

Mathematical background of groundwater modeling

Thomas Heinze

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1 Scale and hydraulic behavior

In a broader sense, groundwater flow is fluid flow in a (fractured) porous media. As such it is part of fluid dynamics and can physically be described using continuum mechanics. In continuum mechanics, the material is considered as a continuous mass instead of consisting of discrete particles. For water this seems quite logic, as probably noone would start describing the movement of single water molecules for groundwater flow. We are used to parameters and variables such as pressure fluid density, and viscosity instead of mean free-length or particle velocity. For a sedimentary aquifer this is maybe less obvious. In continuum mechanics, we do not consider single soil grains or rocks but look at the structure formed by all grains: The porous matrix. This porous matrix is then described by representative parameters such as porosity and permeability. It is known that porosity depends on grain size, shape and sorting. Therefore, continuum mechanics is not neglecting information on the grain scale but it is incorporated into more integrative parameters. With integrative parameters, the volume about which the integral is taken becomes of great importance. If the considered control volume is too small, small than the grain size for example, the obtained value of porosity would depend very much on its location. In an extreme scenario, such a small control volume could fit into a grain resulting in a porosity of zero. On the other hand, just placed a little bit differently it could fit into a pore and result in a porosity of one. Naturally, this is not a statistically meaningful representation for the porous medium. For this sense, the term **representative elementary volume (REV)** has been introduced. A REV is a volume size in which the describing parameters, such as porosity, are statistically meaningful, do not vary within a comparably significant volume range and do not depend on their specific location. The specific size of a REV always depends on soil type and can not be exactly defined. A couple centimeters up to tens of centimeters as lower limit is a good estimation for groundwater applications. For a homogeneous material, there is no upper limit for the REV but for heterogeneous material the REV is constrained by the occurring heterogeneity. If we consider a heterogeneous aquifer system consisting of different sedimentary materials, the REV of one material has to be small enough so that only the characteristics of this material are represented. Heterogeneity is included through different parameters for the different materials.

When subsequently deriving the governing equations for groundwater flow and solute transport, it is important to keep in mind, which spatial scale is considered. Besides the parameters and variables used, also the physical description is scale dependent. To describe flow in pores explicitly, one would use mathematical expressions such as the Navier-Stokes equation based on momentum conservation. With such kind of model, the flow velocity variation within a pore, such as sticking of fluid at the grain surface due to adhesive forces, can be resolved. If instead the effective inflow-outflow relationship across a porous volume is considered, this kind of physical description would be too detailed and too cumbersome to calculate. Different models are more suitable to describe this kind of 'effective' flow and will be introduced below due to their relevance for groundwater flow modeling.

2 The governing equation of groundwater flow

The basic physical principle of groundwater flow is the conservation of mass. In simple words: Any change of the amount of water within a finite volume is balanced by the fluxes inside and outside of this volume or by the sources or sinks of water inside the volume. A classical aquifer can be described as a porous media characterized by its porosity $\phi(-)$. The water is described by its density ρ (kg/m³) and its dynamic viscosity η (Pa s). Using those parameters, we can mathematically express the conservation of mass

$$\frac{d\phi\rho}{dt} = -\rho\nabla\vec{q} + Q. \quad (1)$$

This equation depicts the sentence written above. The fluid mass per unit volume is given as $\phi\rho$, as only the pores are filled with water. Mathematically, a change is expressed through the derivative d . The mathematical symbols $d\phi\rho/dt$ represent the derivation of the product $\phi\rho$ with respect to time t (s). Therefore, the term of the left hand side of the equation is the temporal change of the fluid mass per unit volume over time. The expression 'per unit volume' might sound abstract but just imagine a closed box. We observe how the amount of water inside this box changes over time and relate this change with the water that is flowing through the box or added/removed from inside the box. The expression 'per unit volume' only expresses, that we do not specify the size of this box (just yet). The right hand side of the equation is the change of the flux \vec{q} (kg/m²) and a sink or source term Q (kg/m³s). Note, that \vec{q} is a vector. This means, it has a direction. A vector has as many components as there are spatial dimensions and each component provides the value for the respective dimension. One can write $\vec{q} = (q_x, q_y, q_z)$. Here, the components q_x, q_y, q_z describe the flux in x, y and z direction respectively. In opposition to a vector, a value like porosity is called a scalar. It does not have a direction and is simply one value. The Nabla operator ∇ is a specific mathematical operator. It is a vector and each component of it is the derivative with respect to the direction. The general convention is that the first component is in x direction, the second in y direction and the last one in z direction. The Nabla operator is then equal to $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$. While those direction can be oriented in any way, in this book x and y direction will mark the horizontal directions, while the z direction points towards the depth. If the Nabla operator is applied on a scalar field, it is called a **gradient**. In

a scalar field a scalar value, such as porosity, is associated with every point in space. We write this for the porosity as $\phi(x, y, z)$. This means for any point in our system, assuming each point represents a REV, there is a porosity value. The result of a gradient operation is a vector field because it expresses the change the spatial change of a scalar field in each spatial dimension. If the Nabla operator is applied on a vector field, it is called a **divergence**. In a vector field a vector is associated with every point in space. In the context of groundwater flow, such a vector could be flow velocity. The divergence is then a possibility to quantify the spatial change of this vector field. The result of a divergence operation is a scalar field. The term $\nabla \vec{q}$ marks, describes the change of the flux q in any spatial direction. In other words, $\nabla \vec{q}$ is the difference between outflow and inflow across all six sides of the described box. The flux \vec{q} is the amount of mass through the areas of box, therefore, its unit is kg/m^2 and its mathematical form is a vector. The source or sink term Q is the amount of fluid added or removed inside the box. In a practical application, this could for example be represented through a well or groundwater recharge.

On the left hand side of the equation, there is the derivative of a product: the product of porosity and density. Mathematically, we can resolve this derivative of a product using the chain rule.

$$\frac{d\phi\rho}{dt} = \rho \frac{d\phi}{dt} + \phi \frac{d\rho}{dt} \quad (2)$$

Using this mathematical rule, we have split the derivative of a product of a sum of two derivatives, which we can study separately. The two derivatives represent the change of porosity and fluid density over time. Principally, we can think of many processes that would change the porosity, such as chemical dissolution or precipitation processes or mechanical compaction. Similarly, the fluid density depends on temperature, salinity and pressure. All these processes change porosity and fluid density over time and would therefore be needed to include here. Mathematically, this is expressed through a switch from a total derivatives to partial derivatives. Partial derivatives are derivatives of functions with more than one variable. Here, porosity and density would be functions of the variables pressure P , temperature T , salinity concentration S etc. The total derivative of porosity with respect to time, would then be written as

$$\frac{d\phi(P, T, S)}{dt} = \frac{\partial\phi}{\partial P} \frac{\partial P}{\partial t} + \frac{\partial\phi}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial\phi}{\partial S} \frac{\partial S}{\partial t} \quad (3)$$

with the partial derivation symbolized by ∂ . A partial derivation of a function is conducted by keeping all other variables constant. Of course, a similar formulation could be made for the fluid density.

If many different processes and dependent variables are included, we end up with several coupled differential equations all linking different variables such as contaminant concentration, mechanical stress, temperature and fluid pressure. These kind of problems are complex to solve and go way beyond the topics of this course. Actually, T(hermo)-H(ydraulic)-M(echanical)-C(hemical)-modeling is a whole area of research in the geosciences. An important step in modeling is the formulation of reasonable assumptions to simplify the system! For example, the temperature of groundwater is usually rather constant. Therefore, we can neglect in our specific case the dependence of porosity and fluid density on temperature. Also, mechanical stresses are uncommon to be of importance for

groundwater flow, as is chemical clogging. Note, that the made assumptions have a crucial effect on your model. For example, describing saltwater intrusion into freshwater aquifers along a coastline for example requires density dependent flow and a dependence of water density on salinity. Any neglect of this effect would make it impossible to adequately describe the intrusion process. Assumptions need to be made with care and questioned for each scenario. Many simulations framework have a limited number of effects that are included. The made assumptions and the scenarios to be studied will influence which modeling software can be used. Making the right assumptions to avoid oversimplification but assure efficient solution is one of the most critical task when setting up a model.

In the specific case of groundwater modeling in the most simple case, we can neglect all effects on porosity and density besides the effect of the groundwater level itself. Physically, this effect is quantified through the parameters of compressibility. The compressibility c (1/Pa) of a medium expresses its change in volume as a response to an applied pressure. As there is the change in porosity and density over time, we require two compressibility values.

$$c_\phi = \frac{1}{\phi} \frac{\partial \phi}{\partial P} \quad (4)$$

$$c_\rho = \frac{1}{\rho} \frac{\partial \rho}{\partial P} \quad (5)$$

In principle, the compressibility is another parameter, that itself could depend again to temperature and other variables. Luckily, it can be assumed constant for almost all ranges of temperature, pressure etc. relevant for groundwater flow. However, it is noteworthy here, that there can be quite a variation across rock and soil types. Loose sedimentary materials might show a much higher compressibility depending on grain sorting, than consolidated rocks. Also, porous aquifers might have different values of compressibility than fracture-dominated systems. For the compressibility of the pore space c_ϕ , it is also important to note that based on the derivation here, c_ϕ is a measure of a change of the pore space under the effect of changing pore pressure. This is different than e.g. the compressibility of a rock sample under external mechanical load. Water is assumed incompressible for a reason, because its compressibility under groundwater conditions is really small. The compressibility of the pore space is usually higher than that of water, though still comparably small in the order of $10^{-8} - 10^{-12}$ 1/Pa.

Returning to the right hand side of the conservation of mass, we can now write

$$\rho \frac{d\phi}{dt} + \phi \frac{d\rho}{dt} = \rho \phi (c_\phi + c_\rho) \frac{\partial P}{\partial t} \quad (6)$$

The sum of the compressibility for porous matrix and water is often written as c_t for simplicity. The left hand side includes the temporal changes as before. However, through the replacements we did, there is now the temporal change of pressure instead of the change of fluid density and porosity. Note that the units did not change, as there were also no changes on the right hand side. Introducing the pressure as primary variable is handy because it is our variable of interest in groundwater modeling.

The right hand side of the conservation of mass includes the gradient of the

flux $\nabla\vec{q}$. The dependence of flux and pressure is given through Darcy's law

$$\vec{q} = -\frac{k}{\eta}\nabla P. \quad (7)$$

with permeability k (m²) and dynamic viscosity η (Pa s). The empirical law of Darcy linearly relates the flow through a cross section with the hydraulic gradient along the flow direction. Although the flux \vec{q} has the units of velocity and is therefore often referred to as Darcy velocity, it is important to remember that this is not a true flow velocity but an averaged value. The permeability is a measure of the flow resistance of the rock or soil, while the dynamic viscosity is a measure of the internal friction of the fluid. Through the application of Darcy's law we implicitly assume that all assumptions behind Darcy's law can also be applied to the groundwater model. This is usually the case in groundwater aquifers as the flow can be assumed as continuous, laminar and steady within a saturated soil. Inserting Darcy's law into the conservation of mass

$$\rho\phi c_t \frac{\partial P}{\partial t} = \rho\nabla\left(\frac{k}{\eta}\nabla P\right) + Q, \quad (8)$$

an equation with pressure as primary variable can be obtained and the density can be cancelled out at both sides of the equation. This kind of pressure-based equation is quite common in reservoir modeling but for groundwater modeling the use of the piezometric head h (m) is more applicable because measurements of the groundwater level are made in height of water column.

To transfer the equation from pressure to piezometric head, a simple replacement has to be done, as

$$P = \rho gh, \quad (9)$$

with the gravitational acceleration $g \approx 9.81$ m/s². Using h instead of P , the derived equation can be written as

$$\phi c_t \rho g \frac{\partial h}{\partial t} = \nabla\left(\frac{k\rho g}{\eta}\nabla h\right) + Q. \quad (10)$$

The change from pressure to piezometric head is often accompanied by a change in parameters. The hydraulic conductivity K (m/s)

$$K = \frac{k\rho g}{\eta}, \quad (11)$$

as well as volumetric specific storage S_s (1/m)

$$S_s = \rho g \phi c_t \quad (12)$$

are commonly used. With S_s and K , the equation for the piezometric head is given as

$$S_s \frac{\partial h}{\partial t} = \nabla(K\nabla h) + Q. \quad (13)$$

Please note, that the term Q has now also changed, though it has not been explicitly stated. While the meaning of Q has not been altered, its units have changed.

This type of equation is called a differential equation because it related differentials of a function with the function itself. To be more specific, this equation is a partial differential equation (short:PDE) because it relates partial derivatives of a multi-variable function. The function here is the piezometric head h and the variables are space and time. The order of a differential equation is described by the highest occurring differential, which here is the second order derivative with respect to space. To be even more specific this PDE is called a diffusion equation. All kind of diffusion processes are described by a partial differential equation with a first order differential with respect to time and a second order differential with respect to space. The combination of parameters $\kappa = K/S$ (m^2/s) is called diffusivity. A diffusion equation is also classified as a parabolic partial differential equation, due to the occurring derivatives. The latest separation is primarily relevant for multi-purpose modeling software, as numerical solution strategies depend on the mathematical classification of the PDE.

Usually, a aquifer has a much wider horizontal spread than thickness. Also, the variation with depth is usually not of interest, when modeling groundwater flow. Therefore, it is sometimes convenient to consider a depth-averaged version of the aquifer. In such a scenario, the piezometric head $h(x, y, z, t)$ is only considered as a function of time and the two horizontal coordinates x and y , so $h(x, y, t)$. Any information with depth z is lost. This is sometimes referred to as Dupuit assumption. Mathematically, this is expressed through an integration of the equation over the thickness of the water layer m

$$\int_0^m S_s \frac{\partial h(x, y, z, t)}{\partial t} dz = \int_0^m (\nabla (K \nabla h(x, y, z, t)) + Q) dz. \quad (14)$$

In such a setup, the term transmissivity T (m^2/s) is used, which is the product of aquifer thickness and hydraulic conductivity. Similarly, the term storativity S (-) is used for the product of specific storage and aquifer thickness. Using those parameters, the equation has a similar form than before but with a different set of parameters and meaning respectively

$$S \frac{\partial h(x, y, t)}{\partial t} = \nabla (T \nabla h(x, y, t)) + Q. \quad (15)$$

Besides transmissivity and storativity, also the source/sink term Q changed to a depth integrated version.

This formulation allows a straight forward determination of the parameters S and T using pumping tests. However, through the change to a depth-averaged form, the storativity gained a different interpretation because a change in water layer thickness is now part of the parameter S . Therefore, a differentiation between confined and unconfined aquifers has to be made. In confined aquifers, in which the thickness of the water layer can not change, the storativity is equal to the specific storage S_s times thickness of the water layer. In such a case, the storativity is rather small. However, in an unconfined aquifer, the water level can rise freely. In such a case, compressibility of pore space and water are almost negligible but the accessible pore space can be filled. Storativity, based on the derivation above and the idea of compressibility, represents the change in water volume per unit volume for a change in piezometric head. Therefore, in an unconfined aquifer, the water volume changes by the factor of the effective

porosity per change in hydraulic head. As a result, the storativity is much, much larger in an unconfined aquifer than in an confined aquifer.

The resulting equation for horizontal groundwater flow can be simplified for two common scenarios: steady state and a homogeneous aquifer. The steady state represents a state in which no temporal changes of the piezometric head occur. In such a case, the equation simplifies to

$$\nabla T \nabla h = -Q. \quad (16)$$

In such a case, the hydraulic flow is balanced by the water sources or sinks. In a homogeneous aquifer, the transmissivity is the same everywhere and can therefore put in front of the Nabla operator

$$S \frac{\partial h(x, y, t)}{\partial t} = T \nabla^2 h(x, y, t) + Q. \quad (17)$$

In this form, the mathematical form of a diffusion equation is very obvious. For a steady state in a homogeneous aquifer without sources or sinks, the equation even simplifies to

$$\nabla^2 h = 0. \quad (18)$$

Such an equation is called a Laplace equation, which is an elliptic PDE and very common especially in all field related applications such as in electrostatics. Obviously, with subsequent simplifications, the calculation can become much easier and quicker. However, reaching steady state is often an iterative solution process. Depending on the initial conditions (the first guess), the process of finding a solution can be cumbersome. As an example, the groundwater module of Grass Gis does not intrinsically has a solver for the steady state solution but a steady state solution can be approximated for very long time frames.

3 The governing equation of solute transport

The solute transport is similarly based on the conservation of mass. The temporal change of solute concentration C depends on the difference between in- and outgoing flux $-\nabla \vec{J}$ and the solute generated Q .

$$\frac{\partial C}{\partial t} = -\nabla \vec{J} + Q \quad (19)$$

The flux \vec{J} can be split into separate transport mechanisms, most commonly three for groundwater flow: **diffusion**, **dispersion**, **advection**. The diffusion process is based on Brownian motion, so a random motion of any suspended particle, and driven by the concentration gradient. Diffusion is not unique to solute transport but rather a general concept and can be applied to pressure, temperature but also non-physical quantities such as economics. In the so-called Fickian diffusion, the diffusive flux \vec{j}_{dif} is given as

$$\vec{j}_{dif} = -D \nabla C \quad (20)$$

with a diffusivity D in (m^2/s) . As larger the diffusivity D is, as quicker the diffusion process is taking place and a homogeneous distribution of the concentration C is achieved. The concentration gradient ∇C describes the spatial

change in concentration. If there is a rapid change in concentration across a short distance, then the diffusive flux will be larger than if the gradient is low. This behavior can be easily observed by adding a drop of ink into a water glass. Initially, the concentration gradient is large at the border of the drop, so the diffusion process is quick and progress is visible. Over time, as the ink is beginning to be distributed across the water, the diffusion process is slowing down, meaning the change in concentration over time is small, because the gradient is becoming smaller. While Fickian diffusion is the most common type and a good first guess for solute diffusion in water, it should be noted that for example transport processes in fractures often follow non-Fickian diffusion laws. The applicability of the standard diffusion modeling needs to be evaluated for each specific scenario.

Dispersion is similarly to diffusion driven by the concentration gradient and the dispersive flux can also be described by Fick's first law.

$$\vec{j}_{dis} = -\mathbf{D}_s \nabla C \quad (21)$$

The diffusion coefficient is replaced here by the dispersion coefficient \mathbf{D}_s . In opposite to diffusion, dispersion is usually not an equally directed process in every dimension. The dispersion coefficient is therefore written as a tensor to symbolize this behavior. Anisotropic and heterogeneous behavior and its representation in the mathematical equations and the numerical model will be discussed later on in more detail. In opposite to diffusion, the dispersive flux is caused by non-ideal flow pattern. Dispersion is also often considered scale dependent. From a rather macroscopic perspective, dispersion of a contaminant is caused by complex, tortuous and tangled flow paths within the porous media. Two solute particles starting from the same spot might take different flow paths through the porous matrix, so that after the same macroscopic length, the length of the individual particle's flow path is much longer and different to each other. At a rather microscopic scale, dispersion is caused by the variation of flow velocities across a pores crosssection. While at groundwater flow the flow behavior in individual pores is not considered, as described above, the occurring phenomena still need to be incorporated. It can usually be assumed that water is bound adhesively to grain surfaces, and that water close to this bounded layer will be slower than further away from the grains. This difference in flow velocities also influences the travel time of individual solute particles and increase dispersive effects. The dispersion effect is often considered dominant compared to diffusion.

The advective flux describes the transport of solute through the water movement. The process is not driven by the concentration gradient but directed in the direction of fluid flow q . Therefore, advection is not a process of the solute itself but due to the external force of the flowing fluid.

$$\vec{j}_{adv} = \vec{q}C \quad (22)$$

In further opposition to diffusion and dispersion, advection is shape conserving. This means that a clearly constrained volume of contamination would still be at the exact same volume of the exact same shape, just located at a different spot if advection would be the only transport mechanism in a homogeneous flow field.

Combining all three transport mechanisms into the conservation of mass leads to the following equation.

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\vec{J}_{dif} + \vec{J}_{dis} + \vec{J}_{adv}) + Q. \quad (23)$$

So far, we did not specify any possible source or sink terms for the solute transport. Naturally, there are the obvious sources such as a contamination site or a tracer input. Such kind of sources will be included by a simple rate Q in the respective solute concentration per second. Sinks could be anthropogenic, such as pumping or some kind of filters, or through a chemical or biological processes, such as decay. There are also further natural processes altering the concentration, such as sorption. Sorption is a general term describing that one substance, the solute, becomes attached to another substance, the porous matrix. If the solute is bound through sorption to the porous matrix, its concentration is declining over time.

$$\frac{\partial C_{sorp}}{\partial t} = -\frac{\rho}{\phi} K_d \frac{\partial C}{\partial t} \quad (24)$$

The amount of concentration adsorpt to the matrix depends on the total available concentration and the distribution coefficient K_d . The shown equation here is assuming linear sorption. Depending on the underlying processes, the solute and the matrix, more complex sorption relationships could be applied. Mathematically it is usually more convenient to use the retardation factor R_d .

$$R_d = 1 + \frac{\rho}{\phi} K_d \quad (25)$$

If sorption is considered a sink term, then the conservation of mass reads as

$$\frac{\partial C}{\partial t} = \nabla \cdot (D + \mathbf{D}_s) \nabla C - \nabla \cdot (\vec{q}C) + \frac{\partial C_{sorp}}{\partial t} + Q. \quad (26)$$

Inserting the linear sorption equation for C_{sorp} and bringing it to the left hand side results in

$$R_d \frac{\partial C}{\partial t} = \nabla \cdot (D + \mathbf{D}_s) \nabla C - \nabla \cdot (\vec{q}C) + Q. \quad (27)$$

Often the coefficients for diffusion and dispersion are summarized in a single coefficient, as it is usually cumbersome to quantify both coefficients separately in the field or laboratory.