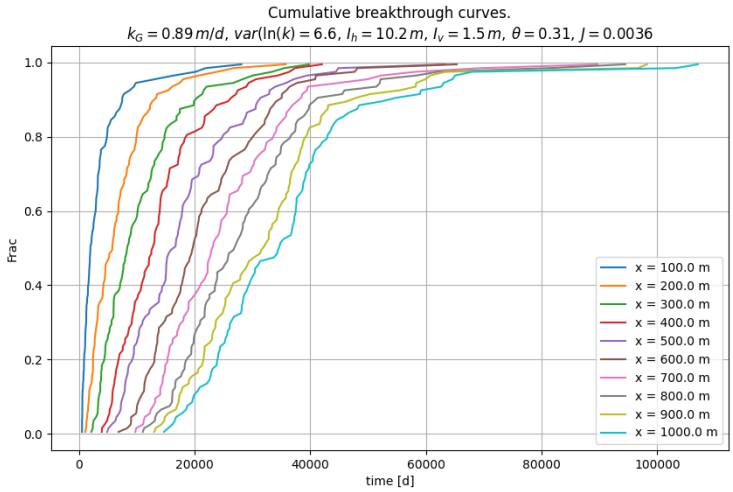


Contents

1 Introduction

According to [De Lange (2020), De Lange (2022), De Lange (2025)] dispersion as we see it through sampling an aquifer, is almost completely caused by groundwater velocity variations on macro-scale and neither on velocity variations at the pore-scale nor on molecular particle movement caused by diffusion. Although pore-scale velocity differences always plays a role whenever groundwater is flowing, and diffusion even when it's not flowing, these two mechanisms are by many scholars believed to play such a small role in most real-world situations, that they can often be neglected when evaluating actual dispersion in the field or when modeling mass transport with dispersion.

So what is dispersion as we see it? Dispersion can be defined based on the gradual concentration increase, the reaching of a peak concentration followed by the slow decrease of a consituent when a well or an observation screen is frequently sampled. Dispersion can also be defined based on the average concentration over the height of the aquifer sampled by many vertically arranged small sampling screens or by sampling a fully penetrating well. With the latter method, using more than one well or series of sampling points at different spatial locations, we may try to outline the extent of a so-called plume of pollutant as it extents at a certain moment in time within the aquifer. We may try to accomplish the same thing by sampling one or multiple wells over time, taking into account the actual velocities of the groundwater, which are oftentimes difficult to determine.

Dispersion has mostly been defined as a process similar to diffusion, in that it is due to velocity differences at the pore-scale, which cause diffusion-aided mixing between adjacent streamlines and thus result in the observed spread of the pollutant both in the direction of the flow as well as perpendicular to it. In this traditional Fickian or Gaussian theory the spreading behaves as if it was driven purely by concentration gradients. In fact, without diffusion, at least, theoretically, a pollutant should not spread perpendicular to the streamlines in all cases where streamlines cannot cross each other. Streamlines can only cross each other in 3D space, and, therefore, such advection mechanisms cannot explain spreading of a pollutant perpendicular to streamlines in 2D space. Nevertheless streamlines can cross each other in 3D space (e.g. in aquifers with hoirzontal layers having main horizontal conductivity axes in different directions [Hemker and Bakker (2004)], [Jankovic et al. (2003), Jankovic et al. (2010)]). This eventually reduces the value of 2D dispersion analyses in a fundamental way as it remains impossible to determined the 3D impact happening in reality using a 2D simulation.

However, major velocity differences occur on macro scale, caused by differences of the hydraulic conductivity and or porosity on the scale of the sedimentation processes that originally formed the aquifer. Notice that we only consider aquifers consisting of sediments, that is, aquifers constructed of layers of particles of different sizes, as show up in borelogs and cross sections alike. These processes have built up the aquifer over large spans of geologic time, in layers, formed in different energetic environments, i.e. by water that carried different amounts of particles the size of which varied depending on the geologic and climatic circumstances. These circumstances have liklely largely varied over the tens of thousands to millions of years, during which the aquifer was formed. Retracting seas during ice ages and rising land cause larger gradients of the earth's surface, due to which erosion increases and more and coarser sediments are laid out over extended areas, generally by wide braided rivers. Their sediments cause coarse-grained inclusions, which are detected in our current-day aquifers. During warmer, more vegetated eras, with higher ocean levels, rivers carry less and finer sediments, While meandering they cut into previously deposited sediment layers to form their characteristic patterns we now observe in cross sections. During cold windy periods with tundras as well as in dry deserts, large-scale areal transport and deposition of fine particles have formed often vast regions with moving dunes, which now show up in cross sections as often thick layers of overlapping sublayers of fine material. They are characterized by their upward curved patterns that witness the original horizonal

progress of the dune-type deposits. Extended clay layers are generally caused by sea transgressions when climate warmed up or land sank. Or they were deposited by rivers that broke through their banks creating extended flood areas with little energy, which allowed fine particles to settle and to form river-clay deposits. We oftentimes witness all such previously active processes play out in the bore-hole profile or in natural or our own man-made cross sections. Looking at such profiles, we are watching how a vast number of geological processes has played out over hundreds of thousands to millions of years to form the aquifer at hand. No wonder the details of the flow of groundwater through an aquifer is complicated. When dealing with the groundwater head in an aquifer or at what rate we can extract water from it by a well, things are far less complicated due to natural averaging of the head between layers and the integration of the flow towards a well screen over all layers that intersect it. However, if we study the spread of pollutants within an aquifer, the details of the structure of the aquifer do matter. And it's obvious that the extremely wide variation of the conductivity within the aquifer, caused by the mentioned varyity of sedimentation (and local erosion) processes, determine the spread of a pollutant more than velocity variations at the porescale. As far as diffusion is concerned, it's important over the long run in stagnant situations and to allow consituents to jump between parallel stream lines. But on local scales and relative short, say sub-century time scales it tends to be of little importance.

While an aquifer tends to be built up over time by repeated fining-up sediment sequences, it is the braided river's coarse material deposition during cold periods that intersects such layered sequences and created inclusions with often sharply distinct hydraulic conductivities. To a somewhat lesser extent, we find „inclusions" (often called facies) caused by meandering rivers that cut into older layers while eroding their outer bends and at the same time deposing fresh material at their inner bends. This way, meandering rivers create their charactistic particle-band patterns in cross sections with their associated conductivity patterns. But we also encounter existing sediment packages that were disturbed, pushed up, shifted and partly or toally turned over by the heavy load of progressing land ice. When retracting and after melting, the deep valley space that was left over, was subsequently filled up by both erosion material from the pushed-up ridges and filled by fine material, especially caused by subsequent sea water rise. Of course, much more can be, and perhaps should be said about the characterisics of the cross sections we encounter in the field. Studying and describing them has been the focus of geologists and especially sedimentologists throughout the world over a long time. However using their discriptions to accurately model the hydrogeneous conductivity field remains a challenge and is mostly not universily successful to say the least.

The fundamental consequence of attributing all „disperision" to spatial conductivity variation in facies and inclusions, i.e. by neglecting pore- and grain-scale processes, is, that, in fact, no mixing can occur in the subsurface because it implies that every particle will stick to its own original streamline over its entire underground life. This would even be true when the streamline changes over time as a result of altered boundary conditions. Hence, with this asusmption, all dispersion, i.e. mixing, occursat the extraction point, where the extracted water is mixed in the screen or the well when pumping or just sampling it. Or, the water is mixed in the computer when we digitally mix the extracted water along the vertical at some point in the aquifer. There may be differences between physical and digital mixing, though. For instance, the mixing in a well screen depends on the flow from each layer that intersects the assumed fully penetrating screen. This makes the layers with the highest conductivities dominant, as we often see when measuring the inflow to a well screen along its length. To get the right comparison, in the computer we must also take the afflux at each elevation along the well screen into consideration, which is not difficult to do. We can also do this over time. But in fact, when mixing the water vertically at a given point in the aquifer and a given point in time, we always mix water from layers with zero consituant concentration with water from layers with non-zero constituent concentration. And, under the assumption that only advection is active, a streamline either has exacly the same concentration it was given at the point of release after passing the point of none. This is a consequence of the assumption of zero mixing within the aquifer, which is what happens as particles stick to their streamline and pore-size processes are ignored. Hence, each streamline either carries a particle of the constituent or none at the moment and point of sampling.

When simulating discrete particle transport in the computer, the probability of hitting any particle at any streamline at the well exactly at the time of sampling may be vanishingly small. Therefore, we have to sample over a given amount of time, to capture at least some particles. Afterwards we integrate over time to get the cumulative probability distribution. Or rather considering an initially sharp front, we simply count the streamlines whose front particle has passed the observation point, sort these times and construct the

cumulative breakthrough curve for this .

How then can we define dispersion when we consider it to be caused by advection through the heterogeneous aquifer alone? One way to do it, is by recording the particles that were initially released at one location and time, as they pass some point downstream. When the particles were initially distributed vertically in such a way that each of them represents the same fraction of water, while the total number of particles make up the entire groundwater flow, then we can construct the cumulative distribution of particles passing the observation location. The shape of this distribution represents the statistics of the advection-dispersion process in its entirety, and its derivative represents the density distribution, allowing for further statistical analysis and statistical generalization.

When we only take advection into account, it is fundamentally impossible to determine the dispersion after releasing particles at a single point and time, i.e. due to a concentration pulse. This impossibility is due to a sudden release of a given number of particles at a single point in the aquifer at a given point in time. This is so, because if this point source is theoretically a single point in the aquifer, then all particles would be on the same stream line and stick to it and would always travel at the same speed. Hence, no dispersion would ever occur within this framework. The fact alone that a point source does generate a growing plume in reality, implies that this concept of pure advection, may have its merits, but also has its limits.

No one dan ignore that diffusion acts in groundwater, as it is caused by molecular movement, which is always present. The spread σ of an initial concentration pulse, or of an initially straight concentration front, is defined by the standard deviation $\sigma = \sqrt{2Dt}$ with D [L^2/T] the molecular diffusion coefficient. With a value of $D \approx 2 \times 10^{-9}$ [m^2/d], we have $\sigma \approx 0.25$ m in one year. This is not nothing. It spread will defnitely does cause particles to step over to adjacent streamlines. In 100 years $\sigma \approx 2.5$ m and in 10000 years $\sigma \approx 25$ m. The latter is of the scale of the vertical exent of the aquifer itself. Hence, on the long run diffusion as a mechanism to spread out pollutants perpendicularly to the streamlines cannot be ignored and will limit the value of the pure advection approach to tens of years rather than hundreds or even thousands of years.

2 Analysis of advection-dominated dispersion using particle tracking in heterogeneous aquifers in 2D vertical cross sections

Assuming that dispersion is caused by macroscale velocity variations due to the aquifer's heterogeneous conductivity field, we can analyze it by means of particle tracking. In order to include diffusion (but still ignoring porescale velocity variations) we would have to include mass transport with diffusion, which is outside our current scope.

Even realizing its limits, we will stick with a vertial, i.e. 2D cross section of uniform height modeled with finite differences using a rectangular mesh with sub layers of equal height. The conductivity of each cell may be unique, and the vertical and horizontal conductivities may be different. Furthermore, also the porosity in each cell may be chosen to be unique. However, the variations of the porosity in a real aquifer tend to be small, even negligible compared to the variations in hydraulic conductivity. For this reason, without loss of generality, we will use a constant porosity of around 35% throughout our analysis.

The boundary conditions of the modeled cross section are a fixed but different head at both ends. This would yield a uniform flow field when the aquifer were homogeneous. However, due to its heterogeneity, the flow field is far from homogeneous and will be determined by a steady-state computation with Modflow. The results allow us to visualize not only the lines of constant head, but also the lines of constant values of the stream function. The stream function allows us to determine uniquely the flow density and the flow direction at any point in the aquifer, even without particle tracking. The stream function permits us to detemrine the elevation of the release points of the particles such that each particle represents the same amount of discharge, which will guarantee keeping the mass balance also with particle tracking.

Particle tracking is done with Modpath7. Modpath guarantees that the governing differential equation of the discharge is fullfilled at every point within every cell of the model. This implies that, although the model is only a limited representation of the actual aquifer, particle tracking the Modpath way does guarantee proper distribution of the particles throughout the aquifer while maintaining the mass balance at any point as well as in the aquifer as a whole.

The procedure to follow is to first generate a conductivity field. Then use Modflow to compute the flow field in the aquifer, with heads and cell-by-cell discharges. This is ollows by the computation of the stream

function using the flow across the right face of the cells that were computed by Modflow. The next step is to place particles along a vertical in the aquifer at elevations obtained from the stream function, such that each particle represents the same amount of discharge along this vertical. After releasing the particles they are tracked with Modpath. Following step is to take the computed pathline file and for each particle compute when exactly it passed a set of given points in the aquifer. Finally we determine the cumulative breakthrough curve for each of these locations. These breakthrough curves represent the cumulative probability density function of the dispersion between the release point and the observation point, they capture the characteristic of the dispersion processes active between the two points. By using more points, the development of the cumulative density function over time or, rather distance, can be studied. These cumulative probability density functions can be converted into breakthrough histograms to unveil the underlying probability density functions. Both cumulative breakthrough curves and the histograms contain the same information.

3 Literature discussion

A vast number of papers has been written on subsurface transport of pollutants (Gelhar, Sudicky ...). This mainly started in the 1980s after it became obvious that hunderds of thousands of waste sites were and have been polluting groundwater and groundwater and as avaluable resource for drinking water and public concern skurocketed. The study of the subsurface displacement and spreading proved difficult due to the heterogeneity of the subsurace and the interaction between pollutants and subsurface material. The studies were plagued by lack of understanding the complexity of the conductivity field that caused preferential flow paths and the mixing processes known as dispersion as well as the role of diffusion in it. The Fickian of Gaussion theory that look so nice on paper, or in math, was time and again challenged in practice, where samples showed that reality adn theory more often than not did not match. Hence long time studies were underrtaken with large-scale and repeated tracer tests to better capture and learn to predict what happens in practice. The Borden en Made studies, both done over 25 years with millions invested in exploring the subsurface structure and sampling the groundwater in great detail were carried out, but in the end did not totally solve our lack of insight and modeling capabilities to correctly predict development of pollution plumes in those and other circumstances.

Sudicky (1986) carefully studied the Borden experiment after others, like Dagan and Gelhar went before him. Hij gives a cross section in both the longidudinal and perpendicular direction to the grounwater flow. His paper is more or less a summarizing evaluation of the work that was done at Borden. Sudicky considers the flow as fundamentally 3D and finishes with a summary worth citing from it.

Zheng et al. (2011) provide a review and overview of over 25 years of research and lessons learned at the Macrodispersion Experiment (MADE) site, located at the Columbus Air Force Base in Mississippi. The site has been instrumental in advancing the understanding of solute transport in highly heterogeneous aquifers. The authors conclude: „In spite of tremendous effort and progress over the past three decades, our ability to predict solute transport processes in highly heterogeneous media remains very limited". They show to expect a lot from future field measurements in a comprehensive suite and carefully designed in a tightly integrated fashion. However, it's doubtful if these new studies will be ever perfomed, given the effort and cost already spent before. It seems that the existing data for the Made and Borden will be revisited in new research for a long time into the future. The authors stress that future work should focus on mapping the hydraulic conductivity distribution and the resulting preferential pathways far beyond what is currently possible given the existing measurement techniques. With this disclamier the authors seem to admit that the problem to fully understand subsurface transport will remain essentially unsolved for a long time in the future.

Gorelick has essentially introduced the dual domain theory and model to better capture the observed dispersion at the very heterogeneous Made site ([Zheng et al. (2011)]). The dual domain was then included in several groundwater transport codes. like MT3SM. The dual domain just discerns between a mobile phase and an immobile phase, with kinetic exchange process between them. It has been quite succesful in Made as is shown in figure 9 in [Zheng et al. (2011)]. It thus seems that a dual domain can compensate for the failure to accurately capture the hydraulic conductiviy field to mimic the transport behavior with preferential flow paths. However, it may well be that the dual-domain model functions well for the wrong reasons by being able to produce a subsurface mass transport that mimics the measurements even if in reality there are not two domains but there is just a very heterogeneous conductivity field. The authors seem to admit

this in their introduction stating that „results from field investigations and modeling analyses suggest that connected networks of small-scale preferential flow paths and relative flow barriers exert dominant control on solute transport processes." Thse connected networks are fundamentaly different from the adsorption process that is modeled by the dual domain seems to make no sense to model consituents that do not sorb like chloride, bromide or tritium. [Fiori et al. (2013)] show that indeed, it is possible to get similar outcomes with a heterogeneous conductivity field without a dual domain with sorption.

Two years after this review paper that should have said it all was picked up by [Fiori et al. (2013)]. They continued the dicussion and tried to model the observed plume dispersion at the Made site. To better tackle the large asymmetry of the pollution plume not described by traditional advection-dispersion models, they propose a multi-indicator model (MIM). With it [Fiori et al. (2013)] essentially subdivide the aquifer into blocks of different independent conductivity drawn from a lognormal distribution. The dispersion generated by the flow of particles through their heterogenious model was the resdult of advection alone. They found that this simple advection model could describe the development of the observed plume „remarkebly well". In their section 3, the authors explicitly motivate their claim that advection is the only process that matters at the Made site. With the few parameters given in their table 1, and used below in this report, their MIM model was capable of mimicking the measured bromide distribution sampled at 6 points of time, but only reasonably. Nevertheless, their MIM model did demonstrate that the observed dispersion can be explained just by the flow as it is distored by the heterogeneity of the conductivity field in the aquifer, even without considering any other processes. The results of this advection-dominated model show the charateristic that proved impossible to model with traditional advecton-dispersion models, which is the large asymmetry (long tail) of the plume development in the subsurface.

The more homogeneous the conductivity field of the aquifer is, the less dominant is the spread of particles caused by advection and the more important diffusion and pore-scale velocity differences will be. Even then these low-scale velocity differences will dominate diffusion, at least in the flow direction. For instance, [Jensen et al. (1993)] show that, even though their Danish aquifer is very homogeneous, the derived longitudinal dispersivity was 500 times larger than the transvese dispersivity and 1000 times larger than the vertical transverse dispersivity. From this, we may conclude that velocity variations caused by local small scale conductivity variations are likely the cause of the large contrast between the vertical and transverse dispersivities. [Jensen et al. (1993)] proved this by showing that inceasing refinement of their model better mimicked the small-scale statistics of the aquifer.

[Jankovic et al. (2006)] show that, even though macrodispersion can be described by velocity variations caused by the conductivity field, and result in largely asymmetric plume shapes with a short front and a long tail, the bulk of the plume can still be described by a Gaussian model with an equivalent mean velocity and a longitudal dispersivity. This does not work for the long tail, but the tail will be of far less importance in practice as it only holds a small fraction of the total mass of the pollutant. Only when the aquifer tends to homogeneity, the Gaussian model will also better predict the plume's tail behavior. [Jankovic et al. (2006)] further conclued from their work, that for very inhomogeneous aquifers, the plume behavior does not approach Gaussian / Fickian behavior even for very long travel distances.

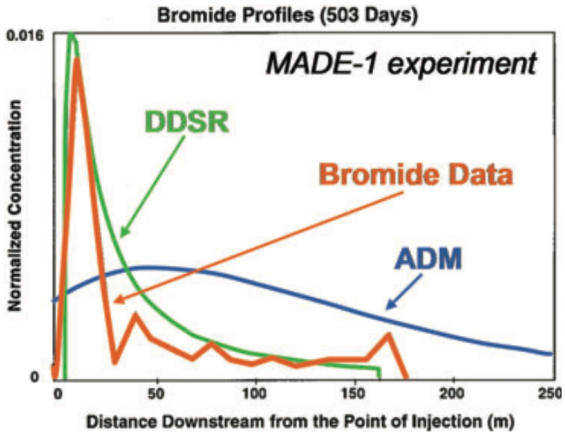


Figure 1: Comparison of the modelled and measured bromide plume extent at the Made site. ADM stands for classical Advection-Dispersion-Mass transfor model, DDSR stands for Dual-Domain Mass Transform Model. The graph clearly shows the rapid progress of a small part of the water while the bulk remain near the source. The intepretation depends on whether the flow rate hat the sampling elevations was included in the analysis. This is probably not the case.

4 Cross sections

4.1 Introduction

A fundamental problem, perhaps the most fundamental one, is that the flow in a 2D cross section misses the thrid dimension. The problem is not that some cross section is bended to follow the curves of a projected streamline, nor that the cross section represents an axially symmetric situation. The essence is that a plain crosss section does not have flow components perpendicular to it. In theory a 2D section does not require flow components perpendicular to it; in practic, this is never fully the case. Wherever the flow and the spread of particles is determined by inhomogeneities, or, in other words, by the heterogeneous conductivity field, due to which the flow direction continuously deviates from the average flow direction in the cross section, one can then be certain that in reality such deviations also occur perpendicular to the 2D plane of the cross section. The inhomogeneities of the real world are never limited to the plane of the cross section, they are just as strong perpendiular to it. [Hemker and Bakker (2004)] and others have shown, that exactly this 3rd component of the groundwater velocity makes that stroomlines can cross each other, and thus cause dispersion, what they never can in a 2D situation. The analysis of the flow in a flat cross section falls fundamentally short to discribe the full mixing process in an aquifer characterized by its heterogeneous conductivty field in all its 3 dimensions. The paper of [Hemker and Bakker (2004)] triggered 3D thinking and made crystal clear the likelihood, or perhaps even the certainty, that a 3D inhomogeneous conductivity field will let streamlines cross each other all the time and everywhere, and thus cause mixing at a scale much larger than that at which molecular diffusion or pore-scale velocity differences play.

And of course particles (molecules) will jump between adjacent streamlines all the time, which, combined by the turnover of streamlines described above, triggers transversal spreading at a rate that far exceeds that of molecular diffusion. Molecular diffusion tends to be slow and becomes increalingly slower over time as expressed by the formula for the grow of the standard deviation of an initially sharp front, i.e. $\sigma = \sqrt{2Dt}$. However, in a porous medium like an aquifer, in which the velocity varies perpendicular to the stream lines everywhere, the concentration gradient perpendicular to the streamlines is kept much sharper. This is a consequence of the washing process associated with particles on adjacent streamlines having different volocities. This washing process cause molecular spreading to be larger than in the theory valid voor a stagnant groundwater.

Finally, it is virtually impossible to determine particle concentration at distinct points in the aquifer. We do not get around the fact what we will always mix water from different streamlines when sampling,

no matter how we do this. This is true for even the smallest sampling screen, for a sampling well and for measuring concentration using some physical device, for instance by measuring electric conductivity or tracer color. If we consider advection to be the dominant or even the only relevant process taking place in the aquifer, then mixing will only take place at the moment we sample or extract. The best we can hope for is the sampling of the passage of a complete front.

To this we must add the the difference between sampling is situ without disturbing flow, for instance by a sounding device, or by extracting using for instance a well. Both methods will often given completely different results as the extraction method mixes the incoming water in proportions proportional to the conductivity along the screen, with some parts yielding most and other parts yielding least water, while sampling in situ measures without considering the amount of flow that its elevation. Mixing these sampling methods can lead to misinterpretations

In conclusion if we ever want to model groundwater mixing appropriately, we must consider 3D velocity components, even when dealing with flat cross sections. When sampling we must realize the mixing we cause or not cause depending on the sampling method as the results may be completely different.

In the analysis for this work, we will at least initially focus on the flow in vertical cross sections without any flow perpendicular to them and should be aware of its limitations.

4.2 Generating cross sections

For any analysis we need a conductivity field first. There are many ways to generate cross sections. One manner is to do this based on a colored picture, by sampling the pixel colors, clustering these colors, and then assigning distinct conductivities to each of them. Although doable, and allowing many pictured cross sections to be used in this way, the resulting sections will always be artificial as no single hand-made image of a cross section can ever grab, even nearly, the real-world conductivity variations that are present in reality. These cross-section pictures have too few colors, and on top of this, the colors tend to picture perceived facies or formations rather than conductivities.

Cross sections may also be obtained from websites that provide them based on borelogs and other physical logs, cores etcetera. Such geological sections are exactly those meant above. However, sites such as Dinoloket.nl provides a full 3D database of the lilelihood of the occurence of a set of materials (sand, clay etc.) for blocks (voxels) of some 100x100x0.5 m across a large part of the Netehrlands. It is straightforward to extract colored cross sections form this website and use them in the way described above. However, these data are also very limited in that the number of voxels is much larger than the resolution of the underlying data, so that they do not represent reality, but instead, the probability of the occurrence of given materials, which can then be associated with conductivities. If we associate one conductivity with each voxel, then the result is likely too coarse to accurately simulate subsurface transport as caused by the more local heterogeneous conductivity field.

One can digitally generate borelholes by using transistion probabilities between adjacent materials as obtained from borehole sampling. The resulting borehole is clearly artificial, but it will at least have some statistical properties similar to that of the real borehole. The problem then becomes how to link manyin this way created boreholes together into a single cross section. Simple interpolation will not be enough as it then ignores the horizontal transitions or at least the scale of them. And it is not clear how to solve this issue without external information, which, in fact, cannot come from boreholes drilled at mutual distances in the order of hundreds to thousands of meters. Such information could come from the study of existing real-world cross sections for similar sedimentological environments. It is likely that the number of real-world cross sections that actually match the sedimentologial environment in the subsurface in which we drill our boreholes, is far too small to yield accurate data.

From such cross sections rather than from individual boreholes that are too far apart, we can extract the statistics of the grainsizes or even the hydraulic conductivity in the horizontal and vertical direction by constructing semi-variograms. Then use these to statistically generate individual cross sections, also know as realisations, which at least have this same statistical properties as the real cross section. The problem is, that each realization is different and no one will mimic the actual field situation accurately. The only thing we can then do, is generate a large number of such realisations and study the properties for the ensemble, the results of which are always statistical themselves.

Finally, we can just generate our 2D cross sections, or even complete 3D conductivity fields digitally

be sampling from conductivity distributions in some way ([Fiori et al. (2013)]) or by placing distinct heterogeneities in a 2D or 3D field ([Jankovic et al. (2003), Jankovic et al. (2006), Jankovic et al. (2010)]), of which the link to reality will remain unanswered.

5 Cross section according to De Lange

in his papers, takes an approach that is similar to that of [Fiori et al. (2013)] et al. He divides his vertical cross sections for the sake of dispersion simulation into blocks, which he calls domains. These blocks have a background conductivity with one embedded elongated facies with a conductivity that is largely distinct from the block's background value. The entire dispersion process takes place inside the block. To simulate a long travel distance, many alike blocks are placed next to each other and on top of each other, thus filling the entire space of the vertical cross section.

We can generate such cross section by creating a conductivity field that mimics De Lange's multiple block aquifer.

5.1 Cross section between De Lange and [Fiori et al. (2013)]

We can also just fill the entire cross section with blocks of the same size, each of which has it's own distinct conductivity drawn from a statistical, i.e. lognormal distribution. The cross section will then be similar to the model domain used by [Fiori et al. (2013)] at al.

5.2 More elaborate cross sections

A next step to more realism is to make sure that not only the probability of encountering certain conductivity values matches that in the real aquifer, while also honouring their spatial covariance or their horizontal and vertical transition probability. This should better mimic the extent of the heterogeneities at the scale of the layers in the aquifer and the horizontal structure that we observe in actual geological cross sections. In fact, doing this, will satisfy the statistics of the real cross section as while keeping it's character determined by adjacent distinct facies, but the aquifer may look completely different that the real one. It's just a computation object required by our model.

5.3 Going fully geostatistical

Going fully geostatistical would be a final stap towards more realistic simulations. However, simple semi-variograms of the distribution of conductivities will not be enough; generating cross sections from it would smear out the distinct boundaries between facies. Hence, going fully geostatistical will require advanced geostatistical methods to allow honouring all features that we observe in real-world cross sections.

5.4 Finally still lacking the third dimension

Even if we go fully geostastical to maximize the match between our digital and real-world cross section, we still miss the third dimension, which may prove essential for mixing by the likely ubiquitous 3D cross-over of streamlines with associated particle exchange. This simply implies that we either include the third dimenension in our cross section or we mimic its effects by introducing some vertical mixing process that mimics it, like vertical dispersion. It's importance may vary though, but totally excluding it may prove wrong, especially in high-conductance zones.

5.5 Choice of the cross section type

Because high-conductive facies of some horizontal extent seem to matter most for the observed pollutant breakthorugh curves, our cross section must reflect this. There are different ways to generate sections with such properties. The one we adopt here is inspired by [Fiori et al. (2013)], [De Lange (2020)] and the sedimentological origin of them as explained in [Coe (2003)].

A rectangular array of conductivity zones is created. Then a cell in the array is arbitrarily chosen to center the next zone. The height and width of the zone are then chosen to label the area of the overal conductivity array. This is done until all cells of the conductivity array have been labeled. As a last step, the conductivties are randomly selected from a log-normal distribution and associated with each of the labels to generate the final conductivity field.

The conductivity field was generated using the data of [Fiori et al. (2013)], table 1.

$K_G = 8.9 \times 10^{-6}$ Geometric mean of K [m/s]

$\sigma_y^2 = 6.6$ Logconductivity variance

$I = 10.2\,m$ Horizontal integration scale (range of the semi-variogram of k_k)

$I_v = 1.5\,m$ Vertical intgration scale (range of the semi-variogram of k_v)

$\theta = 0.31$ Porosity

$J = 0.0036$ Mean head gradient

I did not use the parameters I and I_v directly.

5.6 Made cross section as applied by Fiori at al (2012)

Becaus of their success, we will mimic the the consturction of cross sections used by [Fiori et al. (2013)] in their MIM (multi-indicator) model to simulate plume break-through at the Made site. These sections consists of cubic blocks of equal size, equal to $2R$.

$Y = ln\,(K)$ is normal with $mean(Y) = \ln\,(K_G)$ and variance σ_Y^2 and of stationary symmetric autocorrelation $\rho\left(r^{'}\right)$ where $r' = \sqrt{\left(\frac{r_x^2+r_y^2}{I^2} + \frac{r_z^2}{I_v^2}\right)}$

The conductivity field in figure 2 has been generated according to the parameters used by [Fiori et al. (2013)]. These parameters are in the header of the figure. The zones all have the same width, equal to $2I_h = 21$m. The field was first generated with gstools using an exponetial model with lengths equals to I_h and I_v using the values for the mean conductivity and the variance of its logrithm as given in the figure 2. Next the section was divided into blocks of width $2I_h$ and the conductiviy value generated at its cente was attributed to the entire block. The blocks on overlying layers are shifted relative to each other as was done by [Fiori et al. (2013)].

The k-field was then used in Modflow to compute the heads and flows with fixed-head boundaries at both ends such that the mean head gradient was $J = 0.0036$. The Modflow results permit computing the stream function, which is given in figure 3. No particle tracking is needed for that. The stream lines, which are the contour lines of the stream function, clearly show how the particles flow up and down through the aquifer as caused by the heterogeneous conductiviy field. From these vertical components it should become immediately clear that there must also be components perpendicular to the cross section in real-world circumstances, which are neglected here but could be incorporated with a 3D model generated in the same way.

Figure 4 shows the pathlines as tracked by Modpath. 100 particles were released but only every 5th particle path is shown for clarity. The release elevations based on the stream function, are such that each particle represents the same amount of flow. The pathline pattern matches perfectly that of the streamlines, as they should in a steady-state situation. The heads are not shown here, but they are shown in figure 3.

Figure 5 shows the computed cumulative breakthrough curves at intervals of 100 m along the cross section. The times are quite long, which is due to the length of the section and the enforced gradient $J = 0.0036$. Notice the long tails for the greater x-values. Long tails are expected whenever the mass transport is essentially caused by advection through an aquifer that is heterogeneous on scales that are substantial with respect to the cross section. The size of the heterogeneities of $2I_h = 21$ m in this cross section can be observed in figure 2.

Finally, we compute the histograms from the obtained cumulative breakthrough curves. These overlapping histograms are shown in figure 6. The histrogram for $x = 1000$ m clearly shows the asymmetry of the

density curve with its steep front and long tail, a phenomenon that is characteristic for advection-dominated transport through a hegerogeneous subsurface.

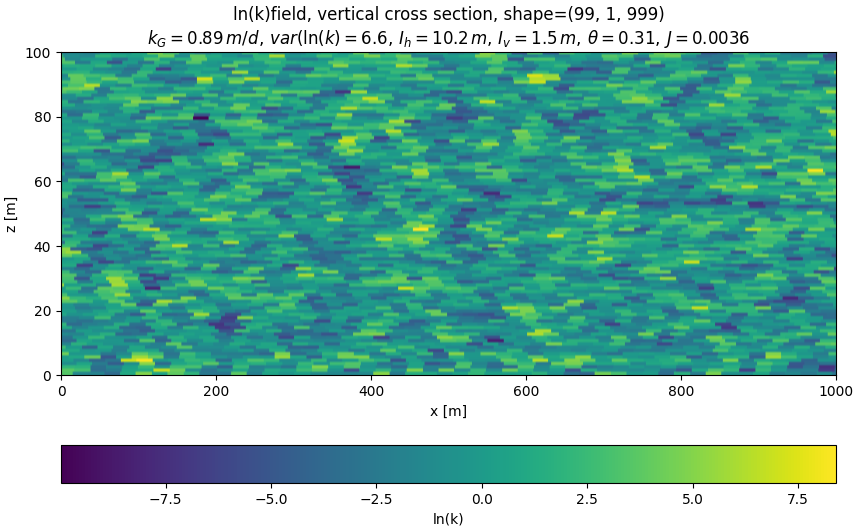


Figure 2: log-K-field, like in [Fiori et al. (2013)] with the same parameters (see header)

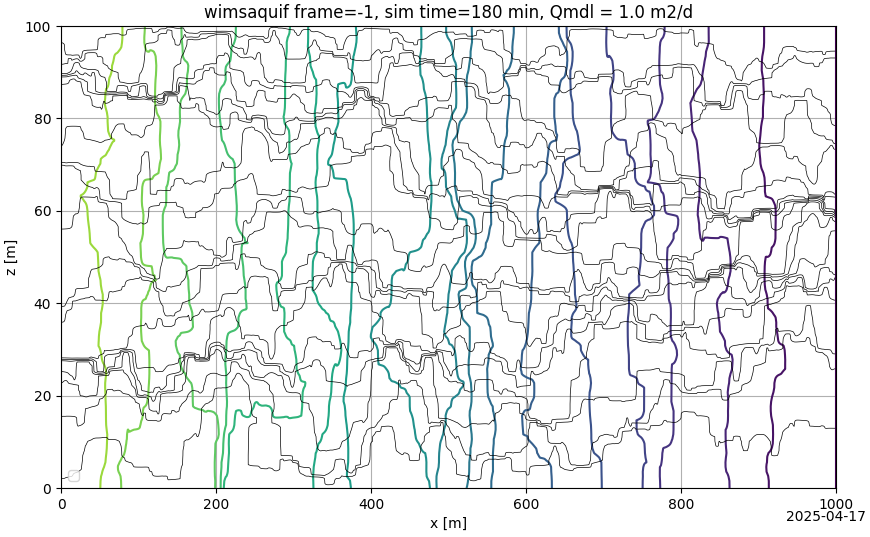


Figure 3: Stream function computed from the flow-right-faces in the cell-by-cell budget file generated by Modflow

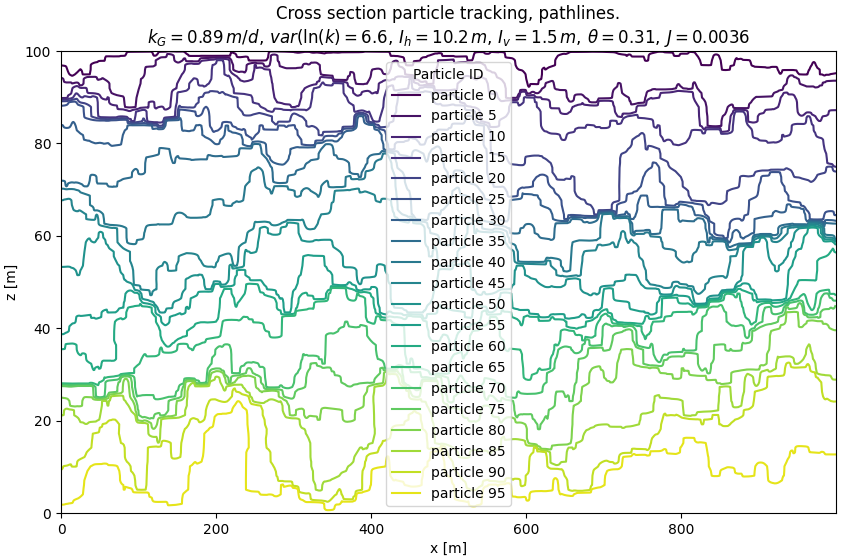


Figure 4: Modpath-computed pathlines.

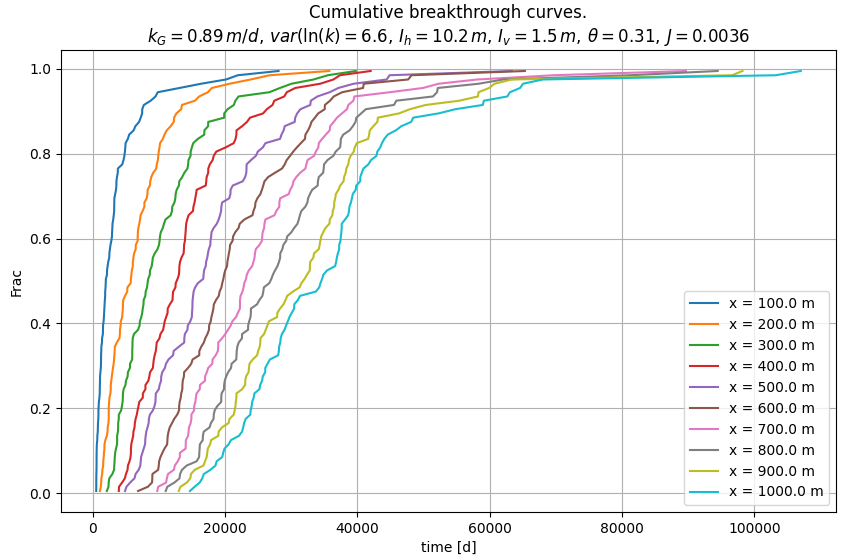


Figure 5: Computed comulative break-through curves

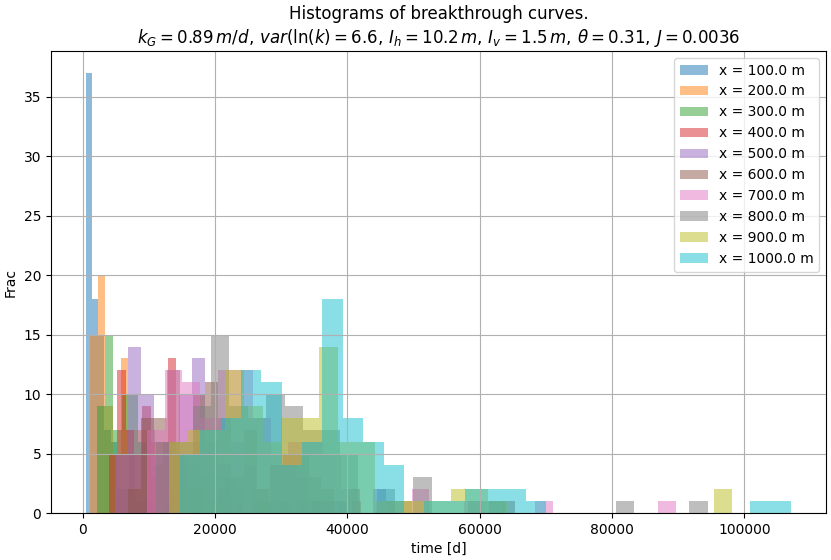


Figure 6: Computed break-through histograms

5.7 The same cross section with the same parameters except for a muck lower variance of the conductivity, namely $var(\ln(k))$ is 1.5 instead of 6.6

The more homogeneous the aquifer, the more the breakthrough will conform to Fickian or Gaussian character with more symmetrical breakthrough curves and histograms. We can test this with the same model by just changing the variance of the $\ln(k)$ field from 6.6 in the previous case to 1.5, a value which I deem more realistic for the more homogeneous aquifers found in the Netherlands. The results are given in the figures below. Figure 7 looks similar to figure 2, however, the colorbar below it shows that the values are different, and less extreme. Figure 8 shows that although the streamlines still go up and down along their paths, these fluctuations are now much less than those in figure 3. Also, the head contours are much more straight in figure 8 than in figure 3. This is also due to the more homogeneous aquifer that we created in this section. As expected, the cumulative breakthrough curves now show much more symmetry about the 50% value, with far a less extreme tail. In fact, except for the small asymmetry in the last curve for $x = 1000$ m, asymmetry are essentially absent for all shorter travel distances. Hence, all breakthrough curves are now essentially Gaussian. The symmetry of the breakthough behavior is also reveiled by the histograms and jumps into the eye when comparing figure 11 with figure 6.

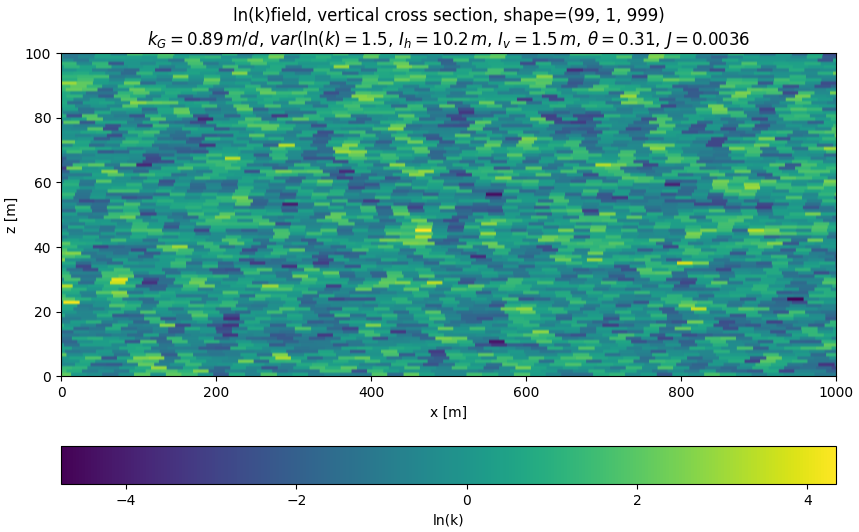


Figure 7: Image of the generated $ln\,(k)$ field for the cross section. For the rest the parameters are the same as in the previous section

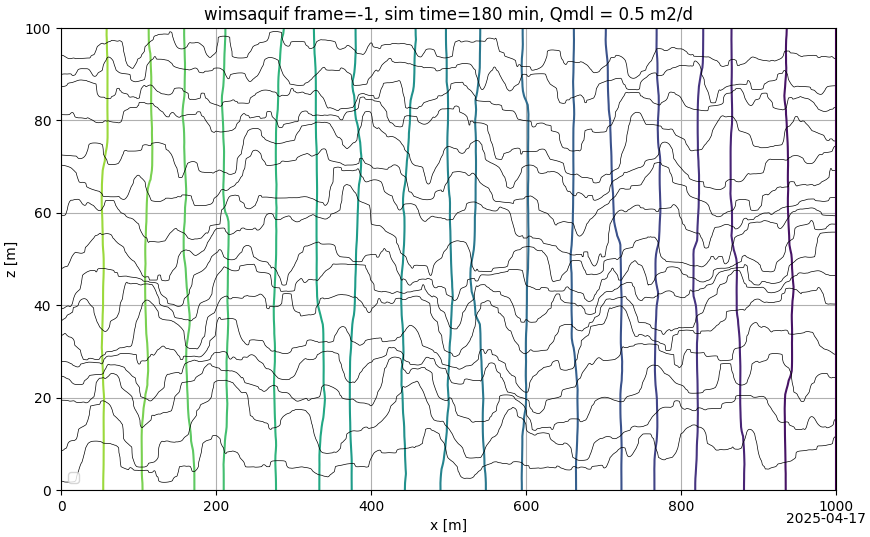


Figure 8: Srteamlines and head contours of the cross section computed using Modflow.

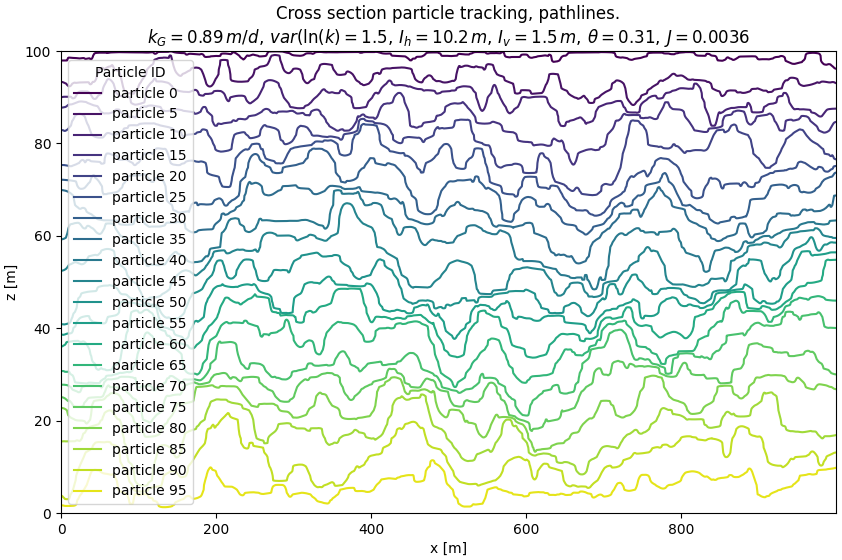


Figure 9: Pathlines, only every 5th particle is shown

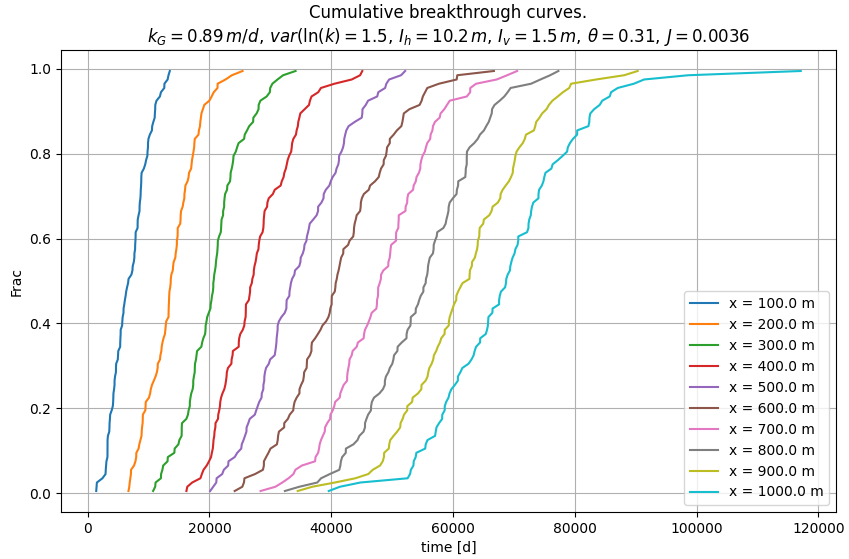


Figure 10: Cumulative break-through curves for different locations in the cross section

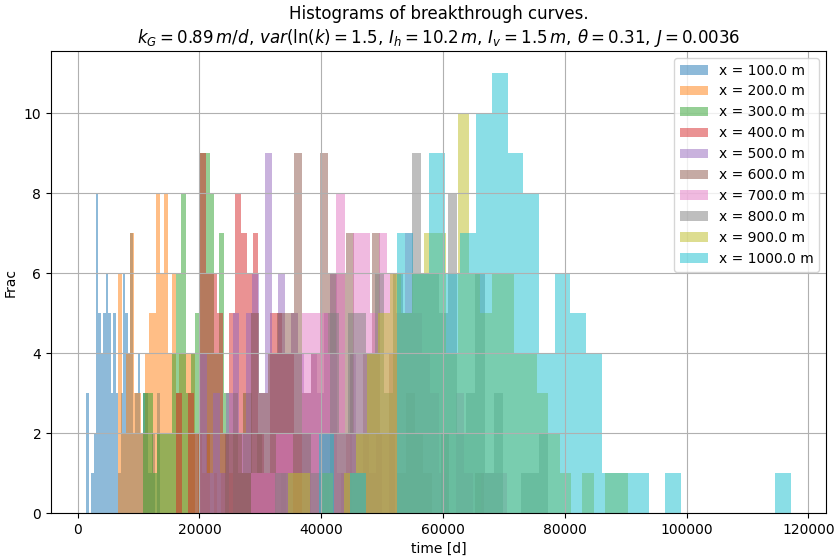


Figure 11: Histogams for the break-through at different locations long the cross section as computed from the cumulatives.

5.8 Regular Gaussian conductivity field with the same parameters as used in the MIM model of section 5.6.

The MIM model to simulate the MADE breakthrough curves in [Fiori et al. (2013)] uses blocks of width $2R$, essentially $2I_h$ with each having a constant conductivity throughout the block, while these block conductivities area conform the statistics for $\ln(k)$, for $var(\ln(k))$ and for the integration lengths I_h and I_v. Instead of using blocks, it may be feasible to simply generate a cross-section that fulfills these condictions but without resorting to the blocks of the MIM model. The cross section generated this way, is shown in figure 12. It lacks the block structure, which characterizes the cross section of figure 2. The stream and head lines in figure 13 are as irregular as in figure 3, which is due to the same large log-conductivity variance used in these two cases. Figure 14 shows the breakthrough curves. The top figure shown those belonging to the current conductivity field, while, for easy comparison, the bottom figure is the same as figure 5 for the model with the block structure, but otherwise the same parameters. Figure 14 makes clear that, also with a fully continuous Gaussian field, similar breakthrough curves are obtained as with a MIM-type model with blocks. Probably it is just the applied range of the horizontal and vertical variograms that matter to get a behavior characteristic of preferential flow path, while it does matter little if a block structure is added. Figure 15, on top, shows the histograms derived from the breakthrough curves for this continuous cross section, and at the bottom, again for easy comparison, those obtained with the block structure and otherwise the same parameters already shown in figure 6. I would argue that both figures are not too different. They are essentially characterized by asymmetry with a large tail, which is what one expects from a strongly heterogeneous aquifer.

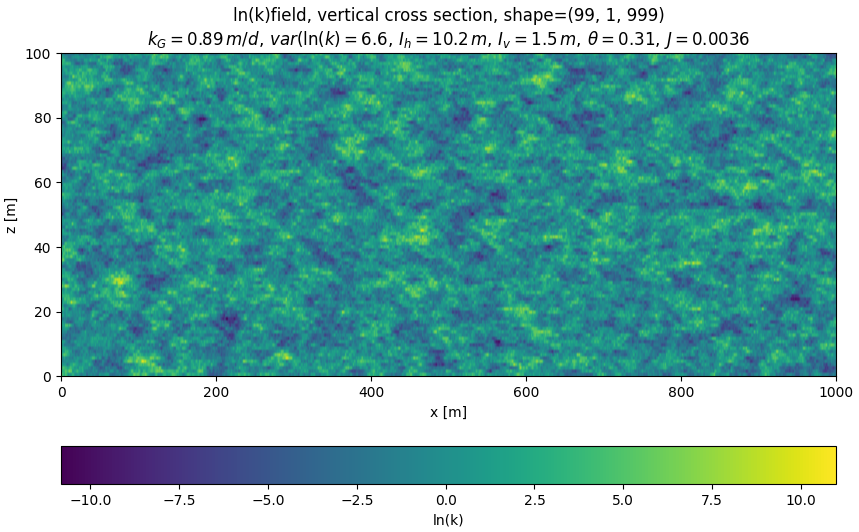


Figure 12: Generated ln(k) field using exponential model with variance and $x_{len} = I_h$ and $z_{len} = I_v$, and the parameters given in the header of the figure.

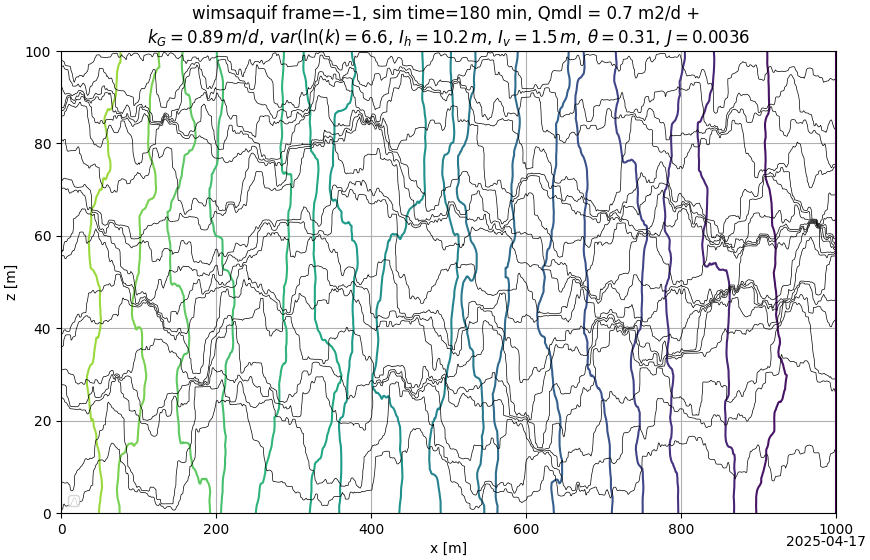
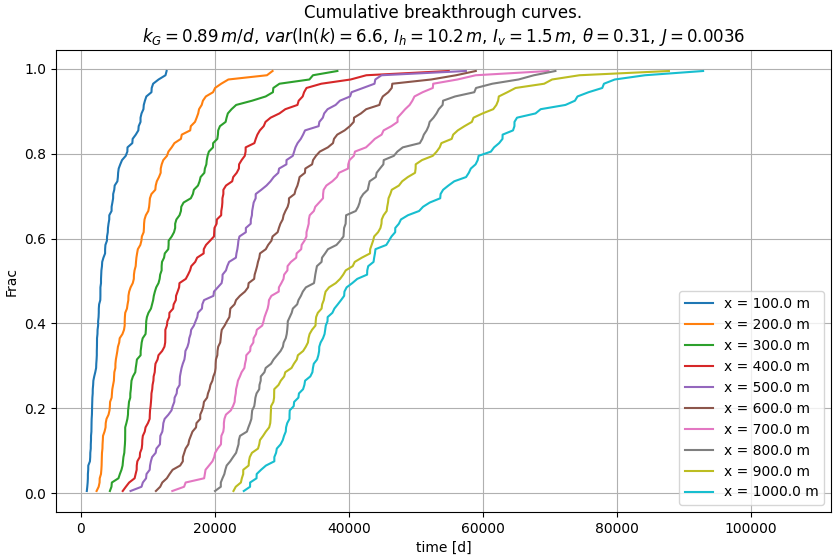


Figure 13: Stream function and head contours after simulating the cross section with the conductivity field in the previous figure.

Gaussian Field



MIM blocks field

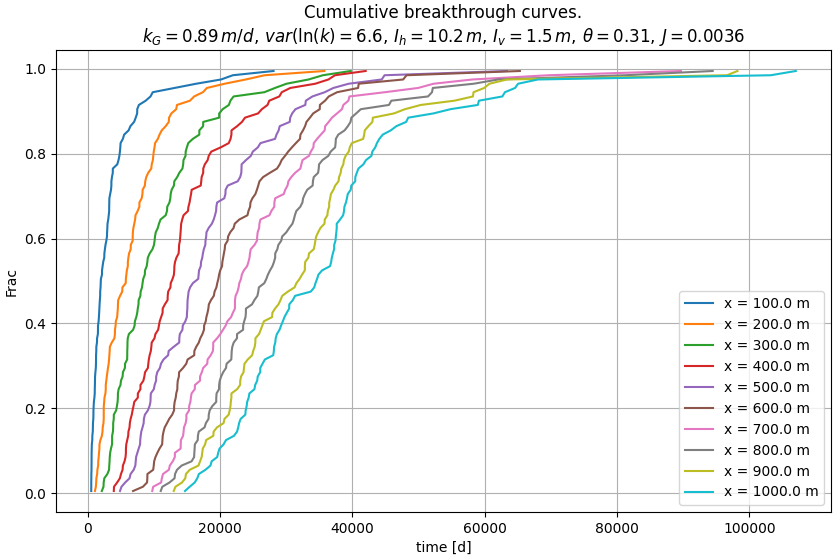
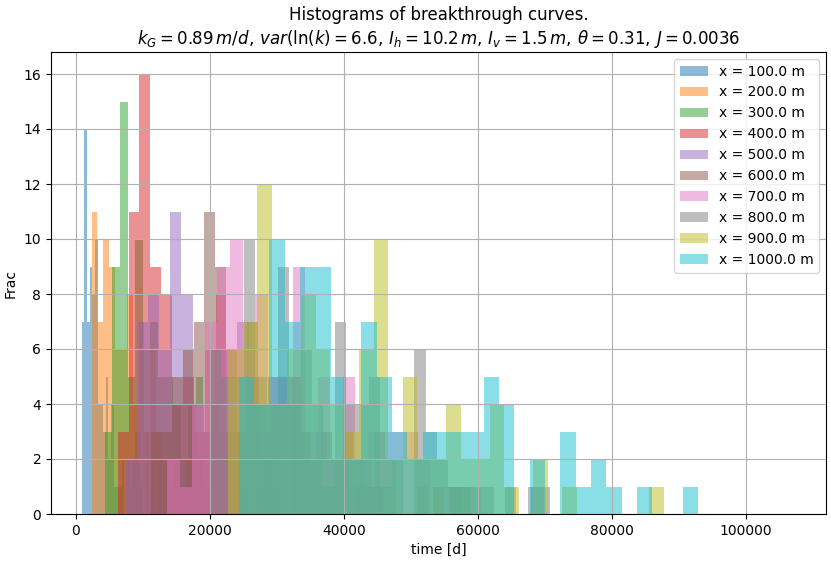


Figure 14: Breakthorugh curves compute using Modpath.

Gaussian Field



MIM block field

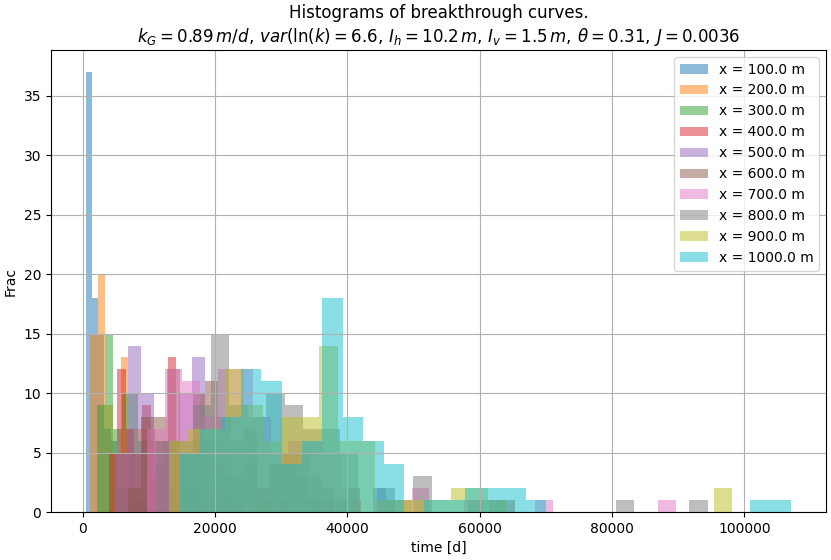


Figure 15: Histograms derived from the breakthrough curves in figure 14

6 Wim's aquifer

In his papers, simulates the dispersion using an artificial aquifer built of blocks, he calls domains of given size that are place next to each other and on top of each other as to fill the entire cross section of the aquifer. Each block as a low background conductivity and includes an elongated facies with a high conductivity. The background and high facies conductivities are the same in each block. For this example they are chose to be 5 and 500 m/d respectively.

Like in the previous examples the cross section has the same size, 100 m deep and 1000 m wide with cells of 1x1 m^2. Each block was given the size of 20 cells along the x-axis and 5 cells along the z-axis. The facies was placed randomly inside each block. The inner facies was given the size of 20 cells along the x-axis and 1 cell along the z-axis. This is about what De Lange uses in his example pictures. The boundary conditions

are the same as in the previous examples, a gradient of 0.0036 and a porosity of 0.31. The results of the simulation are in the following pictures. Figure 16 shows the $\ln(k)$ field, i.e. one background conductivity and one facies conductivity according to the header of the figure. Figure 17 shows the streamline and the head contours. The high-conductive inclusions clearly distort and channel the flow through them. Figure 18 shows the cumulative breakthrough curves for different locations along the cross section. They are not symmetric due to the hetergeneous character of the aquifer. However, the asymmetry can be deemed not so high as expectec. The same conclusion can be drawn from the histograms in figure 19 they are far less asymmetric than expected. Therefore, they might be reasonably modelled by a more tranditional Fickian model. Perhaps the number of inclusions or their lengths are to small to deem this aquifer a really heterogeneous despite the large contract between the background and the facies conductivities.

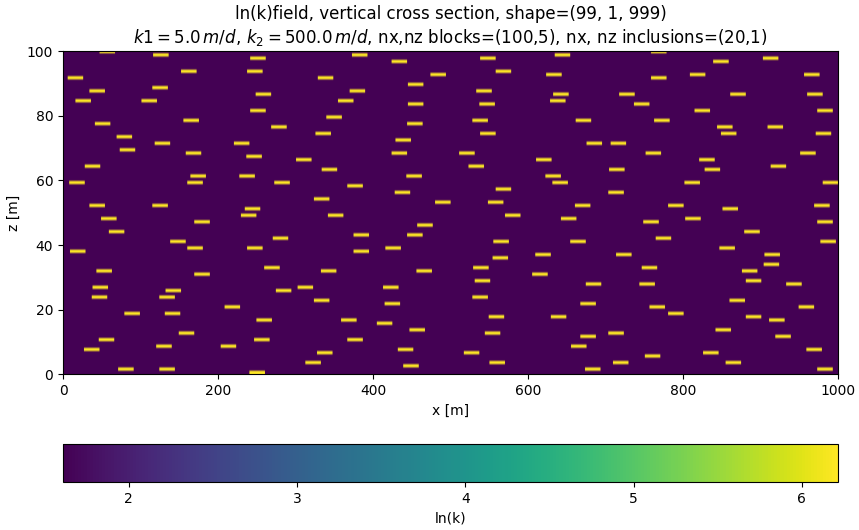


Figure 16: Conductivity field with background and facies data given in the header.

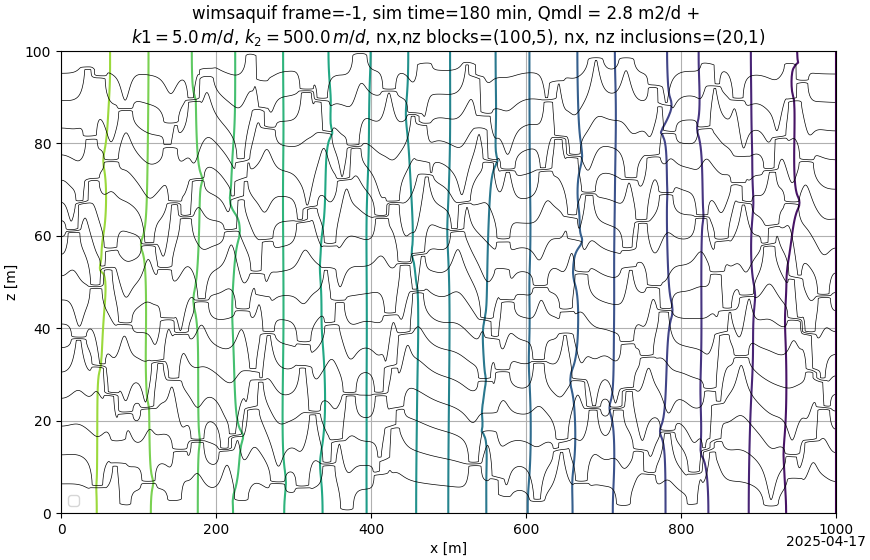


Figure 17: Streamlines and head contours for the simulated cross section. Only every 5th particle is shown.

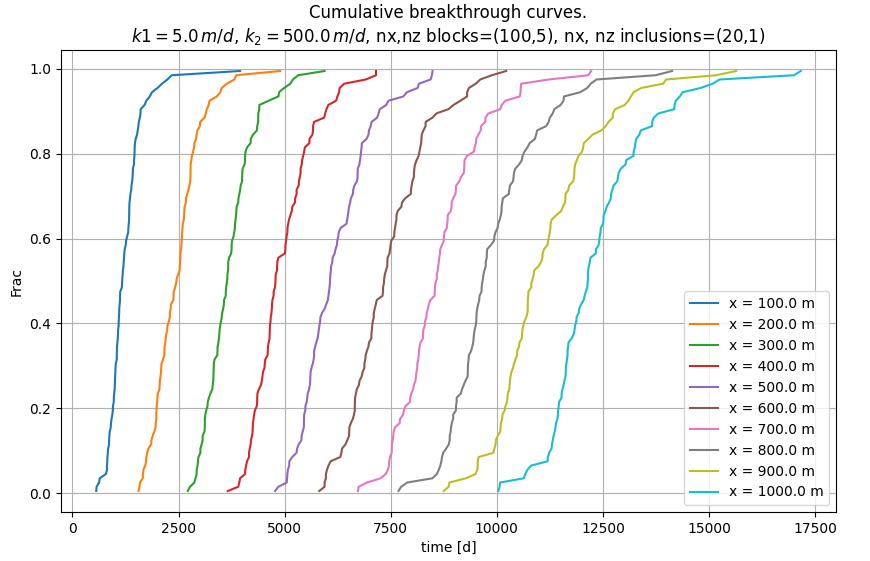


Figure 18: Cumulative breakthrough curves at different locations along the cross section

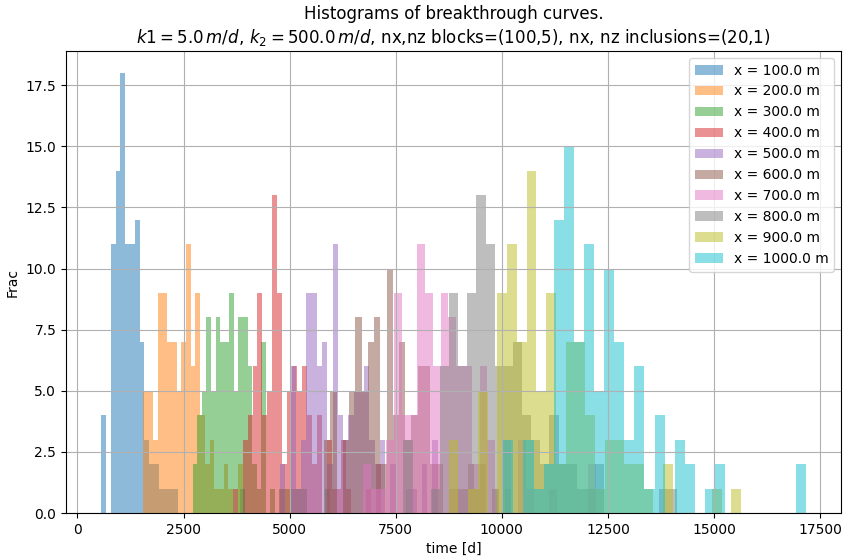


Figure 19: Histograms of different breakthrough points along the cross section

7 Summarizing the discussion on dispersion

A phenomenon, including that of dispersion of a pollutant in moving groundwater, can often be best understood by looking at its behavior or results in extreme situations. We may, therefore, ask ourselves how dispersion develops in the following two extreme cases:

- Uniform flow in a perfectly homogenious aquifer, with grains as fine as the water molucules themselves. Hence, there are no velocity variations.
- Flow in an aquifer that is layered and heterogeneous to the extreme. Hence, it consists of two parallel layers one with (almost) zero conductivity and the other with some distinct conductivity.

Over these cases, we may drape the process of diffusion, which is known to always work and does so at its own pace, irrespective of the actual velocity of the groundwater itself.

In the first case, the only movement of particles is the progress of the front, initally flat and pependicular to the flow, which will always remain sharp and stay perfectly flat. The only thing diffusion does is to cause some spread in longitudinal direction. Without diffusion, the breakthrough curve would be vertical. With diffusion it would still be very steep. The breakthrough curve would be fully described by the average front position and its standard deviation $\sigma = \sqrt{2D_d t}$. Even if the particles would be subject to some small-scale random velocity varations, the front will have the same properties, with a σ that will be larger than that caused by molecular diffusion, probably even be much larger, but would still follow this expression $\sigma = \sqrt{2Dt}$. Only now we have $D = D_v + D_d$ and since the random velocity differences are proportional to the groundwater velocity itself, we would have $D = a_L v + D_d$ and the process would be fully Gaussian and Fickian, with a head and tail of the same length and shape.

In the second extreme case, a part, may be half of the water will be funelled through the high-conductive layer, with the rest lagging far behind. When we call the situation at some point in time also a plume, we see that we have a head and a tail completely defined by the velocities in the two layers. Let the velocity in the two layers be v_1 and v_2 with conductivities k_1 and k_2 respectively and a gradient i and porosity θ, we have

$$v_1 = k_1 i/\theta$$
$$v_2 = k_2 i\theta$$

The total discharge through the aquifer then equals

$$Q\theta = D_1 k_1 i + D_2 k_2 i = D k_m i$$

With D_1 and D_2 the thicknesse of the respective zones and D the aquifer thickness.
Assume that the same amoun of water flows through both zones, so that $D_1 k_1 = D_2 k_2$

$$k_m = 2\frac{D_1}{D} k_1$$
$$k_m = 2\frac{D_2}{D} k_2$$

We are still free to choose k_1/k_2 or D_1/D_2 or D_1/D for that matter. Just take $D_1 = 0.1 D_2$so that $k_1 = 10 k_2$ then

$$k_m = 2\frac{0.1}{1.1} k_1 \approx 0.19 k_1 \rightarrow k_1 \approx 5.3 k_m$$
$$k_m = 2\frac{0.9}{1.1} k_2 \approx 1.64 k_2 \rightarrow k_2 \approx 0.61 k_m$$

We could even take a more extreme case in which $D_1 = 0.001 D_2$ so that $k_1 = 1000 k_2$ yielding

$$k_m = 2\frac{0.001}{1.001} k_1 = 2\frac{0.999}{1.001} k_2 \approx 0.002 k_1 \approx 2 k_2$$

in which still half of the discharge flows through the thin conductive layer and the other half through the thick layer with the lower conductivity. In these, cases, even when equal amounts of water pass through both zones, the distance traveled in the fast, high-conductive zone is more than 5 to 500 times the average traveled distance, and that in the low-conductive zone is about 60% to 50% of the average traveled distance, where 50% is the limit case.

What happens if we sample the water by means of a well that extracts all the water at a certain point? Then, as soon as the fast front passed this point, the relative concentration would jump to 0.5 to remain constant until the tail passes, at which point the relative concentration would jump further to 1.0. From these samples one could conclude that the mean of the front would lie half way between the two mentioned times and that its spread would amount to $\sigma = \frac{t_1 - t_2}{\sqrt{2}}$. On the other hand, if one samples the aquifer without actually extracting water by a well, for instance by means of a device that can measure some quality aspect in situ at any depth, and if we then take the mean along the vertical, a completely different breakthrough curve would emerge. As the fast zone has only one tenth or even one thousandth of the thickness of that of the slow zone, the relative concentration would, after passing the sampling location, only jump up to 0.1 or to 0.001 instead of 0.5 and would rise to 1. 0 after passage of the front in the slow zone. Therefore, the way of sampling may make a huge difference in the outcomes.

What also jumps into mind in this extreme case, is that the spread, i.e. the distance between head and tail, grows proportionally to time and, therfore with distance. In the case of Fickian disperion it grows proportional to the root of time. Reality will likely pop up somewhere in between.

If we drape diffusion or our ignored random small-scale velocity velocity variations over the last situation, there will be some longitudinal dispersion, which may be negligible relative to the fast moving head of the front. However, we will also see some dispersion across the horziontal line separting the two zones. The importance of this sideways spreading depends on the magnitude of the process, or perhaps to the absolute speed of the groundwater relative to diffusion. Nevertheless, if one imagines a very large sideways dispersion, it would cause the head of the front to loose concentration to the water in the slow zone. The larger this process the more the end result will resemble Fickian behavior. Imagine that the fast zone were split into a vast number of subzones spread out over the vertical but still making sure that the combined transmissivity of these fast subzones remains equal to that of the original one. This would make diffusion dominant instead of negligible, even with the same overal transmissivities, conductivities and zone thicknesses; it would completely alter the shape of the front. Hence, size or layering matters. This includes time as it affects the size of the spread by diffusion, which, as we have seen will grow to aquifer-height proportions if

sufficiently long. Even much shorter times may be important if the fast and the slow layers are thin. Reality will always be somewhere in between. The more homogeneous the aquifer, or the thinner the layers, the more Fickian the dispersion process will be. The more heterogeneous in the sense that the flow is more dominated by preferential flow paths, the less Fickian the dispersion will be, and the more its spread with grow linearly with time and distance. Because the streamlines in real-world cases will pass through sequences of zones of higher and lower conductivties of different extent, the spread may grow towards linear with traveled distance, the larger the probability of encountering high-conductivity zones of even larger exent that channel the grounwater along preferential paths.

8 Summary and conclusions

Dispersion during subsurfacde mass transpport was studied based on recent papers as mentioned in the references. The phenomemon of dispersion is still not totally tackeled in models as well as in theory. [Zheng et al. (2011)] mentioned the dual medium feature, adding kinematic sorption, that was built into the MT3DMS mass transport model to better capture the observations of tracer tests in the Made test side [Zheng et al. (2011)]. However, the improved match may well have been reached for the wrong reasons, as there was no sorption active at the site during the bromium tracer test. At least [Fiori et al. (2013)] showed that a similarly accurate result could be reached with their MIM (multi indicator model), which only took advection into account. The problem is believed to has been the impossibility to characterize and model the heterogeneous conductivity field in the subsurface accurately enough, because therein seems to lie the key to successfully model subsurface displacement of pollutants and successfully include match the observed dispersion.

It is generally known that in real-world situations flow along preferential paths is often dominant. At the same time, it is extremely hard to predict beforehand based on methods available to characterize the subsruface's conductivity field in all three dimensions. While in more homogeneous aquifers dispersion tends toward Fickian behavior, in heterogeneous aquifers it does not. Fickian behavior sees dispersion as a Gaussian process, which yields symmetrical breakthrough curves and histograms with the spread that grows according to the square root of the traveled distance. However, non Fickian behavior as observed in hetrogeneous aquifers, show asymmetrical breakhrough curves and histograms, with early breakthorugh and a large tail, with an associated spread that grows linearly with travel distance.

This non-Fickian behavior was shown by modelling a heterogeneous aquifer with the properties of the Made site ([Fiori et al. (2013)]). The aquifer generated with those parameter values, was similar to that by which [Fiori et al. (2013)] were able to reasonably well model the bromide tracer test at the Made site. The results show indeed that the breaktrough curves and breakthrough histograms have an early breakthrough with a long tail. The opposite, more Fickian result was obtained by modeling another cross section generated with the same parameters, but with a far lower $\ln(k)$ variance, which resulted in a much more homogeneous aquifer. The aquifer used by [Fiori et al. (2013)] consisted of blocks with a length of around 20 m based on the horizontal integration scale (range of the semi-variogram). Each block got a conductivity value chosen from a generated random field with the proper statistical values. In the third example, we left the block structure out and directly used the statistically generated conductivity field. The results show that they are similar to those of the first example, generated with the same statistical parameter values (see the header of each figure for the values used). Hence, using the block structure does not seem to add much to the results; only the horizontal and verticla semi-variograms used to generate the random field seem to matter.

Finally, a cross section was generated alike the one De Lange uses in his papers to demonstrate and simulate dispersion in very heterogeneous aquifers. De Lange, for the sake of modelling dispersion, sees the aquifer as layers of equally sized blocks called domains, which are put next to and on top of each other to fill the aquifer. Each block has a low background conductivity (of 5 m/d) and holds an elongated, rectangular inclusion with a high conductivity (of 500 m/d). This cross section was simulated in the same way as the previous ones. Expected was a strong non-Fickian behavior to show up in the breakthrough curves and the histograms. However, this proved hardly the case. So perhaps the cross section was not heterogeneous enough, despite the 100-fold conductiviy contrast between the background and the included facies conductivities.

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