Dispersion according to Wim de Lange

T.N. Olsthoorn

2025-04-23

Inhoudsopgave

1 The generally assumed theory of dispersion (for simplicity only considering 1D) questioned by [de Lange (2020), De Lange (2022), De Lange (2025)])

Dispersion in 1D starting from a sharp front and assuming the front dilutes accoring to a molecular diffusion process, a process that works on the scale of molecules, but is now assumed that it also works due to pore scale velocity variations. Einstens formula for the increase of the standard deviation σ [L] of the concentration front with time for molecular diffusion with a melecular diffusion coefficient D [L^2/T] is

$$\sigma_t = \sqrt{2Dt}$$

For 1D dispersion D becomes the dispersion coefficient, which now also depends on the dispersivity and the velocity of the groundwater

$$\sigma_t = \sqrt{2\left(\alpha_L v + D\right) t}$$

and with $\alpha_L v \gg D$

$$\sigma_t \approx \sqrt{2\alpha_L v t}$$

$$\sigma_L \approx \sqrt{2\alpha_L L} \sim \sqrt{L}$$

This implies that if disperision works as in this generally appied theory, that then the dispersive dilution both in front of and behind of average position of the moving front would be similar to molecular diffusion, i.e. as if it was driven by concentration gradients, and that the σ_L would be proportional to the root of the traveled distance. Furthermore, the head and the tail of the front would be symmetrical with respect to the average location of the moving front.

As De Lange found that these aspects do not comply with the findings of most field studies carried out throughout the world, which I demonstrates by comparing the reported values from these studies, he challenges these basic assumptions in his papers.

2 Assumptions

Wim has recognized from his own experience that, in practice, dispersion does not comply with the theory outlined above. He has been inspired by the work of Jankovic (2003, 2006 etc) who focused on dispersion fully based on flow velocity differences caused by heterogeneities present in the aquifer, so velocity differences between subsurface pathlines that are caused only by advective transport through a porous medium with a heterogeneous conductivity field in which the size of the heterogeneities are of the order of meters and not of that of the pores or the size of the grains. He further basis his theory on the obsevation that in natural aquifers, conductivity contrasts that form the hetergeneities, often have lengths of the size of many to to tens of meters, which easily exceed their vertical size by an order of magnitude. From this he concludes that the main subsurface mixing process causing apparent dispersion at the macro scale is advection distored by the presence of such elongated heterogeneities, facies as know to geologists and sedimentologists. These facies, which are repeatedly encountered by groundwater flowing through the subsurace with have different size and conductivities. Part of them will have conductivities higher to perhaps much higher than the average of the aquifer, while another part will have conductivties that are lower to much lower than the average of the aquifer. The range of conductivities present in the aquifer is mostly defined by the lognormal distribution of sampled conductivity values.

The Lange shows how this mixing works for a single elongated heteregeneity with a conductivity that constrasts with the uniform conductivity of the background aquifer. He the shows that impact this heteregeneity has on the shape of the front in the case of a high-conductive heterogeneity differs fundamentally from that of the distortion of the shape of the front caused by the presence of a low-conductive hetergeneity. The high-conductive elongated heterogeneity mainly causes a relatively wide foward bulb of the front with a small slow-down of the rest. The low-conductive elongated heterogeneity leaves the bulk of the front intact but distorts it by generating a long tail. The combined effect of an elongated high conductive heterogeneity and an elongated low-conductive heterogeneity is a distorted front that is higly asymmetrical around its average moving position.

De lange goes on to quantify seperately the two distortions, i.e. that of the head and the tail of the moving front. In his concept the front distortion is stable from some point after the high-conductive heterogeneity, where the flow has regained its unifromity. The tail distortion, however, will extend over potentially much larger distances after the bulk of the groundwater has passed the low-conductive heterogeneity. The lower its conductivity, the longer (and thinner) the tail-distortion of the nitially flat front. This fundamentally different behavior caused by relative conductivity determines the asymmetry of front distortion encountered in real-world situations, and is caused purely by advection.

3 Real-world aquifers

In the real-world situaiton, there are many heterogeneities of these types, each with a different conductivity and with a different length and thickness. Therefore, to generalize the concept, the connection with the actual real-world aquifer conductivity field has to be made. De Lange accepts the idea that, as an approximation to reality, the conductivy sampled in a real-world aquifer generally shows a lognormal probability distribution.

One way to jump from his concept to the real-world aquifer would be superposition. I.e. super-imposing the effect of many such heterogeneities which got the properties assigned based on the lognormal distribution of the conductivity sampled in the real aquifer while honoring their semi-variograms in both horizontal direction(s). However, it's not clear that superpostion is could be valid when applied to travel-time distortions. But perhaps it is in some sense.

De Lange simply says, without proof, that when the bulk conductivity of the aquifer is taken equal to the geometric mean of the conductivty distribution and that of the elongated k-contrasting heterogeneity is taken equal to that at $+\sigma$ for the high-conductive heterogeneity and at $-\sigma$ for the low-conductive one, the behavior of his model reflects that of the real-world aquifer. Hence he says, with σ the standard deviation of the undelying normal distribution of $\ln(k)$ the the geometric mean of k equal to k_g, or, equivalently, the additive mean of $\ln k$ equal to $\ln k_g$:

$$\ln \frac{k_{+\sigma}}{k_g} = \ln k_{+\sigma} - \ln k_g = \sigma$$

and so

$$k_{+\sigma} = \exp\left(\ln\left(k_g\right) + \sigma\right)$$
$$k_{-\sigma} = \exp\left(\ln\left(k_g\right) - \sigma\right)$$

The other step to be made from reality to model is the translation of real-world integration lengths or semi-variogram ranges to the conceptual model. He describes the plume, where in fact, he is describing the distortion of an initially flat front. The distortion of the front caused by high-conductive zone in domain A is Δs_{Af}, that of caused by the low-conductive heterogeneity is Δs_{At}. The length causing the distortion is the length over which the flow across the vertical is „clearly" not uniform. The distortion lenght can be derived and estimated by hand-calculation. Dropping index A for convenience we get

$$\Delta s_f = \left(1 - \frac{k_g}{k_{+\sigma}}\right) L_{dis,f}$$

$$\Delta s_t = \left(1 - \frac{k_g}{k_{-\sigma}}\right) L_{dis,t}$$

With $k_g \ll k_{+\sigma}$ and $k_g {\gg} k_{-\sigma}$ we get

$$\Delta s_f \approx L_{dis,f}$$

and

$$\Delta s_t \approx -\frac{k_g}{k_{-\sigma}} L_{dis,t} = -e^{-\sigma} L_{dis,t}$$

Fig 3 in de [De Lange (2022)] illustrates that the length of the forward bulge in the front after passing an elongated high-conductive zone is about the length os this zone, whereas it is much longer for the backward tail in the front after passing the low-condutive zone. The length of this tail matches the 5 times lower than bulk conductivity of this latter zone.

In the same way, the thicknes of the wake, or the vertical spread, which can also be derived and hand-calculated. Then, leaving out the ratio of the porisities (assuming this ration ≈ 1), then becomes

$$\frac{W_f}{D} = \frac{1}{1 + \frac{k_g}{k_{+\sigma}}\left(\frac{1}{N} - 1\right)}$$

$$\frac{W_t}{D} = \frac{1}{1 + \frac{k_g}{k_{-\sigma}}\left(\frac{1}{N} - 1\right)}$$

With $k_g \ll k_{+\sigma}$, $W_f \to D$ for $k_g/k_{+\sigma} \to 0$ and with $k_g \gg k_{-\sigma}$ $W_t \to 0$ for $k_k/k_{-\sigma} \to 0$. Hence the $L_{dis,t} \to L$ and $L_{dis,f} \to L + 2D$ or any value between L and $L + 2D$.

If the length of domain A is considered equal to the length over which the mixing is completed, it should equal $L_{dis,f}$, but for the tail it would be much larger.

At this point, it's still not clear how the length of the fundamental mixing box, named domain A is determined.

At this point, we still don't know how mixing occurs in the real aquifer with many zones within each zone.

4 Construction of the proper cross section

To construct a cross section that complies with the concept developed by De Lange (2020, 2022), we have to choose domains A with L a bout 6 λ_h and D about 6 λ_v, given the hint by De Lange that the scale factor N is about 3 while $L_A = 2\lambda_h N$ and $D_A = 2\lambda_v N$ with λ_h and λ_N the horizontal and vertical correlations lengths. But what is not clear, is how to include both the low conductivity zone and the high conductivity zone in a single domain or, for that matter, a single cross section? I could just generate the cross section with two zones in each domain, one low-k and one high-k zone and position them at random within each domain. Or, generate mixing boxes with either a high-k or a low-k zone in them and randomly position these boxes in the cross section. Of one could split the aquifer in two parts, an upper half and a lower half, and fill the upper half with high-k domains and the lower half with low-k domains, and afterwards collect all the particles. But at the same time, we would like to maintain the transmissivity of the entire aquifer the same. It is not clear how to do this, except for running the model and use the computed flow to scale back the result. But then we'll loose the link with the lognormal distribution of the real-world aquifer. Therefore, in fact, I have no clue of how to do this. The most logical approach in my opinion, is to use a conductivity field that is generated with the given real-world aquifer correlation lengths and its lognormal conductivity distribution, which is in fact, what I did already.

I conclude, the simulation with the random conductivity field, with the correct correlation lengths and conductivity, probability is the conductivity field that should generate the most realistic breakthrough curves, which then should be in accordance with De Lange's conceptual model.

5 Front distortion over large travel distances

[De Lange (2022)] writes „In each domain (mixing box) the dispersion process is averaged leasing to linear growth of the plume." I don't yet see that this exactly means. Averaging is mxing, which is what a mixing box is supposed to do. However, the analysis until now just handled what is happening in a single box due to passing an single inhomogeneity. I would expect an analysis of the shape of the cumulative probability density distribution of the pollutant concentration leaving the box, when the shape was sharp at the front of left side of the box. Once we have this, we could place many such boxes next to each other and observe or compute change the shape of the cdf after each box passed. We can then analyze this using the theory developed by [Maas (1994)] in his thesis. This would seem to me a straight-forward exercise because the math lies ready, at least for indepent successive mixing boxes. I suspect the variances should be added, same increment after each box.

Maas proves this in chapter 2 of his thesis. He also proves that, with successive mixing boxes passed, the mean distance increases linearly as does the variance of the break-through curves. The result approaches a Gaussian or normal type of breakthrough after an infinite number of boxes passed. On page 16, he addresses the fact that breakthrough curves of practical tests are often considerably skewed. Which, when it happens, implies that the Gaussian limit has not yet been reached. In fact, this is the subject of De Lange's papers. Maas refers to [Chatwin (1980)] who fitted longitudinal dispersion, which he found to be definitivily non-Gaussian. Maas continues to elaborate the skewness of breakthrough functions and finally finds the Pearson type III distribution as a modification of the generalized gamma distribution (Abramowitz and Stegun, 1964, p255). This Pearson III distribution has only 3 degrees of freedom and generates breakthrough curves (i.e. cdfs) that are very skewed for early times and then, with increaring time, gradually evolve towards the normal distribution as the cenral limit theorem demands (Figure 1). Maas writes that the gamma distribution along with the lognormal distribution have been proposed earlier by [Jury & Roth (1990)]. They speak about Travel Time Probability Density Functions and regard them as an integral soil property to be measured in the field. I like to agree with their conclusion and I would say that we can measure this propertie also in the model by letting particles flow through a given conductivity field with predescribed properties (and compare it with physical experiments, of course).

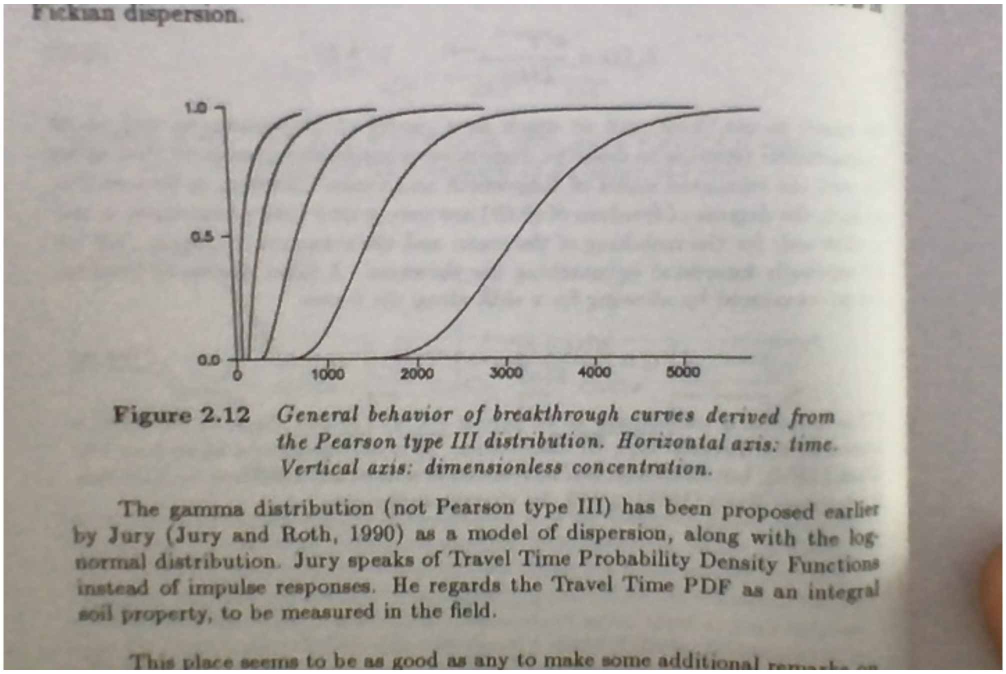
Fickian dispersion.

Figure 2.12 *General behavior of breakthrough curves derived from the Pearson type III distribution. Horizontal axis: time. Vertical axis: dimensionless concentration.*

The gamma distribution (not Pearson type III) has been proposed earlier by Jury (Jury and Roth, 1990) as a model of dispersion, along with the log-normal distribution. Jury speaks of Travel Time Probability Density Functions instead of impulse responses. He regards the Travel Time PDF as an integral soil property, to be measured in the field.

This place seems to be as good as any to make some additional

Figuur 1: From [Maas (1994)], showing time-breakthrough curves according to the Pearson type III distribution.

6 ChatGPT

6.1 Question 1 to ChatGPT

W.J. de Lange as published two or three papers since 2020 on dispersion in Journal Groundwater. What is actually his message?

Answer from ChatGPT W.J. de Lange has contributed significantly to the understanding of dispersion in groundwater systems through his publications in the journal Groundwater. His research focuses on the role of advective transport phenomena in explaining dispersion observed in field conditions, challenging traditional reliance on Fickian diffusion models.ngwa.onlinelibrary.wiley.com+1ngwa.onlinelibrary.wiley.com+1

Key Messages from de Lange's Work:

Advective Transport as a Primary Mechanism:

De Lange emphasizes that dispersion in groundwater is predominantly governed by advective processes resulting from aquifer heterogeneity, rather than solely by diffusive mechanisms. He illustrates how variations in hydraulic conductivity within aquifers lead to differences in flow velocities, causing spreading of solute plumes.

Asymmetry in Plume Development:

His studies highlight the asymmetric nature of plume dispersion, where the plume front and tail develop differently due to the presence of high and low conductivity zones. High-conductivity zones tend to accelerate the plume front, while low-conductivity zones retard the tail, leading to an uneven spread that traditional models may not accurately capture.

Introduction of the Macroscale Dispersion Correlation Coefficient (r):

De Lange introduces a correlation coefficient to quantify the degree of dependency in dispersion across successive domains within an aquifer. This parameter helps in understanding whether dispersion processes are independent or correlated, which has implications for predicting plume behavior over larger scales.

Practical Tools for Field Application:

Recognizing the need for accessible methods in engineering practice, de Lange provides analytical expressions and tools, such as spreadsheets, to calculate dispersivities and plume spreads. These tools are designed to be user-friendly for practitioners dealing with real-world groundwater contamination issues.

In summary, de Lange's work advocates for a shift towards models that incorporate advective transport phenomena and aquifer heterogeneity to better understand and predict dispersion in groundwater systems. His contributions offer both theoretical insights and practical tools for engineers and hydrogeologists.

6.2 Question 2 to ChatGPT

W.J. de Lange in his 2020 and 2020 paper on advective dispersion in journal Ground Water develops a framwork with which he explains and quantifies the development of asymmetric breakthrough curves caused by a heterogeneous conductivity field passed by groundwater. He takes much time to explain is so-called domain A. However, I can't find on what he basis its size or scale factor N. Can you figure that out for me?

Answer from ChatGPT In W.J. de Lange's 2020 and 2022 publications in Ground Water, he introduces a framework to explain and quantify asymmetric breakthrough curves resulting from groundwater flow through heterogeneous conductivity fields. Central to this framework is the concept of "domain A," a representative volume within the aquifer that encapsulates the effects of local heterogeneities on solute transport.

Definition of Domain A and Scale Factor N

Domain A is conceptualized as a repeating unit within the aquifer, each containing a discrete, elongated zone with contrasting hydraulic conductivity. These zones are characterized by their horizontal and vertical correlation lengths, denoted as λ_h and λ_v, respectively. The dimensions of domain A are directly related to these correlation lengths through a scale factor, N. Specifically: Wiley Online Library

* Length of domain $A(L_a) : L_a = 2\lambda_h N$

* Thickness of domain $A(D_a) : D_a = 2\lambda_v N$ Wiley Online Library+2hess.copernicus.org+2TU Delft Research Portal+2

This scaling ensures that each domain A encompasses a conductivity zone of size $2\lambda_h$ by $2\lambda_v$, effectively capturing the local heterogeneity's influence on flow and transport. Wiley Online Library

Determination of Scale Factor N

While the mathematical relationship between domain A's dimensions and the correlation lengths is clearly defined, the specific value or method for determining the scale factor N is not explicitly detailed in the available publications. The choice of N likely depends on factors such as the degree of heterogeneity in the aquifer, the scale of interest for modeling, and the desired resolution of the simulation. In practice, N may be selected based on empirical data, calibration against observed breakthrough curves, or sensitivity analyses to ensure that the model accurately captures the dispersion behavior observed in the field.

For a more precise determination of N, consulting the full texts of de Lange's publications or related supplementary materials would be beneficial. These resources may provide case studies or examples where N is assigned specific values based on empirical observations or modeling requirements.

If you have access to the full articles and can provide more context or specific excerpts, I can assist further in interpreting the methodology for selecting N.

6.3 Question 3 to ChatGPT

De Lange in his two papers seems step from the real world from which he gets his lognormal distributed conductivities to his conceptual model, which is definitely not the real world. I would like to know what the underlying logic of plausibility is te make such a step, so that the conceptual model will bear a strong link to reality. The other factors are of course the length scales he uses and the real world origin of those. Can you help me figure this out?

Answer from ChatGPT W.J. de Lange's framework, as presented in his 2020 and 2022 Ground Water publications, bridges real-world aquifer heterogeneity with a conceptual model to elucidate and quantify asymmetric breakthrough curves resulting from groundwater flow through heterogeneous conductivity fields. Central to this framework is the concept of "domain A," a representative volume within the aquifer designed to encapsulate the effects of local heterogeneities on solute transport.

Constructing the Conceptual Model: Domain A

In de Lange's model, the aquifer is partitioned into repeating units termed "domain A." Each domain contains a discrete, elongated zone with contrasting hydraulic conductivity, reflecting the natural variability observed in real aquifers. The dimensions of these domains are directly linked to the aquifer's statistical properties:

* Horizontal dimension $(L_a) : L_a = 2\lambda_h N$

* Vertical dimension $(D_a) : D_a = 2\lambda_v N$

Here, λ_h and λ_v represent the horizontal and vertical correlation lengths of the hydraulic conductivity field, respectively, and N is a scale factor determining the size of domain A relative to these correlation lengths. This scaling ensures that each domain A encompasses a conductivity zone of size $2\lambda_h$ by $2\lambda_v$, effectively capturing the local heterogeneity's influence on flow and transport. ngwa.onlinelibrary.wiley.com

Determining the Scale Factor N

While the mathematical relationship between domain A's dimensions and the correlation lengths is clearly defined, the specific value or method for determining the scale factor N is not explicitly detailed in the available publications. The choice of N likely depends on factors such as the degree of heterogeneity in the aquifer, the scale of interest for modeling, and the desired resolution of the simulation. In practice, N may be selected based on empirical data, calibration against observed breakthrough curves, or sensitivity analyses to ensure that the model accurately captures the dispersion behavior observed in the field.

Linking the Conceptual Model to Reality

De Lange's approach ensures that the conceptual model maintains a strong connection to real-world aquifer behavior by:

1. Statistical Grounding: Utilizing statistical parameters (mean, variance, correlation lengths) derived from field data to define the properties of domain A.

2. Physical Representation: Modeling the effects of discrete conductivity zones within each domain to replicate the impact of heterogeneities on solute transport.

3. Scalable Design: Employing the scale factor N to adjust the size of domain A, allowing the model to be tailored to different scales of heterogeneity and ensuring that it remains representative of the actual aquifer conditions.

By integrating these elements, the conceptual model serves as a simplified yet robust representation of the complex processes governing solute dispersion in heterogeneous aquifers.

For a more precise determination of N and a deeper understanding of the model's application, consulting the full texts of de Lange's publications or related supplementary materials would be beneficial. These resources may provide case studies or examples where N is assigned specific values based on empirical observations or modeling requirements.

Referenties

[Chatwin (1980)] Chatwin, PC (1980) Presentation of Longitudinal Dispersion Data. ASCE Journ. of Hydro. Div. 71-83

[de Lange (2020)] Advective Transport Phenomena to Better Understand Dispersion in Field and Modeling Practice. Groundwater 58, 46–55. https://doi.org/10.1111/gwat.12883

[De Lange (2022)] Lange, WJ de (2022) Quantification of Advective Transport Phenomena to better Understand Dispersion in the Field. Ground Water Vol. 60, No. 3, May-June 2022 (319-329)

[De Lange (2025)] Using Advective Transport Phenomena In Modeling To Better Understand Mechanical Dispersion: Step One. Submitted.

[Maas (1994)] Maas, C (1994) On Convolution Processes and Dispersive Groundwater Flow. PhD Thesis TU-Delft, 13-June 1994.

[Jury & Roth (1990)] Jury A & K. Roth (1990) Transfer Functions and Solute Movement through Soil. Theory and Applications. Birkhäuser Verlag Basel. (Ref from Maas 1994)