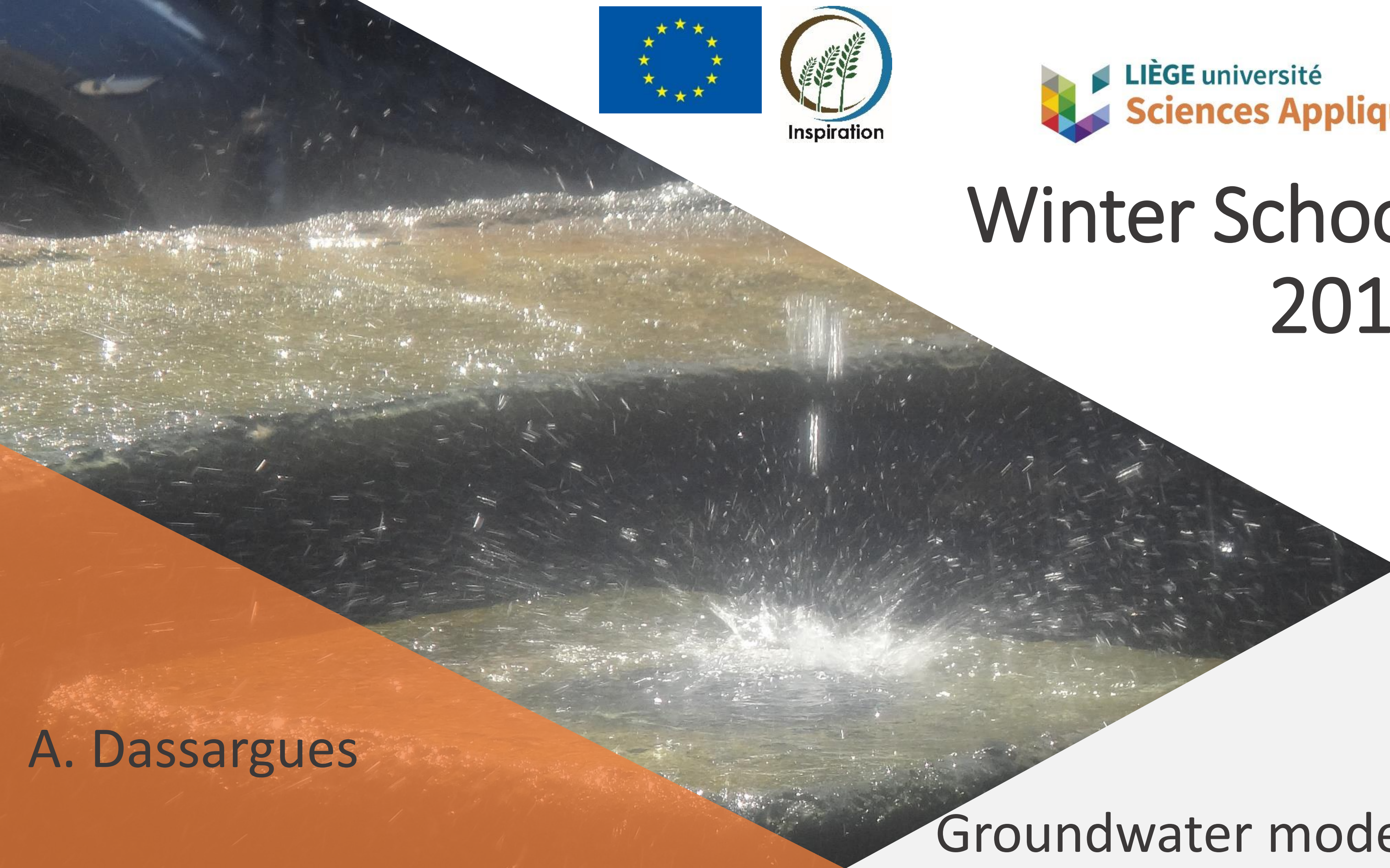


LIÈGE université
Sciences Appliquées

Winter School 2019

A. Dassargues

Groundwater modeling at the catchment scale: **mathematical and numerical aspects**

Reference: Chapters 12 and 13 in Dassargues A., 2018. Hydrogeology: groundwater science and engineering, 472p. Taylor & Francis CRC press

Groundwater modeling at the catchment scale : mathematical and numerical aspects

- *Terminology and General methodology*

- *Groundwater flow equations*
- *Flow Boundary Conditions*
- *Introduction to solving methods*
- *Time integration scheme*

- *Solute transport equations*
- *Transport Boundary Conditions*
- *Pe and Cr numbers*
- *Introduction to solving methods*

- *References*

A model ?

- *a model is a tool for simulating reality in a simplified form*

  (Wang and Anderson 1982)

- *a mathematical description of the physical reality can already be considered as a mathematical model*

- *a mathematical model can be solved or computed analytically or numerically*

- *'Any type of modeling includes subjective decisions and simplifying assumptions because the true complexity of a natural system is never fully represented and data about properties and variables include uncertainties'* *(Fienen 2013)*

Terminology

Black-box model: a set of mathematical equations is developed by empirical or statistical fitting of parameters to reproduce historical records of the main variable ('data driven' model) *(Anderson et al. 2015)*

… all is relative, any model is always a simplification of the reality,

- *'black box'*
- *'grey box'*
- *physically based but not spatially distributed*
- *spatially distributed but not physically based*
- *spatially distributed and physically consistent*

Various possibilities for catchment scale models

Terminology

$x_1, x_2, \ldots, x_j, \ldots x_n$ *independent variables*

Stress factor

pumping,
recharge,
change in stress,…
contaminations,

Aquifer parameters

$p_1, p_2, \ldots, p_i, \ldots p_k$

Geometrical characteristics,
properties of the considered domain

Deterministic

Reaction/answer

$y_1, y_2, \ldots, y_i, \ldots y_n$ *dependent variables*

piezometric heads, pressures, concentrations, …

Stochastic/probabilistic *using Monte Carlo multiple simulations, the same schema can be used with multiple equally likely sets of parameters, independent variables, and dependent variables.*

(Konikow and Mercer, 1988, Dassargues 2018)

Terminology

Deterministic models versus Stochastic/Probabilistic models:

- ***Deterministic Model:*** *the answer (reaction) of the simulated system, under a set of considered stress factors, is unique and defined in a pure deterministic process (even if the new simulated scenario is out of the stress range of the calibration)*

- ***Stochastic/Probabilistic Model:*** *in addition, the possible uncertainties on the parameters, on the initial conditions, on the BC's, …*
  - *combined resolution (can be very heavy)*
  - *most often, n resolutions of n equiprobable cases, and then statistics for estimating results dispersion and confidence intervals*
  - *allows to take into account 'soft-data'*

Terminology

…more about stochastic modeling

Sources of uncertainty are multiple and of different types:

1) associated to subjective conceptual choices made to simplify the reality into a model

(Cooley 2004, Rojas et al. 2008, Wildemeersch et al. 2014 and many others)

2) embedded in parameters data uncertainty

(de Marsily et al. 2005, Brunner et al. 2012 and many others)

3) highly parameterized models, where parameters value determination represents an ill-posed problem

(among others: Carrera and Neuman 1986a, Moore and Doherty 2005, Hill and Tiedeman 2007, Beven 2009)

4) from initial and boundary conditions

Terminology

…more about stochastic modeling

For predictions, the uncertainty of the <u>stress factors</u> linked to each simulated scenario can be integrated

(e.g. Rojas et al. 2010c, Sulis et al. 2012, Goderniaux et al. 2015 and many others)

A formal stochastic formulation in the partial differential equations for flow and solute transport can be used

(see many books, among others: Dagan 1989, Gelhar 1993, Kitadinis 1997, Zhang 2002, Rubin 2003)

In practice, the most commonly-used : Monte Carlo simulations with multiple equally-likely realizations of the model parameter sets that are conditioned on the existing data

(e.g. Vecchia and Cooley 1987, Deutsch and Journel 1998, Huysmans and Dassargues 2006, Tonkin et al. 2007 and many others)

Multiple simulations ➡ multiple responses statistically treated assuming (most often) Gaussian behavior

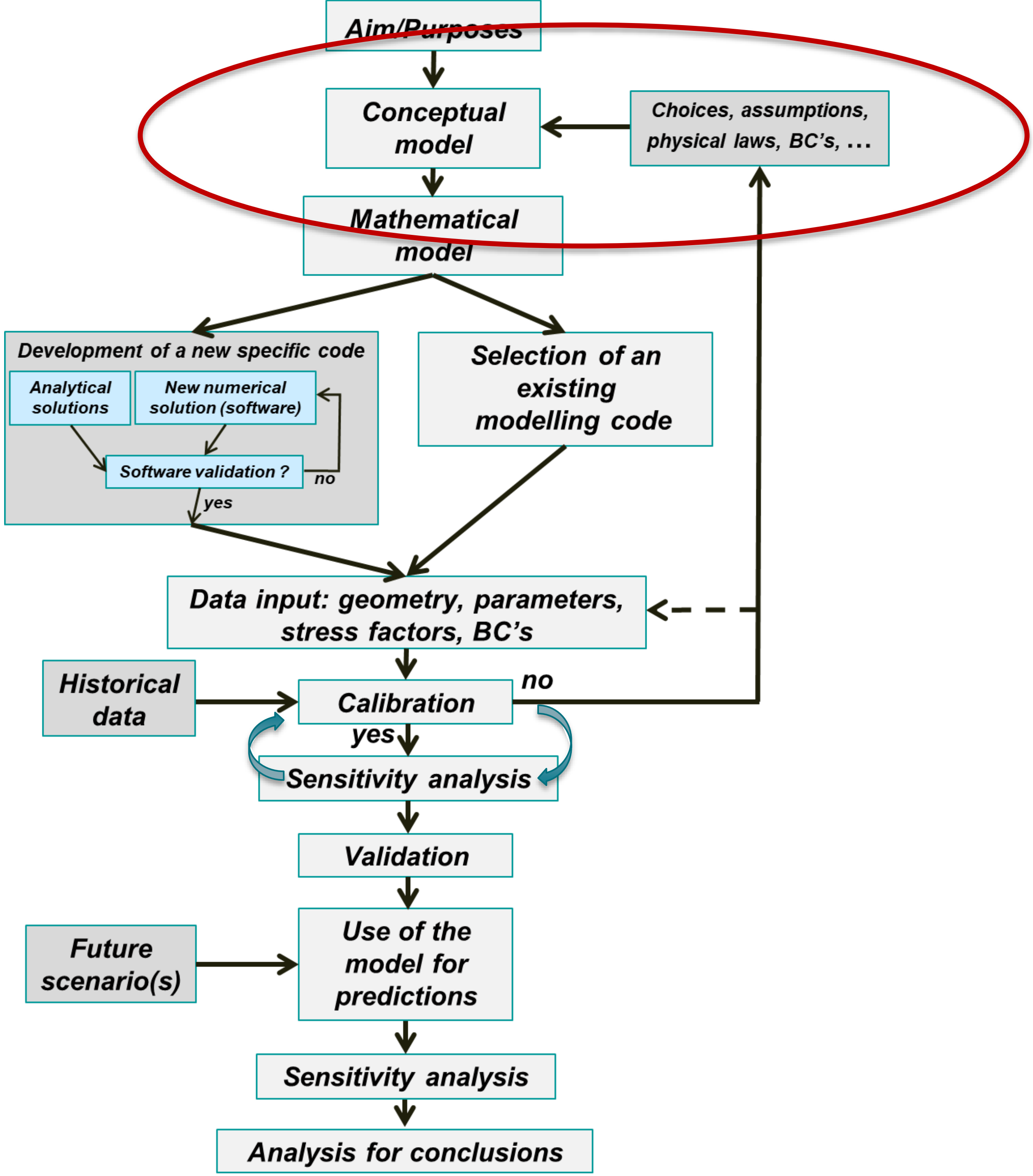
➡ *results in statistical distributions*

➡ *probability distribution for each response based on the statistical distribution of data, parameters and stress factors*

General methodology

Different steps of a groundwater numerical model :

- *clear definition of the final aim*
- *conceptual model*
- *mathematical model*
- *numerical model, development or choice of an existing code*
- *data input*
- *calibration and then validation*
- *sensitivity analysis*
- *application (use) of the model*
- *results analysis with regards to the initial question*
- *redaction of a report*


Aim/Purposes
Conceptual model
Choices, assumptions, physical laws, BC's, …
Mathematical model
Development of a new specific code
Analytical solutions
New numerical solution (software)
Software validation ?
no
yes
Selection of an existing modelling code
Data input: geometry, parameters, stress factors, BC's
Historical data
Calibration
no
yes
Sensitivity analysis
Validation
Future scenario(s)
Use of the model for predictions
Sensitivity analysis
Analysis for conclusions

General methodology

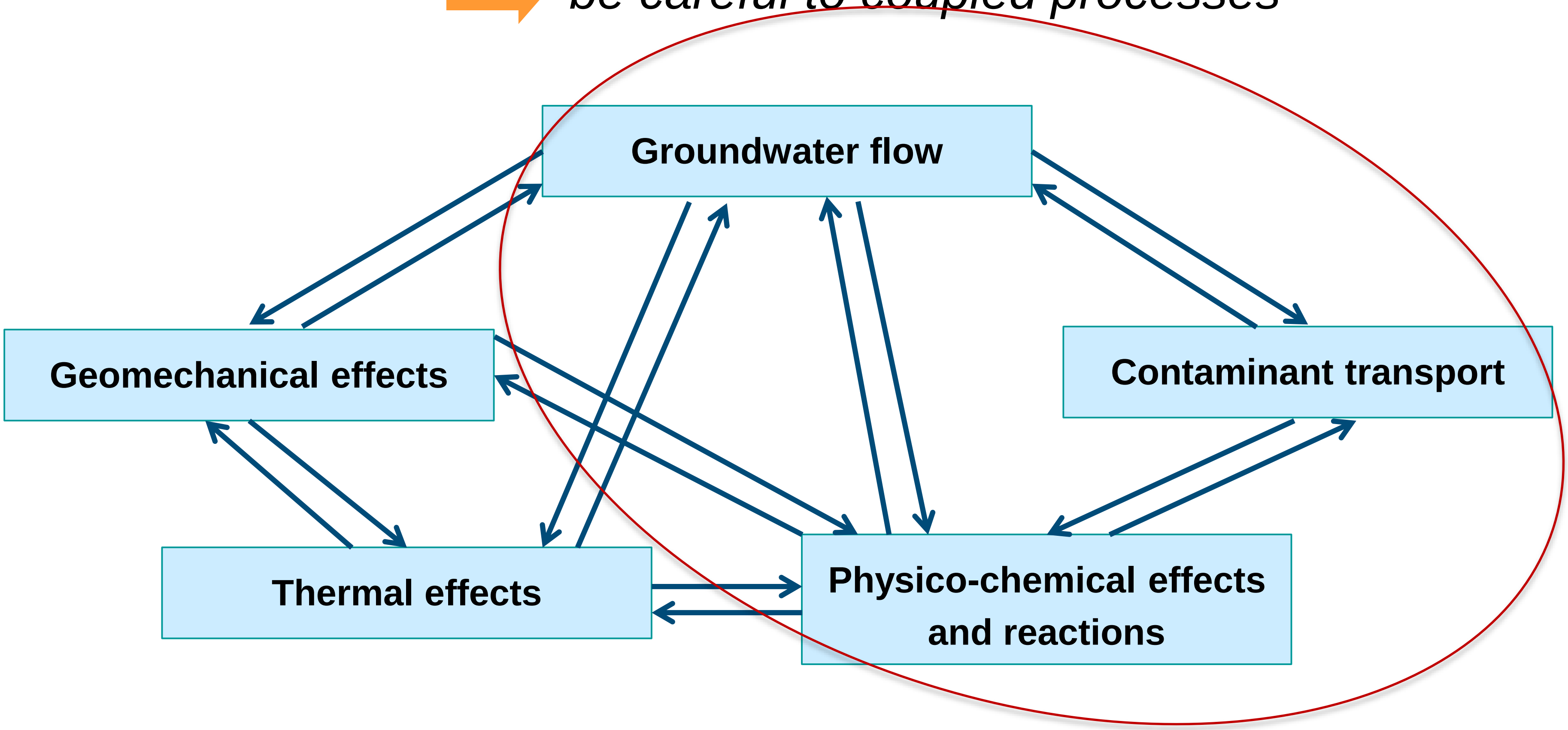
- *Definitions, terminology, aims*
- *Methodology*
- ***Conceptual model***
- *Choice of a software & numerical main characteristics*
- *Data needs and model implementation*
- *Model calibration and sensitivity*
- *Evaluation/reporting*

General methodology: conceptual model

(Anderson et al. 2015)

… the way in which reality is translated in a model

be careful to coupled processes



(Rosbjerg and Madsen 2005, Dassargues 2018)

General methodology: conceptual model

Conceptualisation of an hydrogeological problem consists in a fundamental step where the main assumptions of the modelling are chosen:

- *scale level*
- *steady state or transient analysis*
- *model dimensionality: 1D, 2D vertical, 2D horizontal, quasi-3D, 3D*
- *boundary geometry and location, boundary conditions*
- *geological media (porous / fissured / double porosity / …)*
- *homogeneity/heterogeneity, isotropy/anisotropy, properties changes in function of time*
- *initial conditions within the domain*
- *…*

… 'poorly justified assumptions can potentially discredit an entire groundwater model' *(Peeters 2017)*

General methodology: conceptual model

– *Steady state*

- *it does not exist in the reality*
- $\Delta Res = 0$ *and* $Q_{in} = Q_{out}$
- *when piezometric heads and fluxes can be considered as relatively stable*
- *when transient data are lacking (first guess, …)*
- *with data allowing to deduce a 'mean behaviour' of the system :* R_{mean}, Q_{mean}, H_{mean}…
- *for starting with a problem, before going to transient conditions*
- *adopted for simplification, considering extreme conditions and being on the 'security side'*

can be difficult to converge when data are not realistic or when non linearities are not considered

➔ *transient simulation with constant conditions + time step increasing*

General methodology: conceptual model

- ***Transient simulation***
  - *requires generally more data*
  - *takes more CPU time*
  - *sometimes needed in function of the context*
    - *transient character of the gw flow conditions*
    - *transient transport (it is generally the case) on a supposed steady gw flow*

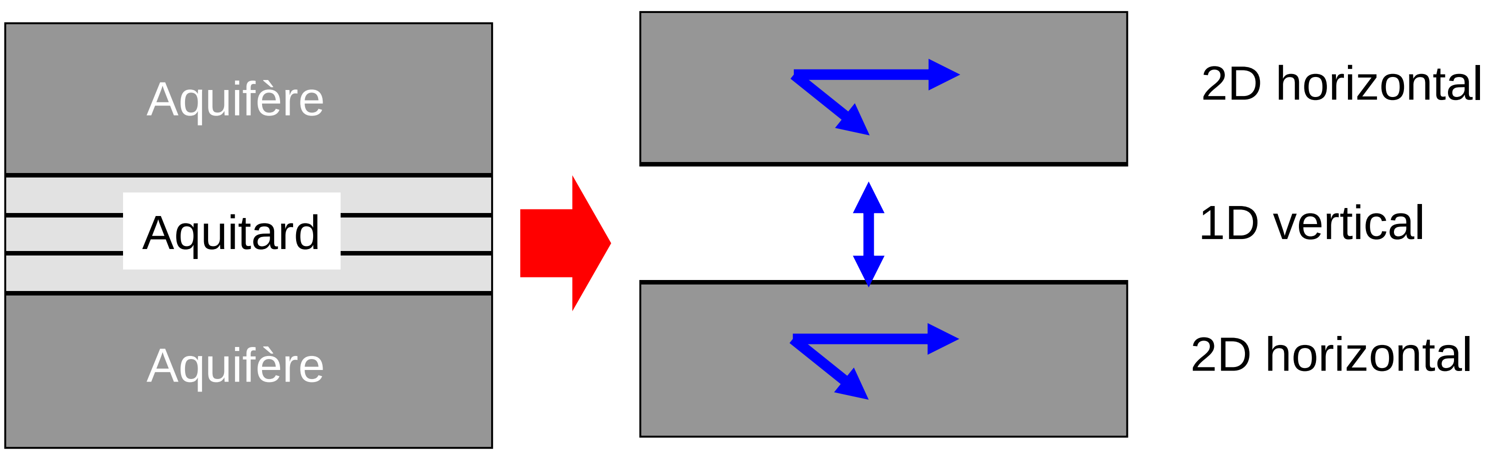
General methodology: conceptual model

- ***Initial conditions**: initial values of the main variable (generally piezometric head h) in each node of the mesh*
  - *1st used values for a steady state computation (1st approximation)*
    - *influence the convergence process and the CPU time for reaching the steady state equilibrium*
    - *if the convergence is not ideal, results can be affected*
  - *actual initial state of the sytem at time t_0 for starting a transient simulation*
    - *if h_i are not consistent with BC's and stress factors, then Δh calculated can be completely strange*
    - *very often: starting with a steady state and continuing with a transient simulation*

General methodology: conceptual model

Extension and dimensionality

- *pseudo-3D or quasi-3D*
  - *multi-layers system with 2D gw flow in each of them*
  - *strictly vertical flow in aquitards calculated by applying the Darcy's law*



General methodology: conceptual model

(Hill 2006, Gómez-Hernández 2006, Wildemeersch 2012,)

Parsimony or complexity: merits and pitfalls

- *any process-based model becomes complex and remains uncertain*
- *complexity could be considered through the use of stochastic approaches conditioned on the available data*

(Beven and Freer 2001, Gómez-Hernández 2006, Beven and Binley 1992, Hoeting et al. 1999, Neuman 2003, Rojas et al. 2008 and 2010a)

- *complexity could be introduced in a stepwise fashion, from simple to complex*
- *preserve refutability and transparency*

each chosen hypothesis can be tested

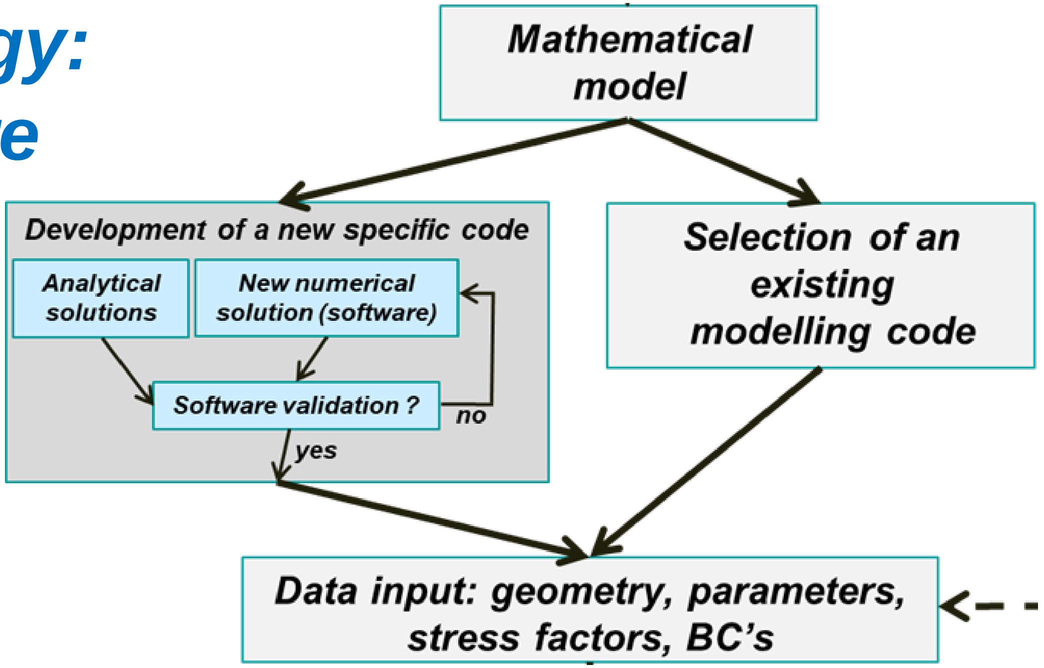
modelled processes remain understandable

(Ward 2005, Schwartz et al. 2017, Kurtz et al. 2017)

- *to determine if a simple model provides reliable results, its results should be compared to results from a more complex one*

(de Marsily et al. 2005)

General methodology: choice of a software



- *if a new code is developed: it must be validated for the same kind of processes*
- *choose your code in function of your conceptual model*
- *many existing codes for different purposes*

Do not use a hammer to drive a screw

or do not use a screwdriver to drive a nail !

General methodology: numerical models main characteristics

- *study area represented by a mesh of elements or cells to which nodal points (or nodes) are associated*
- *in those subdomains (cells, elements, volumes) the medium is assumed homogeneous*
- *the continuous variable by a discrete variable (the solution will be found at discrete points of the spatio-temporal domain)*
- *a finer spatial discretization means a better approximation of the solution*
- *partial differential equations are replaced by a system of algebraic equations*
- *the state variables are the unknown*
- *a solution obtained for each specified set of parameter values*
- *…*

General methodology: numerical models main characteristics (2)

- *iterative procedures more efficient than direct matrix inversion methods*
- *solution = values at discrete locations in the simulated domain generated from the spatial discretization*
- *if transient problem, the time scale is also discretized in time steps*
- *solution at the n discrete nodes and for all time steps, then interpolations at any location in space and time*

(Wang and Anderson 1982)

General methodology: numerical models main characteristics (3)

For an iterative solution,

***Convergence** = computed values converge towards the exact values, in particular when the spacing between nodes is decreasing*

***Stability** = the numerical errors (truncation + roundoff) should not increase in the solution computation within one time step or from a time step to the next ones*

*(Volume, mass or energy) **conservation** is preserved (i.e. the numerical solutions must preserve and satisfy balance equations at the local as at the global scales)*

(Bear and Cheng 2010, Diersch 2014)

General methodology: numerical models main characteristics (4)

Physical consistency *is dependent on the conceptual choices to simplify the reality for an efficient modelling*

Numerical consistency *is ensured if truncation errors tend to zero for decreasing mesh increments and time steps*

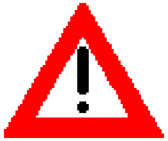
Accuracy *= describing the (lowest as possible) modeling errors (truncation and roundoff errors + conceptual and calibration errors)*

Resolution *= the smallest increment or decrement of the considered variable value that can be calculated by the model*

(Paniconi and Putti 2015)

REV *concept = considered volume of geological medium for quantifiying properties at the appropriate scale (by averaged equivalent values)*

(Bachmat et Bear 1986, Bear et Verruijt 1987, de Marsily, 1986, Dagan, 1989)



a very useful concept that implicitly assumes a continuum and a porous medium *(Molz 2015)*

General methodology: modeling errors

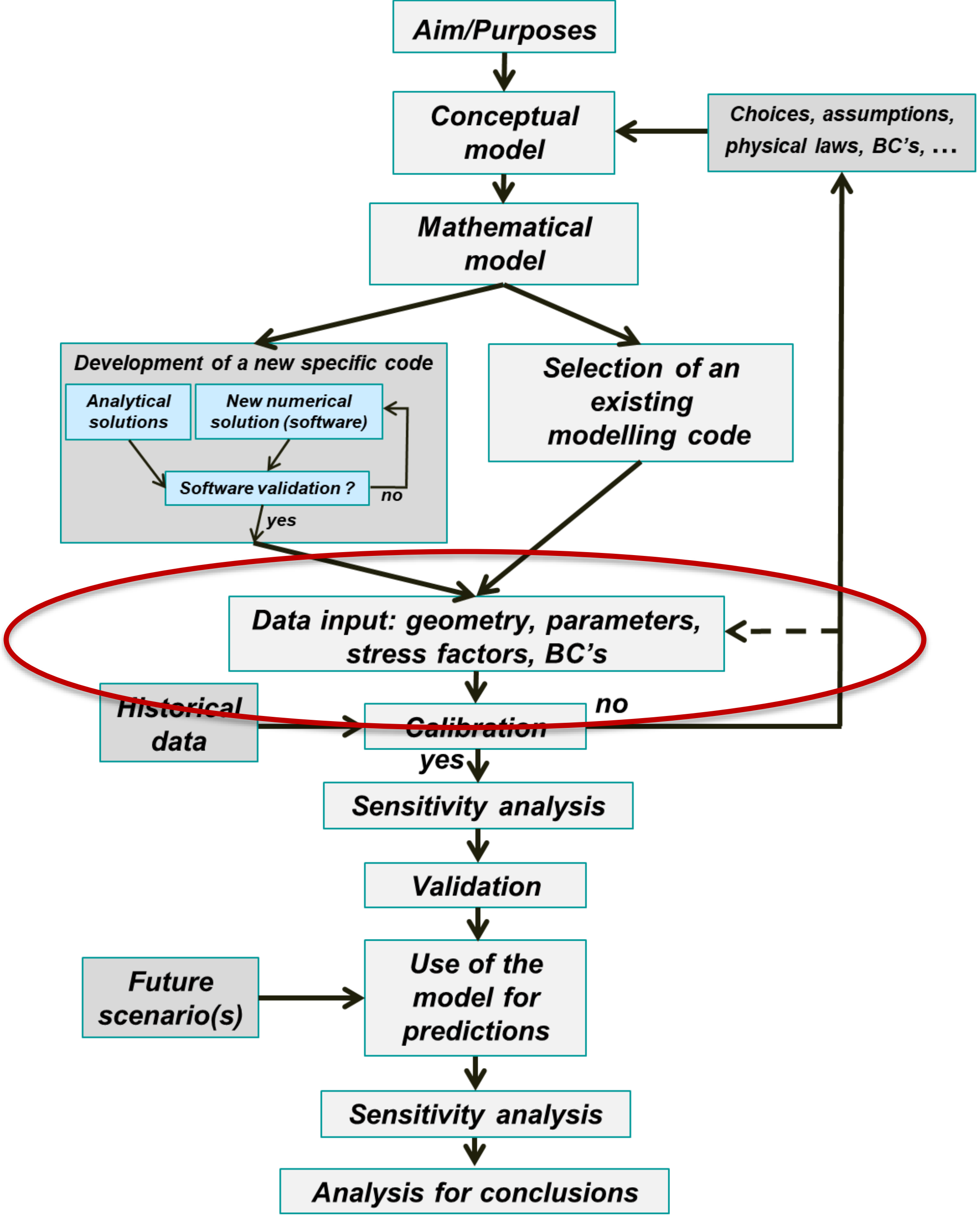
- *conceptual errors (linked to main conceptual choices, systematic)*
- *approximation errors (linked to the chosen spatial/temporal resolution)*
- *numerical errors (linked to the numerical method adopted for solving the system of equation, truncation and roundoff errors, …)*
- *measurement errors (implicitly introduced during the calibration process, see next section)*

Scale issue: measurement scale is

very different model scale

General methodology

- *Definitions, terminology, aims*
- *Methodology*
- *Conceptual model*
- *Choice of a software & numerical main characteristics*
- ***Data needs and model implementation***
- *Model calibration and sensitivity*
- *Evaluation/reporting*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General methodology: data needs

Summary and generalization: only 4 kinds of data

- *1D, 2D or 3D geometry of the modelled zone (geology, topography, hydrology, concerned problem, scale, …)*
- *values for the properties (parameters) playing a role in the modeled processes (i.e. for gw flow: K and S_s or T and S, for solute transport n_e, a_L, a_T, R, …)*
- *stress factors applied on the modelled domain (i.e. for gw flow: recharge, pumping, injections, for solute transport mass injection or removal)*
- *historical (measured) data concerning the main problem variable (i.e. for gw flow: piezometric heads, for solute transport: concentrations) or its first derivative (i.e. for gw flow: flow rates or fluxes, for solute transport advective or dispersive mass fluxes) … distributed data in the domain that will be used for calibration (or inverse modeling) procedure*

General methodology: model implementation

discretisation, parameters, stress-factors and historical data

Conceptual model → *translated in a usable form for modelling:*

→
- *Spatial discretisation* → *grids with cells*
- *Time discretisation* → *time steps*
- *Boundary Conditions (BC's)*
- *Sink /source terms*
- *Initial values for the main variable*
- *Initial values for possible useful other state variables*

General methodology

- *Definitions, terminology, aims*
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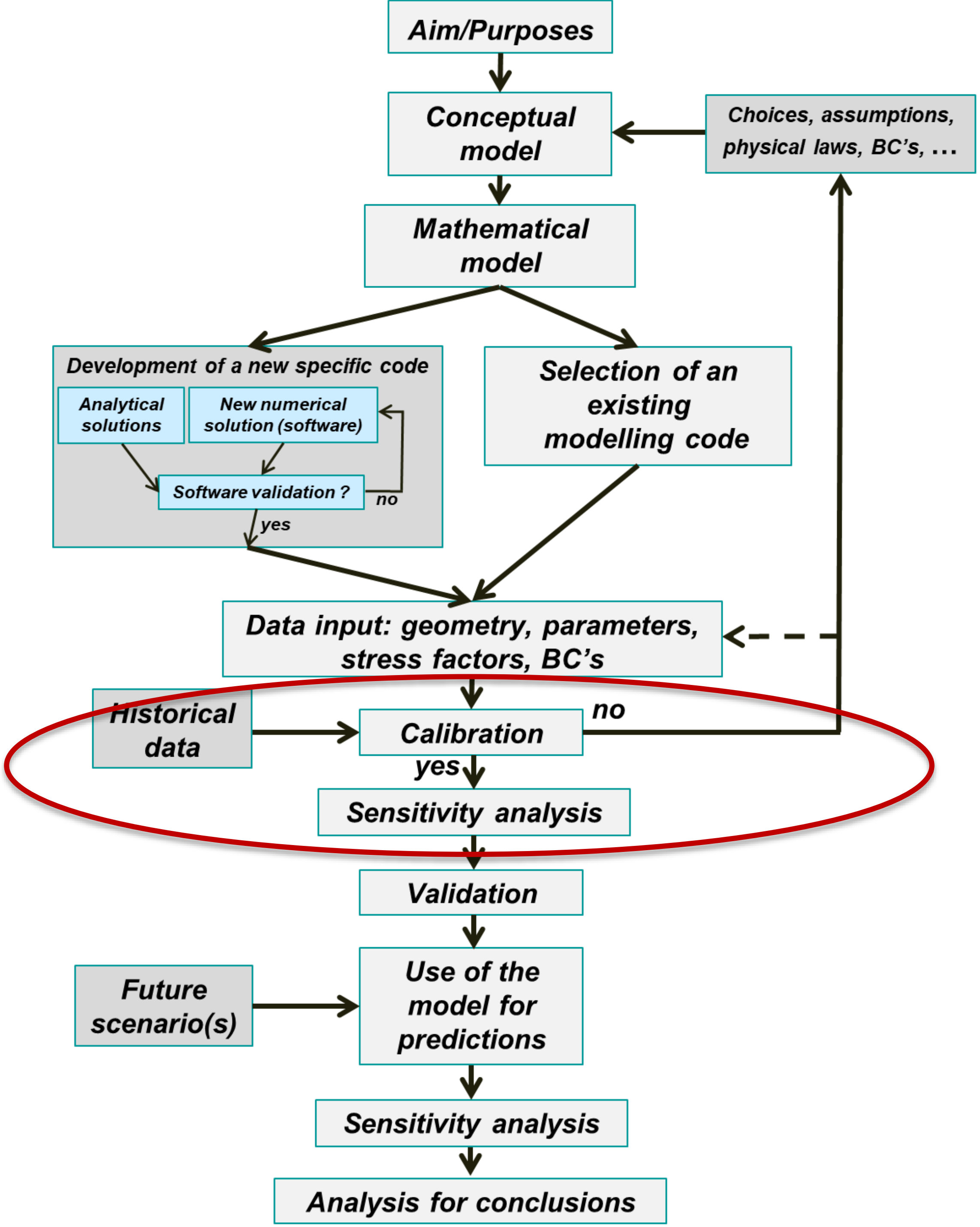
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General methodology: model calibration

Change (adaptation) of the parameters values and distribution … for a better simulation of the reality

➡ *… this reality is considered as represented by historical data sets*

How to quantify objectively the good fit ?

accounting for the discrepancies between observed and computed values of the main variables and/or one or more of their derived variables

Different steps :

- *Objective function formulation (be careful: any objective function is subjective !)*
- *Sensitivity analysis*
- *Change in parameters values (inverse problem);*
- *Validation using another data set (most often another time period, for transient modelling)*

General metodology: performance criteria for calibration

➡ *weighted least square*

$$\varphi\ (\boldsymbol{b}) = \sum_{i=1}^{n} w_i \left[y_i^{obs} - y_i^{sim}(\boldsymbol{b})\right]^2$$

weighting factors for different kind of data

for the relevant process to answer the initial question !

(Beven and Binley 1992, Refsgaard and Henriksen 2004, Rojas et al. 2010b and 2010c, Wildemeersch 2012)

If the aim is to simulate the baseflow evolution in a watershed:

$$\varphi_{NS}\ (\boldsymbol{b}) = 1 - \frac{\sum_{t=1}^{nt}\left[q_t^{obs} - q_t^{sim}(\boldsymbol{b})\right]^2}{\sum_{t=1}^{nt}\left[q_t^{obs} - \mu^{obs}\right]^2} \quad \in\ ]-\infty, 1]$$

(Nash and Sutcliffe 1970, Wildemeersch 2012)

General methodology: model calibration = inverse modeling

could be helpful to gain a full understanding of the physical behavior of the simulated system

- *manual trial-and-error procedure*
- *automatically non-linear regression methods = inverse modelling*

more efficient to produce useful statistics

- *main issues : the non-uniqueness of the solution*
- *introduce prior information on the parameter values to avoid as far as possible an ill-posed inversion*

(Carrera et al. 2005, Hill and Tiedeman 2007, Carrera and Neuman 1986b)

General methodology: sensitivity analysis = calibration tool

the amount the simulated value would change given a change in the parameter value

the amount the simulated value would change given a 1% change in the parameter value

the importance of observations as a whole to a single parameter

- *simple sensitivities*
- *dimensionless scaled sensitivities (dss)*
- *composite scaled sensitivities (css)*

(Hill 1992, Anderman et al. 1996, Hill et al. 1998, Hill and Tiedeman 2007)

(example in Goderniaux et al. 2015)

- *calculated using inverse modeling codes as PEST and UCODE*

(Doherty 2005, Skahill and Doherty 2006, Poeter et al. 2005)

the degree of correlation between couple of parameters and/or stress factors

- *+ parameter correlation coefficients*

General methodology

- *Definitions, terminology, aims*
- *Methodology*
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- *Model calibration and sensitivity*
- ***Evaluation/reporting***

General methodology: evaluation & reporting

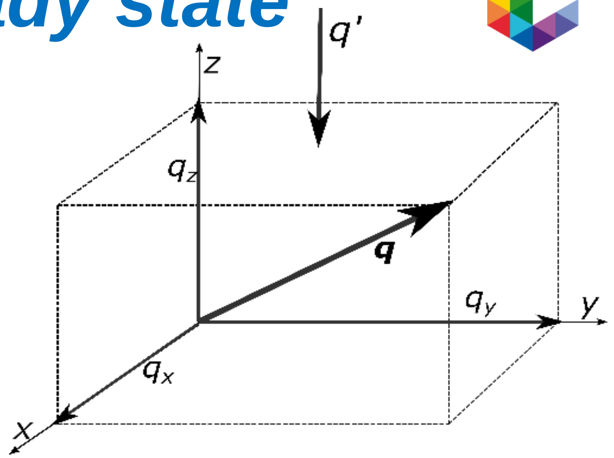
- *very important to analyse and evaluate the reliability of model results and adopted conceptual choices <u>with regards to the question to be answered</u> …*

Reporting

- *modelling study realised step by step … these steps must be described in the final report to establish clearly the reliability of the results despite the simplifying assumptions of the conceptual model*

- *the reader must be able to understand the justification of the conceptual choices and the rigour of the followed approach*

Groundwater flow equation in steady state



$$\nabla \cdot (\rho\, \boldsymbol{K} \cdot \nabla h) + \rho q' = 0$$

terms are kg/(m³s)

$$\frac{\partial}{\partial x_i}\left(\rho K_{ij} \frac{\partial h}{\partial x_j}\right) + \rho q'_i = 0$$

in indicial notation

$$\frac{\partial}{\partial x}\left(K_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy} \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial h}{\partial z}\right) + q' = 0$$

if density is assumed constant and the principal anisotropy directions of the K tensor are known and aligned with the selected coordinate system – terms are in s^{-1}

$$\frac{\partial}{\partial x}\left(K_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial h}{\partial z}\right) + q' = 0$$

if 2D vertical flow, terms are in s^{-1}

$$\frac{\partial}{\partial x}\left(T_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy} \frac{\partial h}{\partial y}\right) + q'' = 0$$

if 2D horizontal flow, terms are in m/s

2D groundwater flow equations in transient conditions (horizontal flow)

confined aquifer

$$\nabla \cdot (\boldsymbol{T} \cdot \nabla h) + q'' = S\frac{\partial h}{\partial t}$$

terms are in m/s

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) + q''_i = S\frac{\partial h}{\partial t}$$

in indicial notation

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) + q'' = S\frac{\partial h}{\partial t}$$

principal anisotropy directions aligned with the selected coordinate system

unconfined aquifer

$$\nabla \cdot (\boldsymbol{T}(h) \cdot \nabla h) + q'' = n_e\frac{\partial h}{\partial t} = S_y\frac{\partial h}{\partial t}$$

terms are in m/s

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) + q''_i = n_e\frac{\partial h}{\partial t} = S_y\frac{\partial h}{\partial t}$$

in indicial notation

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) + q'' = S\frac{\partial h}{\partial t}$$

principal anisotropy directions aligned with the selected coordinate system

Groundwater flow equations including the partially saturated zone

$$\nabla \cdot \rho\left[\boldsymbol{K}\left(h_p\right) \cdot \nabla h_p + \boldsymbol{K}\left(h_p\right) \cdot \nabla z\right] + \rho q' = \rho C\left(h_p\right)\frac{\partial h_p}{\partial t}$$

(Celia et al. 1990)

with water pressure head as main variable

terms are kg/(m^{3}s)

$$\nabla \cdot \rho\left[\boldsymbol{K}(\theta) \cdot \nabla h_p + \boldsymbol{K}(\theta) \cdot \nabla z\right] + \rho q' = \rho\frac{\partial \theta}{\partial t}$$

(Richards 1931)

in a mixed way as a function of the water content and the pressure head

needs relations between

- *θ and h_p*
- *θ and K*

…

… van Genuchten relations and others

Flow Boundary Conditions

- *Dirichlet conditions: prescribed piezometric head*
- *Neumann conditions: prescribed flux*
- *Cauchy or mixed conditions: flux depending on piezometric head*

Flow BC's

Prescribed piezometric head

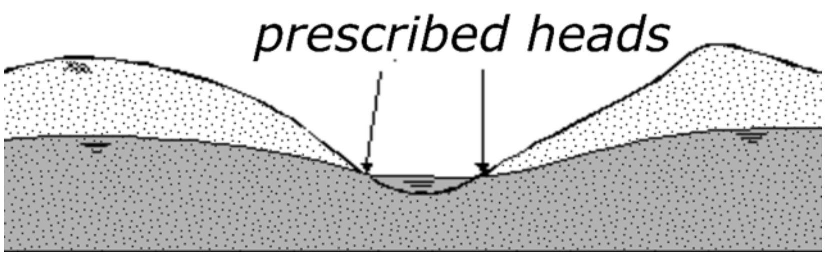
(Dirichlet condition)

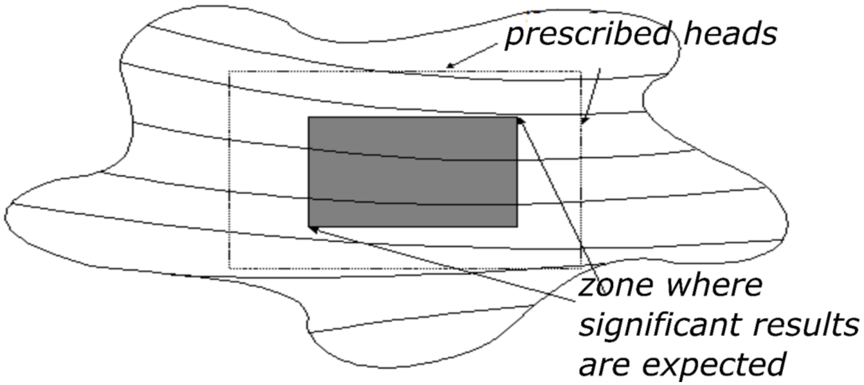
Prescribed piezometric head on the concerned boundary:

$$h(x, y, z, t) = f'(x, y, z, t)$$

f' *can vary in space and time*
(one value per node and per time step)

➡ *a flux will be computed per concerned node*





Flow BC's

Prescribed flux (Neumann condition)

The first derivative of the piezometric head is prescribed on the concerned boundary:

$$\nabla h \cdot \boldsymbol{n} = \frac{\partial h}{\partial n}(x, y, z, t) = f''(x, y, z, t)$$

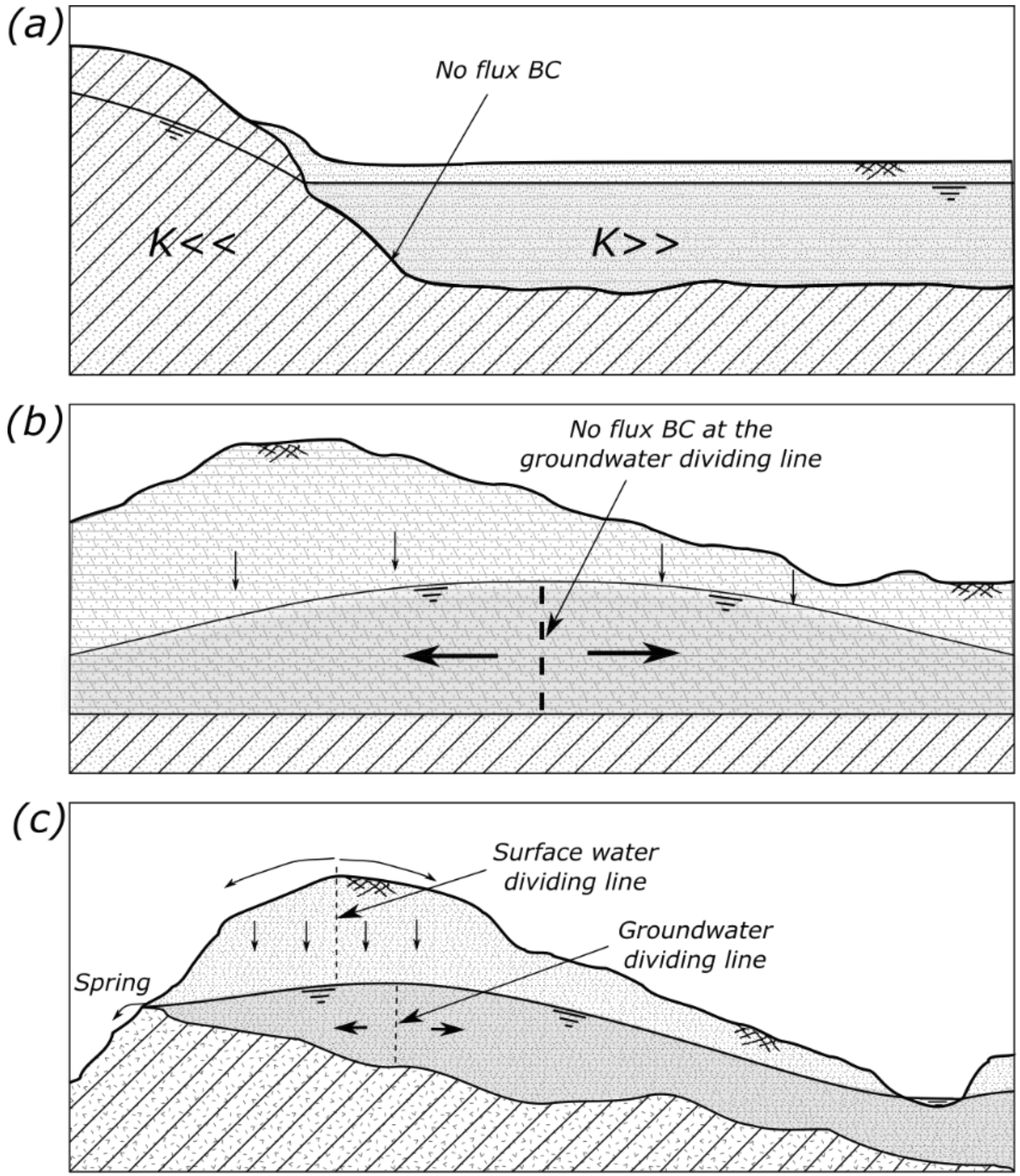
f'' *piezometric gradient normal to the concerned boundary, its value can vary in space and time (one value per concerned node and per time step) Applying the Darcy's law, it is a way of prescribing the water flux through the boundary:*

$$K \frac{\partial h}{\partial n}(x, y, z, t) = q''(x, y, z, t)$$

q'' *: precribed flux through the boundary (m/s)*

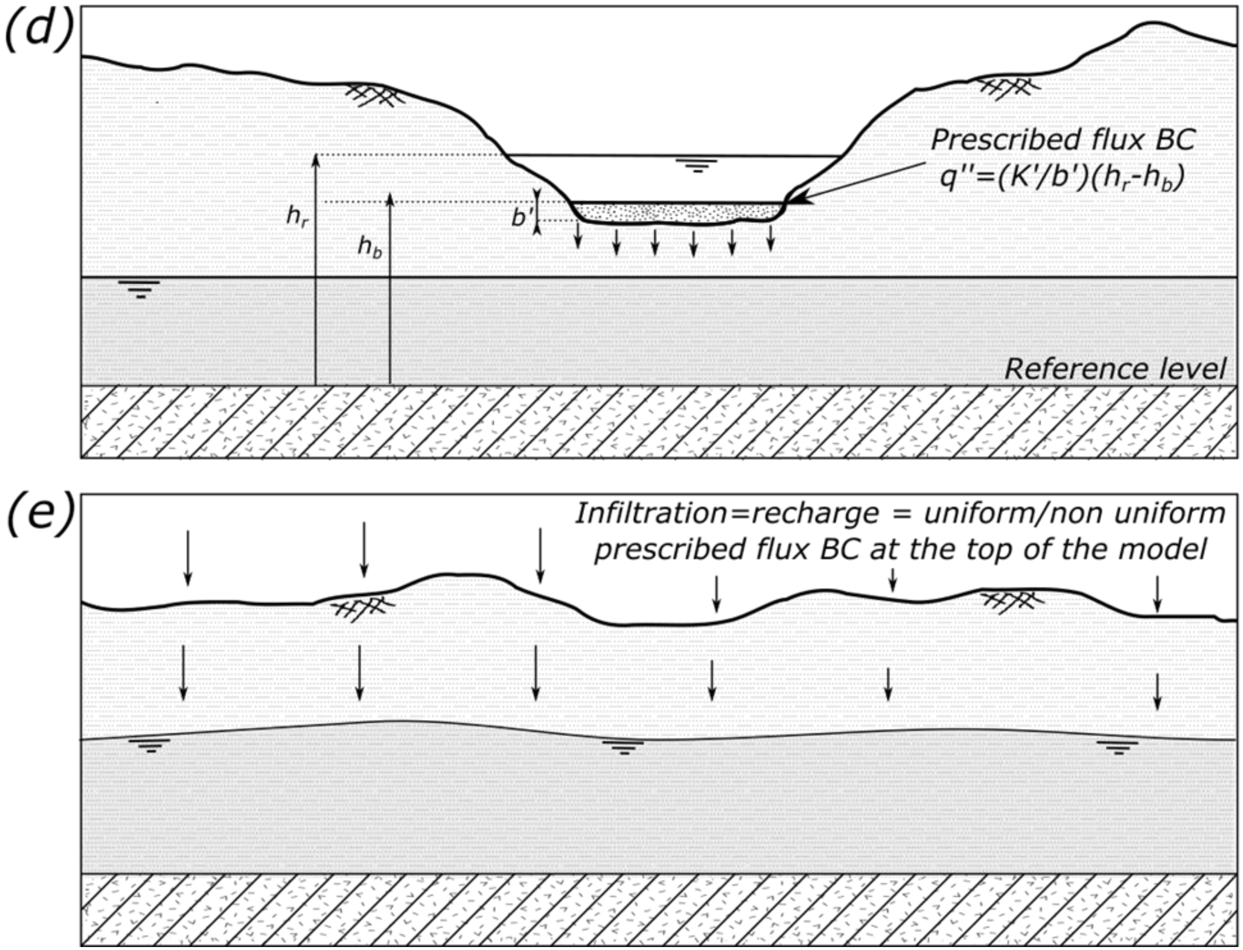
particular case: $f'' = 0$

Flow BC's *Prescribed flux (Neumann condition)*



(Dassargues, 2018)

Flow BC's *Prescribed flux (Neumann condition)*



(Dassargues, 2018)

Flow BC's

Flux depending on the piezometric head

(mixed condition or Cauchy condition)

A combination (linear relation) of the piezometric head and its first derivative is prescribed on the boundary:

$$a.\frac{\partial h}{\partial n}(x,y,z,t)+b.h(x,y,z,t)=f'''(x,y,z,t)$$

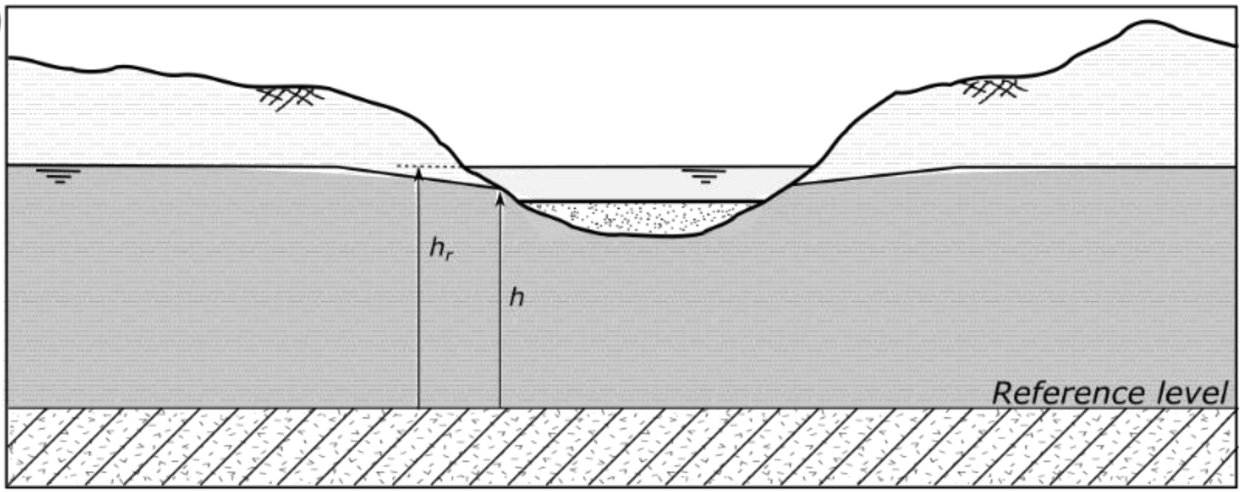
f''' *can vary in space and in time*

(one value per concerned node and per time step)

- *interactions between surface water bodies and groundwater*
- *interactions between different aquifers*

Flow BC's *Flux depending on the piezometric head (mixed condition or Cauchy condition)*

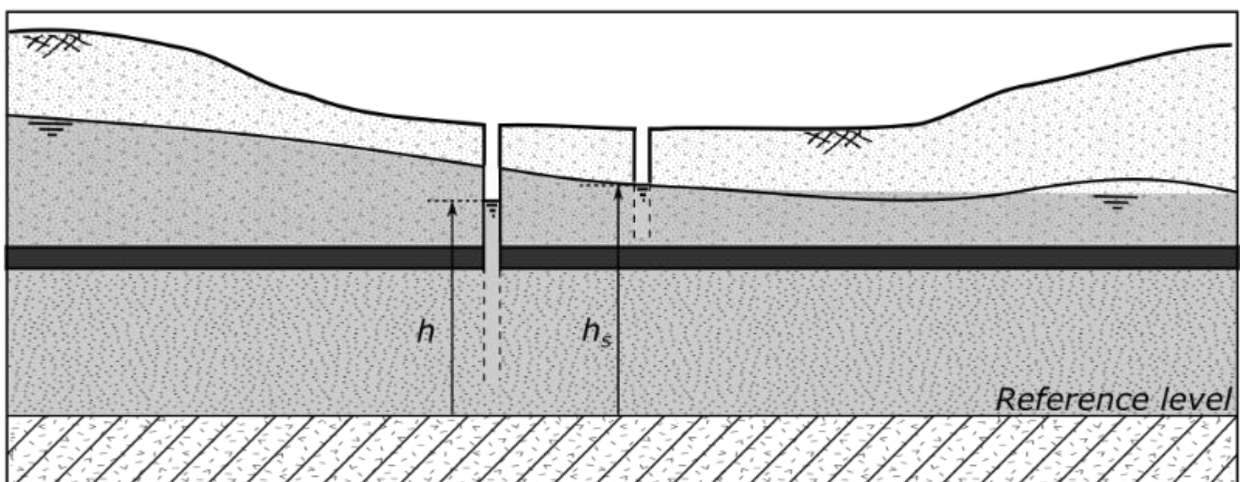
(a)



conductance

$$q'' = -K\frac{\partial h}{\partial n} = \frac{K'}{b'}(h_r - h)$$

(b)

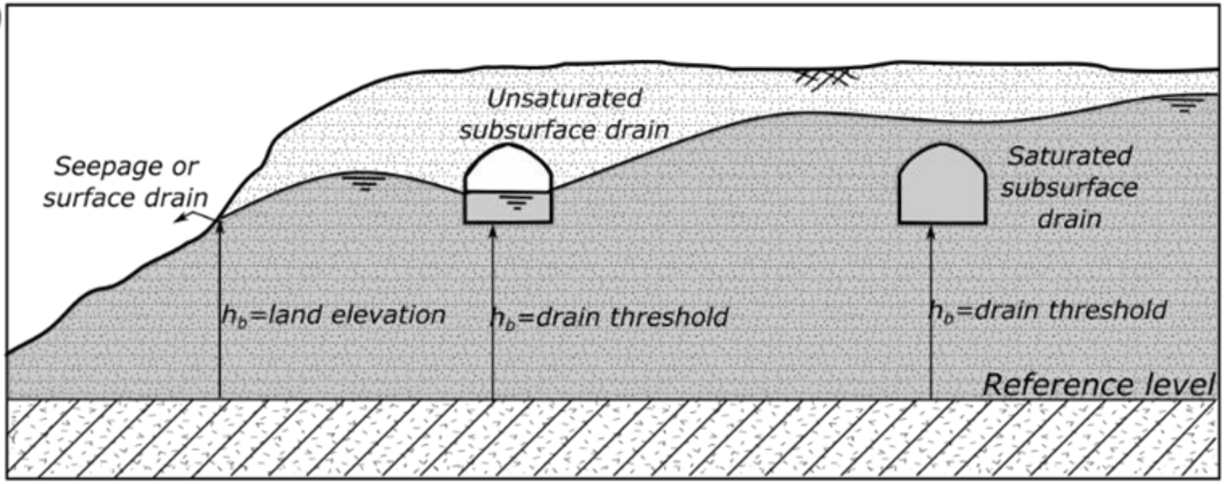


conductance

$$q'' = -K\frac{\partial h}{\partial n} = \frac{K'}{b'}(h_s - h)$$

Flow BC's *Flux depending on the piezometric head (mixed condition or Cauchy condition)*

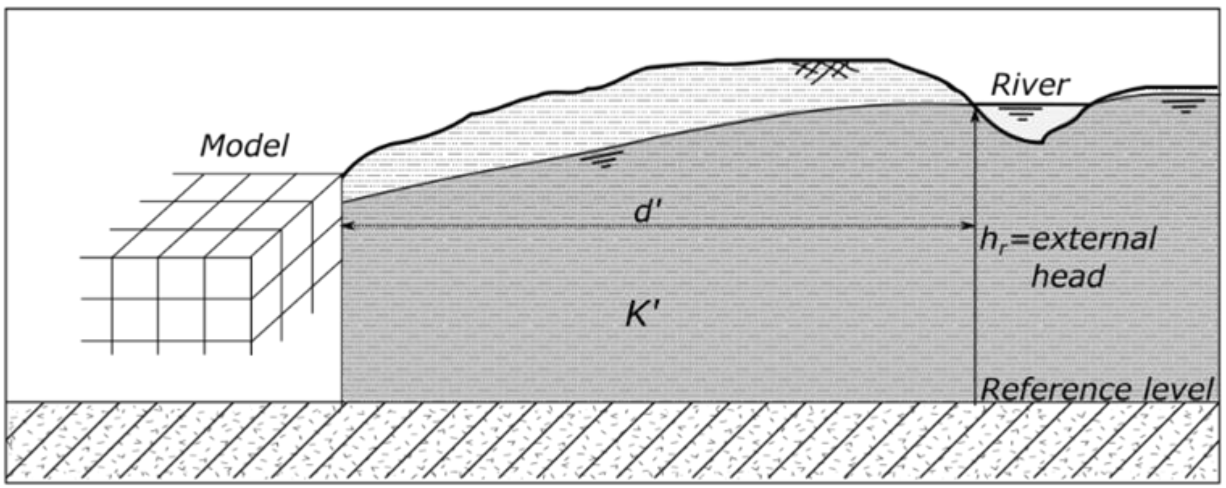
(c)



conductance

$$q'' = -K\frac{\partial h}{\partial n} = \frac{K'}{b'}(h_b - h)$$

(d)



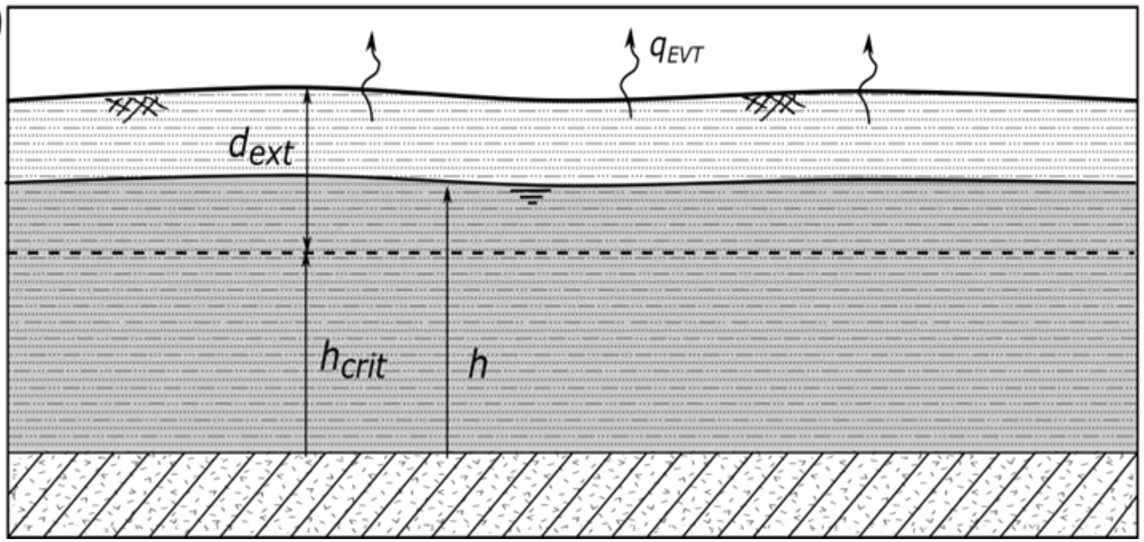
conductance

$$q'' = -K\frac{\partial h}{\partial n} = \frac{K'}{d'}(h_r - h)$$

prescribing an 'external head' (i.e. not on the true boundary but outside the modelled zone) so that a groundwater flux across the boundary is computed from the difference between this 'external head' and the piezometric head on the model boundary using a given conductance

Flow BC's *Flux depending on the piezometric head (mixed condition or Cauchy condition)*

(e)



in arid and semi-arid zones

conductance

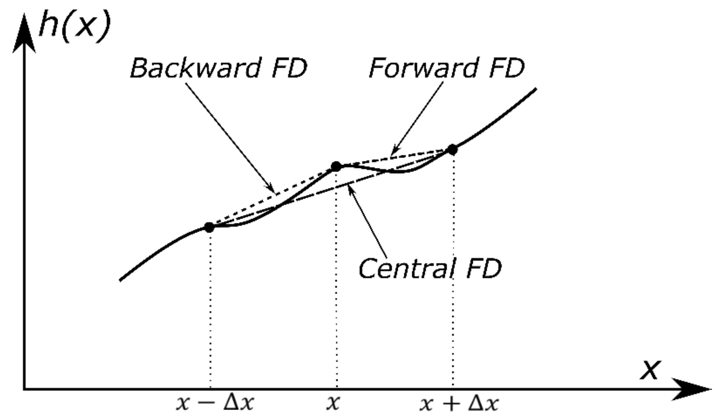
$$q_{EvT} = \frac{R_{EvT}}{d_{ext}}\left(h(x,y,z,t) - h_{crit}(x,y,z,t)\right)$$

(Anderson et al. 2015)

represent an evapotranspiration flux leaving the model but dependent on the 'depth to water' (i.e. the land surface elevation minus piezometric head). An extinction depth d_{ext} corresponding to a critical head h_{crit} can be defined so that EvT occurs only if the water table is higher

Introduction to solving methods: FD

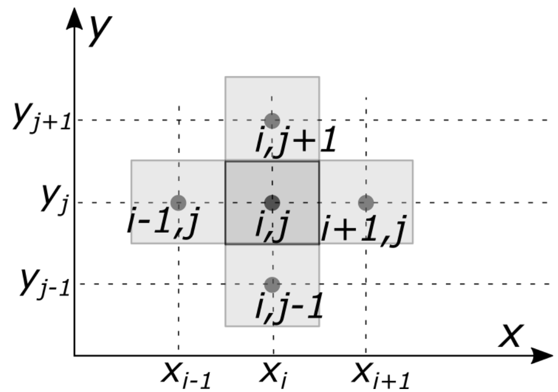
1D spatial approximation of the gradient by a finite difference:



Forward FD $$\frac{\partial h}{\partial x} \approx \frac{h(x+\Delta x)-h(x)}{\Delta x}$$

Central FD $$\frac{\partial h}{\partial x} \approx \frac{h(x+\Delta x)-h(x-\Delta x)}{2\Delta x}$$

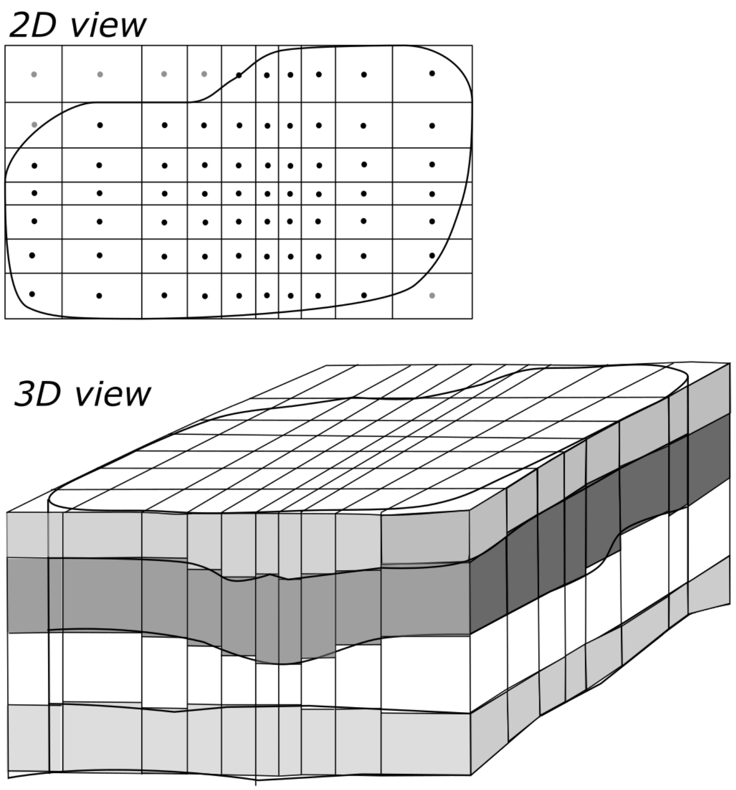
$$\frac{\partial^2 h}{\partial x^2} \approx \frac{h_{i+1j}-2h_{ij}+h_{i-1j}}{(\Delta x)^2}$$

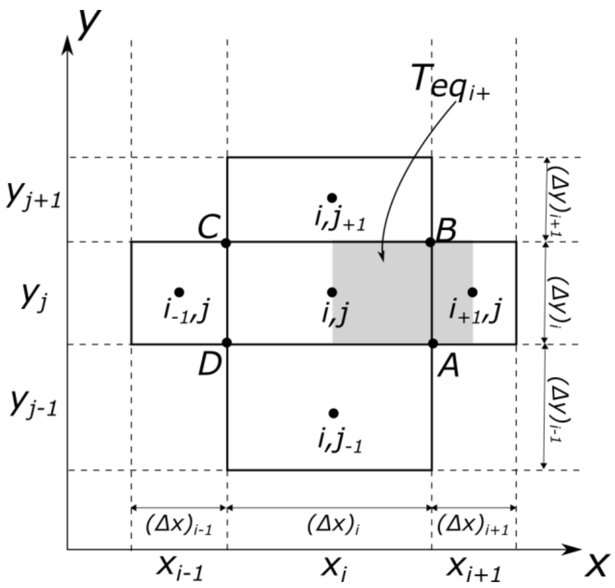


In 2D, with a 2nd order accurate FD:

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2} \approx \frac{\left(h_{i+1j}+h_{i-1j}+h_{ij+1}+h_{ij-1}-4h_{ij}\right)}{(\Delta m)^2}=0$$

Introduction to solving methods: BCFD



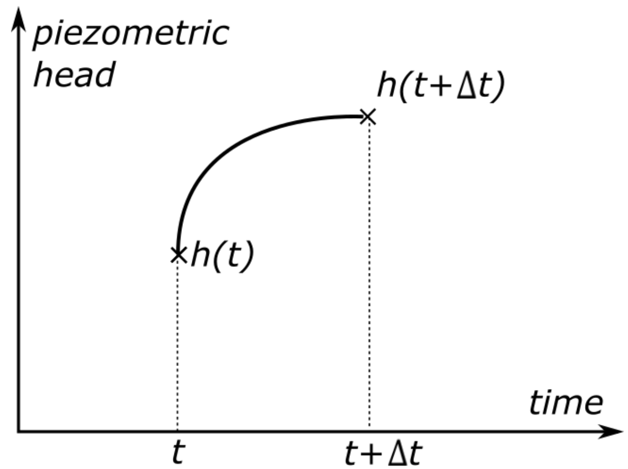


$$T_{eq_{i+}} = \frac{2T_{i+1j}T_{ij}}{T_{ij} + T_{i+1j}}$$

Introduction to solving methods: time integration scheme

$$T\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\approx T\frac{\left(h_{i+1j}+h_{i-1j}+h_{ij+1}+h_{ij-1}-4h_{ij}\right)}{(\Delta m)^2}=S\frac{\partial h}{\partial t}$$

$$\frac{\partial h}{\partial t}=\frac{h(t+\Delta t)-h(t)}{\Delta t}$$



at what time do we consider the piezometric head values?

$$\frac{T}{(\Delta m)^2}\left(\overbrace{h_{i+1j}+h_{i-1j}+h_{ij+1}+h_{ij-1}-4h_{ij}}\right)+Q_{ij}=S\frac{h_{ij}(t+\Delta t)-h_{ij}(t)}{\Delta t}$$

Explicit

$$h_{ij}(t+\Delta t)=h_{ij}(t)+\frac{Q_{ij}\Delta t}{S}+\frac{T\Delta t}{(\Delta m)^2 S}\left(h_{i+1j}(t)+h_{i-1j}(t)+h_{ij+1}(t)+h_{ij-1}(t)-4h_{ij}(t)\right)$$

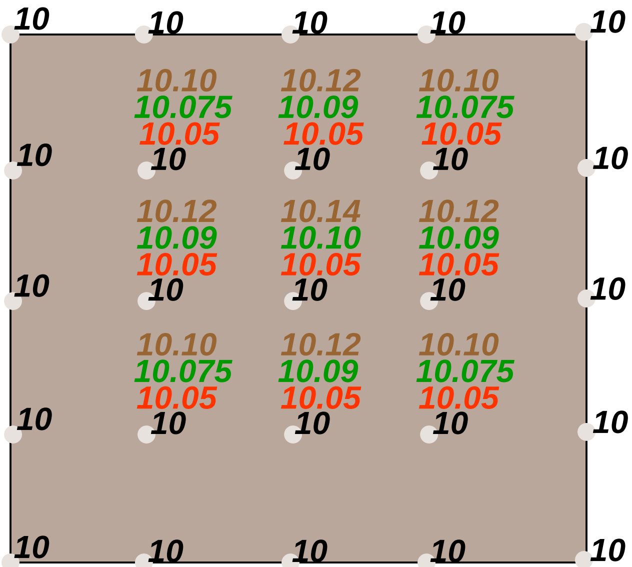
- *physically: not so accurate*
- *numerically: stability problem when the time step becomes larger*
- *respect a stability criterion*

$$T=Cst$$

$$\Delta x=\Delta y=\Delta m=Cst$$

Explicit method

$$h_{ij}(t+\Delta t)=h_{ij}(t)+\frac{I.\Delta t}{S}+\frac{T.\Delta t}{(\Delta m)^2.S}.\left(h_{i+1\,j}(t)+h_{i-1\,j}(t)+h_{i\,j+1}(t)+h_{i\,j-1}(t)-4h_{ij}(t)\right)$$



Example:

- *squared island*
- *initial value h = 10 m*
- *BC's : h = 10 m*
- *infiltration: 0.002 m/day*
- *S = 0.4 ; T = 100 m²/day*
- *Δt =10 days Δm =50m*

$$\frac{I.\Delta t}{S}=0.05 \qquad \frac{T.\Delta t}{(\Delta m)^2.S}=0.25$$

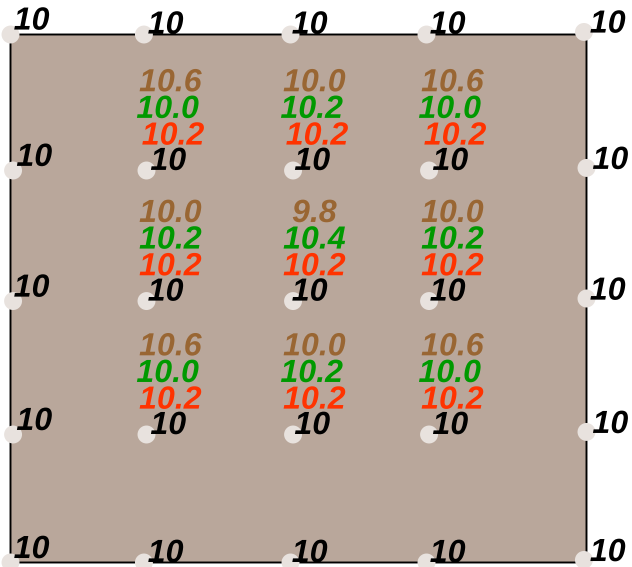
… computation:

- *1st time step;*
- *2nd time step;*
- *3rd time step;*
- *…*

… no problem

Explicit method

$$h_{ij}(t+\Delta t) = h_{ij}(t) + \frac{I.\Delta t}{S} + \frac{T.\Delta t}{(\Delta m)^2.S}.\left(h_{i+1\,j}(t) + h_{i-1\,j}(t) + h_{i\,j+1}(t) + h_{i\,j-1}(t) - 4h_{ij}(t)\right)$$



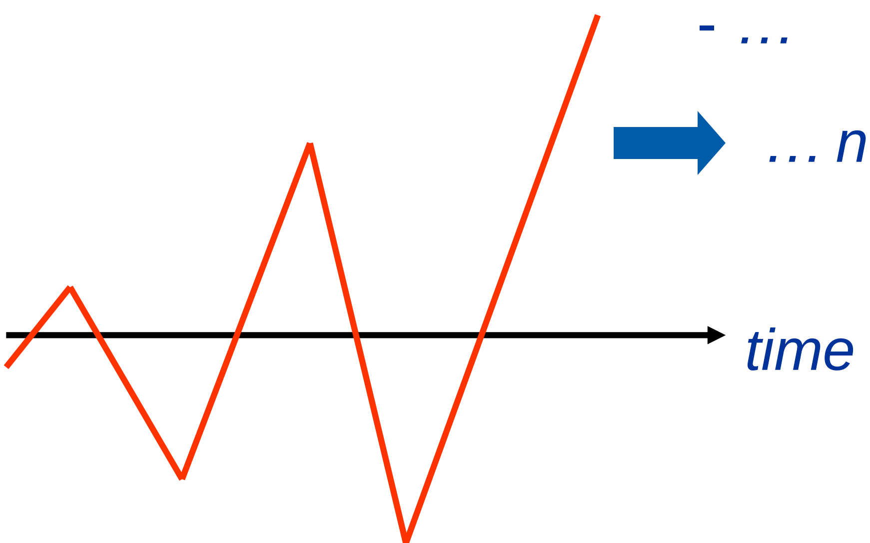
… now with a Δt = 40 days

$$\frac{I.\Delta t}{S} = 0.2 \qquad \frac{T.\Delta t}{(\Delta m)^2.S} = 1$$

… computation:

- 1st time step;
- 2nd time step;
- 3rd time step;
- …

… numerically not stable



Explicit method: stability criterion (example)

$$h_{ij}(t+\Delta t) = h_{ij}(t) + \frac{I.\Delta t}{S} + \frac{T.\Delta t}{(\Delta m)^2.S}.\left(h_{i+1\,j}(t) + h_{i-1\,j}(t) + h_{i\,j+1}(t) + h_{i\,j-1}(t) - 4h_{ij}(t)\right)$$

… worst case

$$\frac{I.\Delta t}{S} = 0 \qquad \frac{T.\Delta t}{(\Delta m)^2.S} = \alpha$$

	10 + ε	
10 + ε	**10 - ε**	**10 + ε**
	10 + ε	

$$h_{ij}(t) = (10-\varepsilon)$$

$$h_{ij}(t+\Delta t) = (10-\varepsilon) + 0 + \alpha(8\varepsilon)$$

$$h_{ij}(t+\Delta t) = 10 + (8\alpha - 1)\varepsilon$$

… for obtaining the stability :

$$(8\alpha - 1)\varepsilon \leq \varepsilon$$

$$\alpha \leq 1/4$$

$$\frac{T.\Delta t}{(\Delta m)^2.S} = \alpha \leq 1/4$$

Introduction to solving methods: time integration scheme

Implicit

… at the time $t + \Delta t$

$$h_{ij}(t+\Delta t)[1+4\alpha] = h_{ij}(t) + \frac{Q_{ij}\Delta t}{S} + \frac{T\Delta t}{(\Delta m)^2 S}\left(h_{i+1j}(t+\Delta t) + h_{i-1j}(t+\Delta t) + h_{ij+1}(t+\Delta t) + h_{ij-1}(t+\Delta t)\right)$$

implicit equation

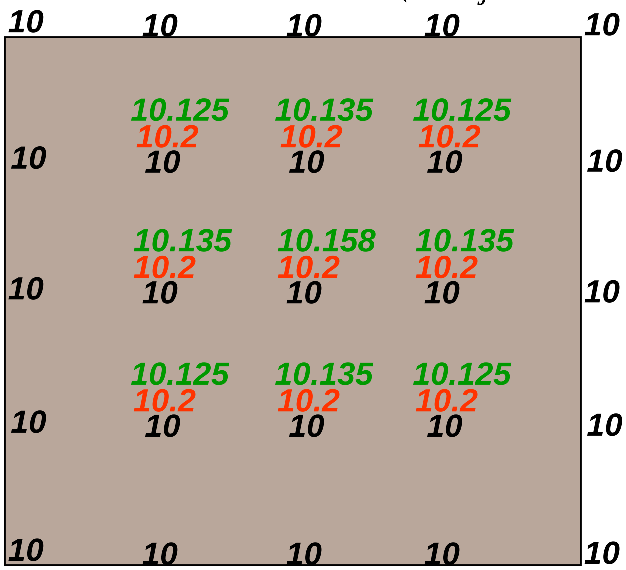
the unknown cannot be deduced from one equation
you need the whole system to be solved

- *physically: not so accurate (error increases with time step)*
- *numerically: unconditional stability*
- *mathematically: more complex/heavy*

(Bear and Cheng 2010)

Implicit method

$$h_{ij}(t+\Delta t).\left[1+4.\alpha\right] = h_{ij}(t) + \frac{I.\Delta t}{S}$$
$$+\alpha.\left(h_{i+1\,j}(t+\Delta t) + h_{i-1\,j}(t+\Delta t) + h_{i\,j+1}(t+\Delta t) + h_{i\,j-1}(t+\Delta t)\right)$$



… even with a Δt = 40 days

$$\frac{I.\Delta t}{S} = 0.2 \qquad \frac{T.\Delta t}{(\Delta m)^2.S} = 1$$

… computation:

- *1st time step;*
- *2nd time step;*
- *…*

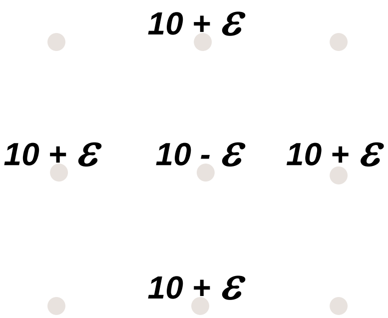
➡ *… numerical stability*

Implicit method: stability can be proven

$$h_{ij}(t+\Delta t).[1+4.\alpha] = h_{ij}(t) + \frac{I.\Delta t}{S} + \alpha.\left(h_{i+1\,j}(t+\Delta t) + h_{i-1\,j}(t+\Delta t) + h_{i\,j+1}(t+\Delta t) + h_{i\,j-1}(t+\Delta t)\right)$$

… the worst case

$$\frac{I.\Delta t}{S} = 0 \qquad \frac{T.\Delta t}{(\Delta m)^2.S} = \alpha$$



$$h_{ij}(t) = (10-\varepsilon)$$

$$\Rightarrow h_{ij}(t+\Delta t)(1+4\alpha) = (10-\varepsilon) + 0 + 4\alpha(10+\varepsilon)$$

$$h_{ij}(t+\Delta t) = \frac{(10-\varepsilon)+4\alpha(10+\varepsilon)}{(1+4\alpha)}$$

⇒ *for obtaining stability :*

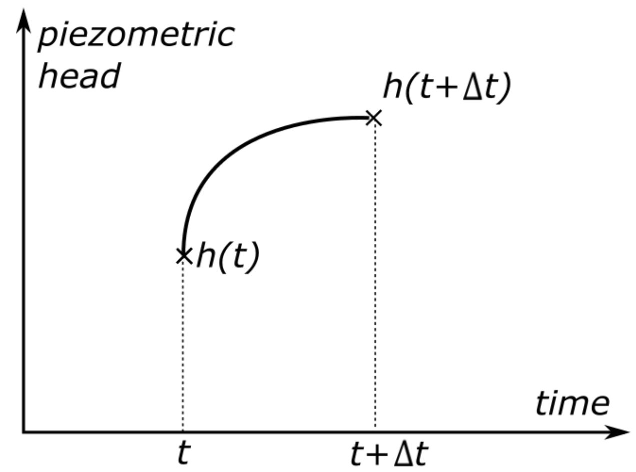
$$\boxed{h_{ij}(t+\Delta t) - 10 \leq \varepsilon}$$

$$\Rightarrow \frac{(10-\varepsilon)+4\alpha(10+\varepsilon)}{(1+4\alpha)} - 10 \leq \varepsilon$$

$$\Rightarrow 10-\varepsilon+40\alpha+4\alpha\varepsilon < 10+\varepsilon+40\alpha+4\alpha\varepsilon$$

…always the case

Introduction to solving methods: time integration scheme



Crank-Nicholson method

- … at the time $t+\Delta t/2$
- physically: more accurate
- numerically: implicit procedure, unconditional stability

Galerkin method

- … at the time $t+2\Delta t/3$
- physically: most accurate
- numerically: implicit procedure, unconditional stability

Introduction to solving methods: time integration scheme

$$\frac{T}{(\Delta m)^2}\left(h_{i+1j}+h_{i-1j}+h_{ij+1}+h_{ij-1}-4h_{ij}\right)+Q_{ij}=S\frac{h_{ij}(t+\Delta t)-h_{ij}(t)}{\Delta t}$$

$$\frac{T}{(\Delta m)^2}(1-\theta)\left(h_{i+1j}(t)+h_{i-1j}(t)+h_{ij+1}(t)+h_{ij-1}(t)-4h_{ij}(t)\right)$$
$$+\frac{T}{(\Delta m)^2}\theta\left(h_{i+1j}(t+\Delta t)+h_{i-1j}(t+\Delta t)+h_{ij+1}(t+\Delta t)+h_{ij-1}(t+\Delta t)-4h_{ij}(t+\Delta t)\right)$$

$\theta = 0$ ➡ *Full explicit time integration*

$\theta = 1$ ➡ *Full implicit time integration*

$\theta = 1/2$ ➡ *Crank-Nicholson implicit*

$\theta = 2/3$ ➡ *Galerkin implicit*

➡ *stability criterion only for explicit schemes* $\theta < 1/2$

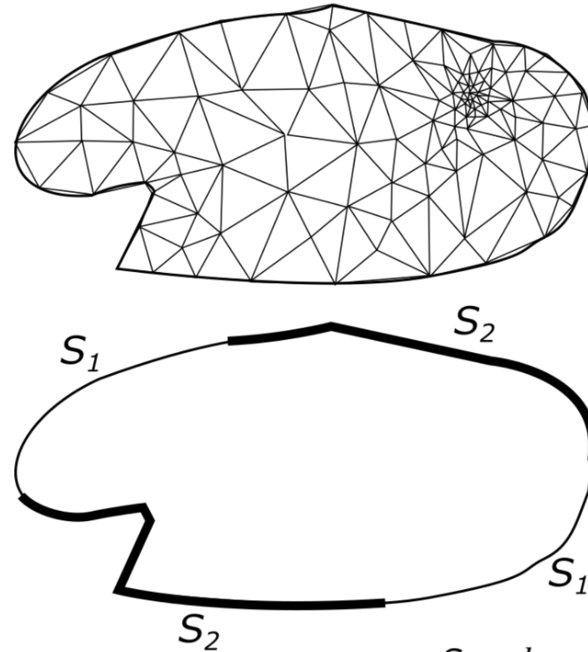
time integration schemas used in all numerical techniques

Introduction to solving methods: FD practical recommendations

- *an initial field of values for the main unknown variable (piezometric head) needed for initiating the iterative solving*
- *accuracy increases with the number of cells but portability (i.e. computing efficiency) decreases*
- *use smaller cells where a steep gradient of the main variable is expected.*
- *spatial discretization: nodes located at pumping wells and observation piezometers*
- *avoid distances between nodes greater than 1.5 the previous one*
- *avoid ratios greater than 1/10 for the cell dimensions (bad numerical conditions for solving the system of equations)*
- *boundaries with a prescribed head should correspond to nodes (central points of the cells, if BCFD)*
- *boundaries with a prescribed flux should correspond to sides of the cells (where the flux condition is calculated) if BCFD.*
- *…*

Introduction to solving methods: FE

- discrete elements, unstructured FE mesh
- better for irregular boundaries, spatial variations, and exact locations for stress-factors and observation measurements
- optimized mesh generation to reduce the needed memory space

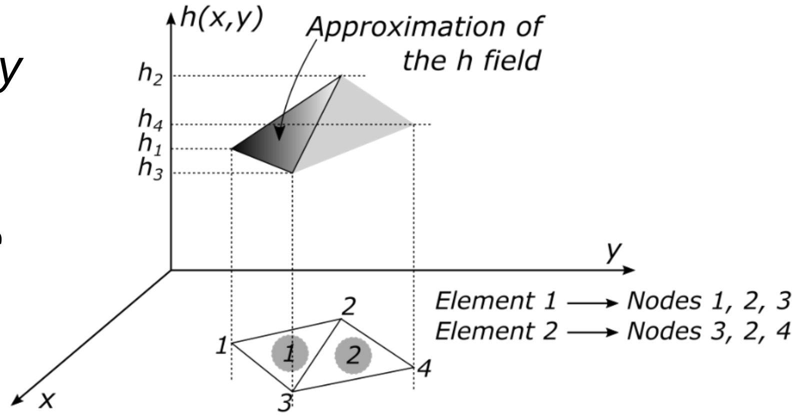


S_1 : $h = f(x,y)$
S_2 : $\partial h/\partial n = 0$ $(or\ cst)$

(refs among others: Narasimhan et al. 1978, Huyakorn and Pinder 1983, Bear and Verruijt 1987, Wang and Anderson 1982, Fitts 2002, Rausch et al. 2005, Bear and Cheng 2010, Anderson et al. 2015, Diersch 2014, Pinder and Celia 2006, Dassargues 2018)

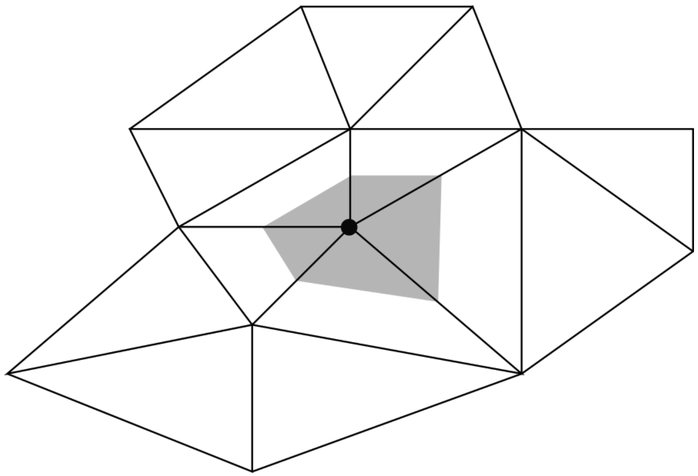
Introduction to solving methods: FE

- *the continuous field of the variable (i.e. piezometric head) approximated typically by interpolation functions (here also referred to as basis functions)*
- *piezometric field described in each finite element by a plane*
- *the discrete unknowns are the nodal values*
- *an integral approach expressing the weak formulation (i.e. a variational form integrating the governing partial differential equation of the process with its BCs and initial conditions) for obtaining a global continuum balance statement*
- *two ways:*
  - *(1) minimum of a natural variational functional (when it exists)*
  - *(2) method of weighted residuals (applicable to all types of partial differential equations)*



Introduction to solving methods: FV

- *common features with FD and FE*
- *FD for unstructured grids*
- *if triangles: similarities with triangle FE*
- *as for FE, FV approximates the main variable using basis functions in the triangular element*
- *Finite Volume refers to the volume surrounding each node point in a mesh with nodal basis function = 1 only at the considered node and 0 at all others*
- *conservation law is satisfied locally for a given control volume with respect to its neighboring volumes (similar to FD not to FE)*
- *balance relies on evaluation of surface integrals on the boundaries (i.e. the conservation must be satisfied across the boundaries of the adjoining control volumes)*



(refs among others: Patankar 1980, Baliga and Patankar 1983, Chung 2002, Diersch 2014, Narasimhan and Witherspoon 1976, Rausch et al. 2005, Fletcher 1988, Idelsohn and Onate 1994, Forsyth et al. 1995, Therrien and Sudicky 1996, Pinder and Celia 2006, Therrien et al. 2010)

Solute transport equations

$$R\frac{\partial C^v}{\partial t} = -\nabla\cdot(\boldsymbol{v_a}C^v) + \nabla\cdot(\boldsymbol{D_h}\cdot\nabla C^v) - R\lambda C^v + \frac{M^v}{n_m}$$

Remarks and assumptions:

- *degradation occurs in both the mobile mass phase as well as the sorbed phase*
- $R = \left(1 + \frac{\rho_b}{n_m}K_d\right)$ *and* n_m *is the mobile water porosity for transport, isothermal linear relation for adsorption/desorption*
- *source/sink term represented by* M^v *in kg/m³s [ML⁻³T⁻¹]*

  (a) source/sinks of solute mass linked to a groundwater flow rate exchanged with the external world $= q_s C_s^v$

  (b) source/sinks of solute mass resulting from chemical reactions and immobile water effects/matrix diffusion

Solute transport equations

multi-species reactive transport in mobile groundwater

$$R_i \frac{\partial C_i^v}{\partial t} = -\boldsymbol{v}_{\boldsymbol{a}_i} \nabla C_i^v + \nabla \cdot (\boldsymbol{D}_{\boldsymbol{h}} \cdot \nabla C_i^v) - R_i \lambda_i C_i^v - \frac{q_s}{\theta_i}(C_i^v - C_{s_i}^v)$$

$$\boxed{+\frac{1}{\theta_i} \sum_{j=1}^{N_s} S_{ij}(C_1^v, \dots, \quad C_n^v)} \qquad i = 1, \dots, N_s$$

can be solved separately by PREEQC (for example)

where S_{ij} *= source/sink term representing the effect of reactions (kg/m³s)[ML⁻³T⁻¹],*

θ_i*= groundwater specific volume fraction of the REV where species* i *is located*

There are as many equations as species being considered in the reaction system: N_s*, which are coupled through the* $S_{ij}(C_1^v, \dots, \ C_n^v)$ *terms. If all reactions occur in the water phase,* θ_i *are all equal to* n_m *and the components of* $\boldsymbol{v}_{\boldsymbol{a}_i}$ *are all equal to* $\boldsymbol{v}_{\boldsymbol{a}}$ *(i.e. the advection velocity), which is defined as a homogeneous reaction system. On the contrary, if a part of the involved species is on the solid matrix or in the immobile water, the reaction system is defined as heterogeneous,* $\boldsymbol{v}_{\boldsymbol{a}_i}$ *and* $\boldsymbol{D}_{\boldsymbol{h}}$ *being equal to zero for the species in those immobile phases.*

(Kinzelbach 1992, Rausch et al. 2005, Dassargues 2018)

Transport Boundary Conditions

Full analogy with gw flow problem, 3 kinds of BC's:

- *Prescribed concentration (Dirichlet condition)*
- *First derivative of the concentration is prescribed (Neumann condition)*
- *A relation between the concentration and its first derivative is prescribed (Cauchy or mixed condition)*

BC's for a solute transport problem

Prescribed concentration *(Dirichlet BC)*

$$C(x, y, z, t) = g'(x, y, z, t)$$

g' *can vary in space and timevarier dans l'espace et le temps (one value per concerned node and per time step)*

in some cases, a non zero prescribed concentration is used for simulating a continuous (long term) source of contamination

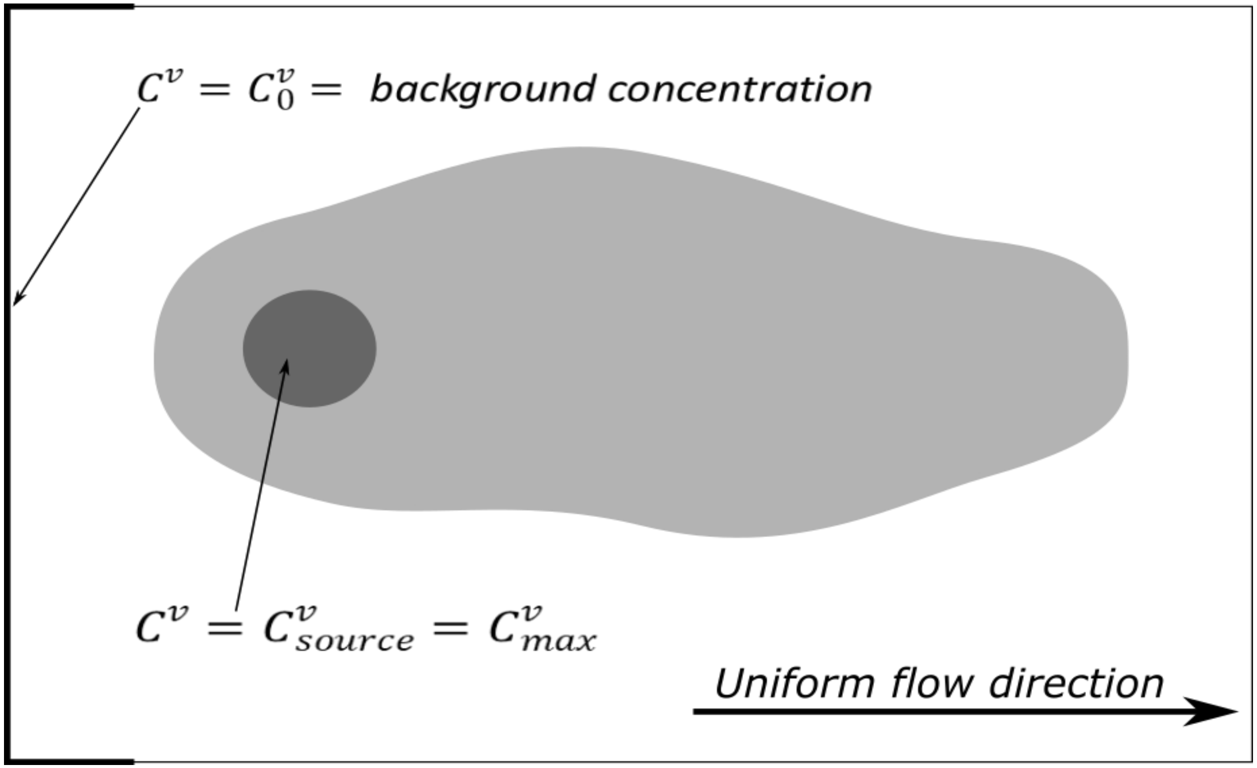
however, for numerical reasons, it induces large numerical dispersion

→ *a huge concentration gradient is prescribed abruptly to the system inducing artificial (numerical) dispersion*

BC's for a solute transport problem

Prescribed concentration (Dirichlet BC)

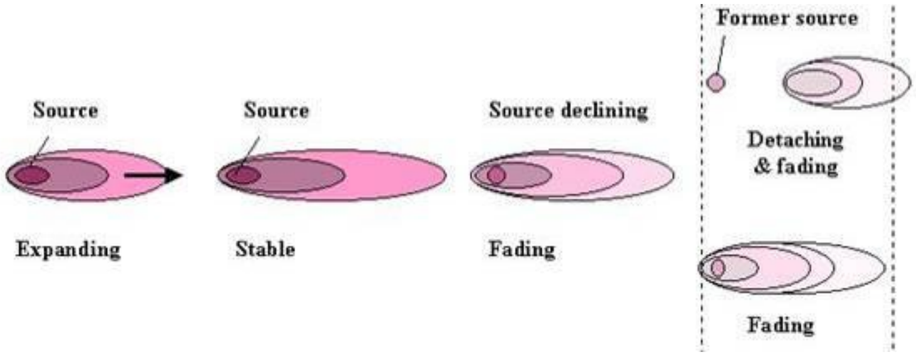
Typical case: a zero (or background) concentration prescribed upwards to the problem



also used for a source of contaminant prescribing C^v_{max} in place of $M_s = q_s C_s^v$

BC's for a solute transport problem

- *main discussion point: how to translate in the model the actual source of contaminant corresponding to the pollution ?*
- *through the sink/source term ? or through prescribed concentrations ?*
- *conceptually, 3 periods in a pollution event*
  - *First release … recent contamination*
  - *Possible stable period*
  - *Decline period … old contamination*



BC's for a solute transport problem

Prescribed first derivative of the concentration

(Neumann BC)

$$\nabla C^v \cdot \boldsymbol{n} = \frac{\partial C^v}{\partial n}(x,y,z,t) = g''(x,y,z,t)$$

g'' *the concentration gradient normal to the boundary can vary in space and in time (one value per node and per time step)*

➡ *… a way of prescribing the dispersion mass flux (hydrodynamic dispersion) on the boundary*

In practice, this kind of condition is often used with a zero value for the diffusion-dispersion mass flux through the boundary:

$$g''=0$$

➡ *the advective component of the mass flux is computed on the boundary by the code*

BC's for a solute transport problem

Prescribed first derivative of the concentration

(Neumann BC)

$$\boldsymbol{n} \cdot (-n_m \boldsymbol{D_h} \cdot \nabla C^v) = -n_m D_{h,n} \frac{\partial C^v}{\partial n}(x,y,z,t) = q''(x,y,z,t)$$

$q''(x,y,z,t)$ *diffusion-dispersion mass flux prescribed on the concerned boundary (kg/(m^2.s))*

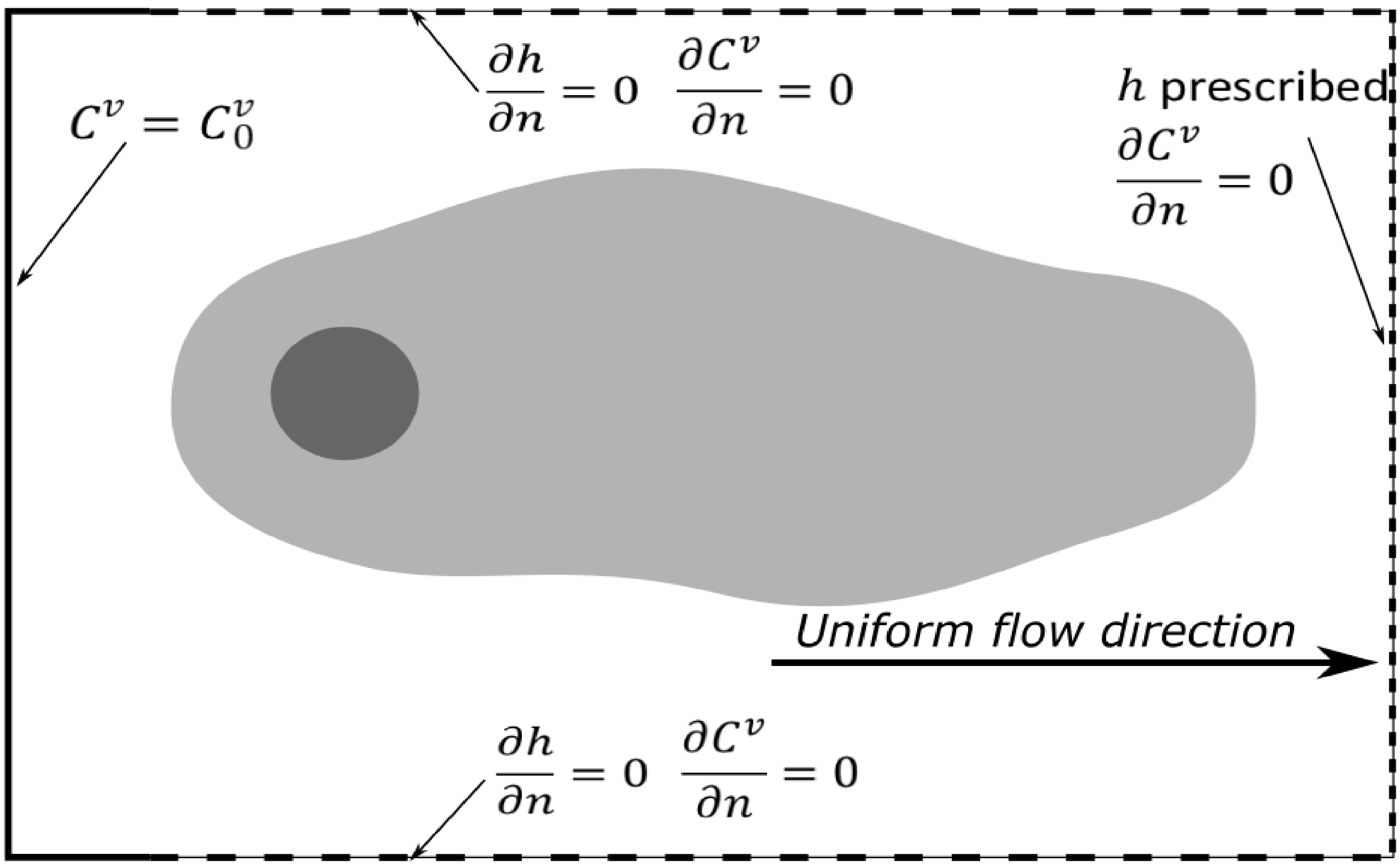
$D_{h,n}$ *normal (to the boundary) component of the hydrodynamic dispersion tensor*

BC's for a solute transport problem

Prescribed first derivative of the concentration

(Neumann BC)

example:



but $\underline{n}.(\rho.v_e.C) \neq 0$

BC's for a solute transport problem

Prescribed relation linking concentration and its first derivative *(Cauchy or mixed Neumann BC)*

a linear combination of the concentration and its first derivative is prescribed on the concerned boundary:

$$a \frac{\partial C^v}{\partial n}(x, y, z, t) + b\, C^v(x, y, z, t) = g'''(x, y, z, t)$$

g''' *can vary in space and time (one value per concerned node and per time step)*

➡ *a combination (most often the sum) of advection and hydrodynamic dispersion mass fluxes is prescribed*

BC's for a solute transport problem

Prescribed relation linking concentration and its first derivative *(Cauchy or mixed Neumann BC)*

advection + diffusion-dispersion :

$$\boldsymbol{n} \cdot (\boldsymbol{q} C^v - n_m \boldsymbol{D_h} \cdot \nabla C^v) = q_n C^v(x,y,z,t) - n_m D_{h,n} \frac{\partial C^v}{\partial n}(x,y,z,t)$$

$$= q'''(x,y,z,t)$$

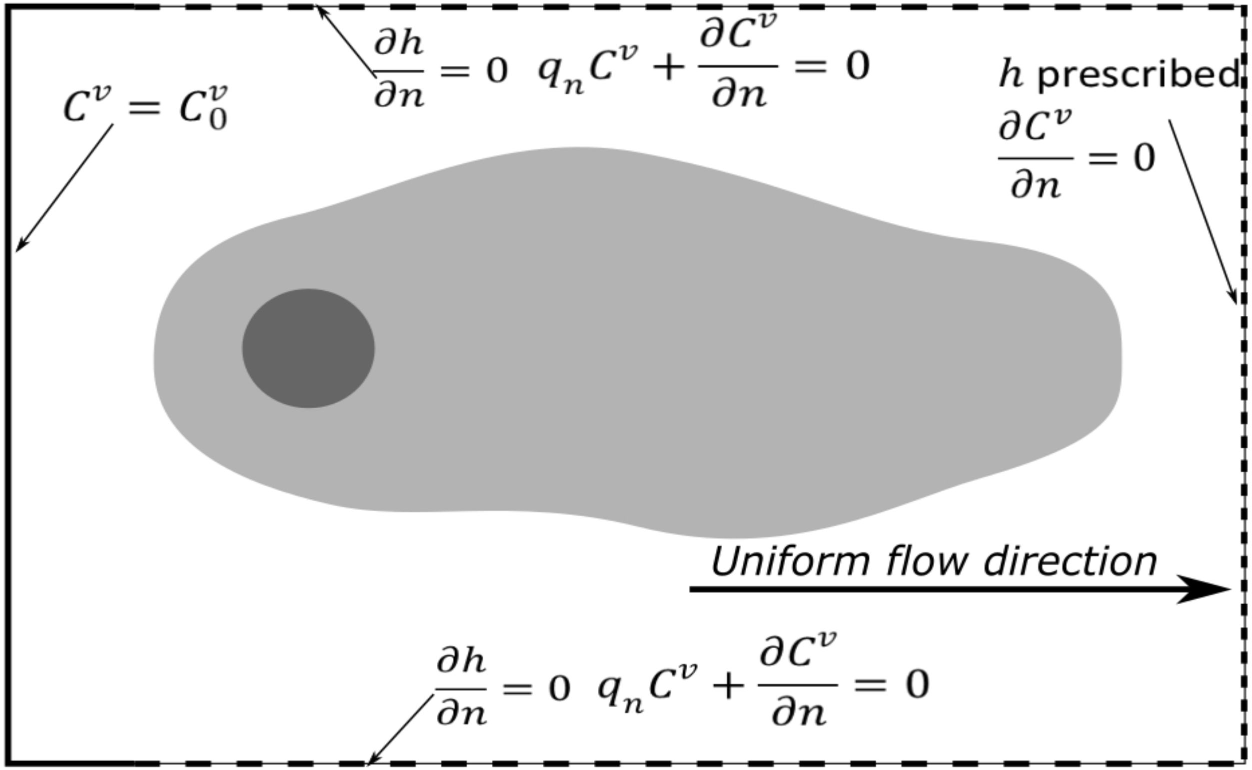
$q'''(x,y,z,t)$ *total prescribed mass flux (advection + diffusion-dispersion) normal to the concerned boundary (kg/(m^2.s))*

… mostly used for prescribing a zero total flux on a boundary:

$$g'''=0$$

BC's for a solute transport problem

Prescribed relation linking concentration and its first derivative *(Cauchy or mixed Neumann BC)*



… equivalent to a zero flux (Neumann) gw flow BC associated with a transport zero Neumann BC:

no advection and no diffusion-dispersion through the boundary

a totally impervious boundary

Introduction to solute transport solving methods

… solving the transport equation is never a simple operation …

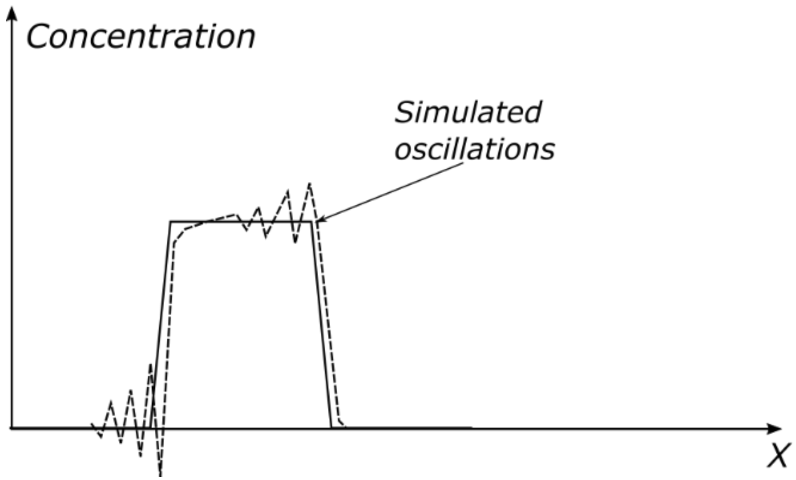
partial derivatives of the 1st and 2nd order in the same equation (parabolic and elliptic equation)

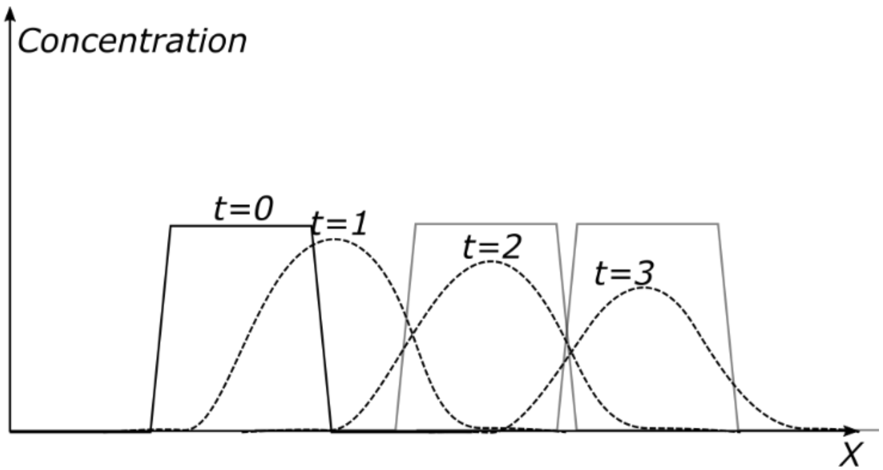
- *numerical dispersion*
- *artificial oscillations*
- *more memory*
- *more CPU*

Introduction to solute transport solving methods

… solving the transport equation is never a simple operation ...

- *partial derivatives of the 1st and 2nd order in the same equation (parabolic and elliptic equation)*
- *numerical dispersion*
- *artificial oscillations*
- *more memory*
- *more CPU*





Introduction to solute transport solving methods

… solving the transport equation is never a simple operation …

partial derivatives of the 1st and 2nd order in the same equation (parabolic and elliptic equation)

with regards to a fixed axis system

with regards to a moving axis system (referential) at v_a /R velocity along a streamline

- *Pe and Cr numbers*
- *Eulerian methods*
- *Eulerian-Lagrangian methods*
- *Multi-reactive transport*

Numerical Peclet and Courant numbers

- *dimensionless Peclet number = ratio between advection and dispersion* $Pe = \frac{v_a \Delta x}{D}$

  simplified in $Pe = \frac{v_{a_x} \Delta x}{a_L v_{a_x}} = \frac{\Delta x}{a_L}$

  ➡ $\Delta x < 2a_L$ *to avoid oscillations when using classical grid-based numerical methods* *(Price et al. 1966)*

- *dimensionless Cr number = ratio between advection travel during a time step and the grid dimension* $Cr = \frac{v_a \Delta t}{\Delta x}$ *(Daus and Frind 1985, Rausch et al. 2005)*

  ➡ $Cr < 1$ *to allow the transfer of information from a grid cell (element) to the next without losing information*

Time integration schemes

- *explicit integration schemes ($\theta < 0.5$) : conditionally stable*
- *time integration on the implicit side ($\theta \geq 0.5$): unconditionally stable*
- *Crank-Nicolson scheme ($\theta = 0.5$) provides 2nd order accuracy (i.e. proportional to $(\Delta t)^2$) and is just unconditionally stable*

  the reduction of the time step by a factor of 2 reduces the approximation error by a factor of 4.

- *time weighting can be combined to different spatial weighting (i.e. upstream weighting) for a variety of different methods*
- *in general, weighting more toward the implicit side will produce less oscillations but more numerical dispersion*
- *Crank-Nicolson scheme is often adopted as a compromise*
- *with spatial and temporal discretizations adequately chosen in relation to Peclet and Courant constraints*

Introduction to solute transport solving methods

Eulerian methods

concentration calculated at a given node should be more influenced by the concentration at the upstream node (i.e. with respect to the advective transport) than by concentrations at the other neighboring nodes

- *more weight should be given to upstream values in the finite difference or finite element approximations of the advective term*
- *other terms of the solute transport PDE are treated by the standard approximations (i.e. similarly to what is done for solving the flow equation*

- *a series of upwind or upstream numerical techniques to decrease oscillations but at the cost of creating numerical dispersion (using upstream information artificially smooths the simulated gradients, which corresponds to numerical dispersion)*
- *Note: in many numerical books, oscillations = 'dispersive error' and numerical dispersion = 'diffusive error'*

Introduction to solute transport solving methods

Eulerian methods

- *similar when applied to FDM, FVM and FEM*
- *upwind or upstream techniques require to compute beforehand the advection direction (i.e. groundwater flow direction) for the time step*
- *two types of upwind techniques: central-in-space upwind weighting and upstream weighting*
- *combined with different time integration schemes gives rise to a series of different methods*
- *for FD with uniform grid:*

central-in-space

$$\frac{\partial C}{\partial x} \approx (1-\alpha)\frac{C(x+\Delta x)-C(x)}{\Delta x} + \alpha\frac{C(x)-C(x-\Delta x)}{\Delta x}$$

where α *is the upwind coefficient,* $\alpha \in [0,1]$

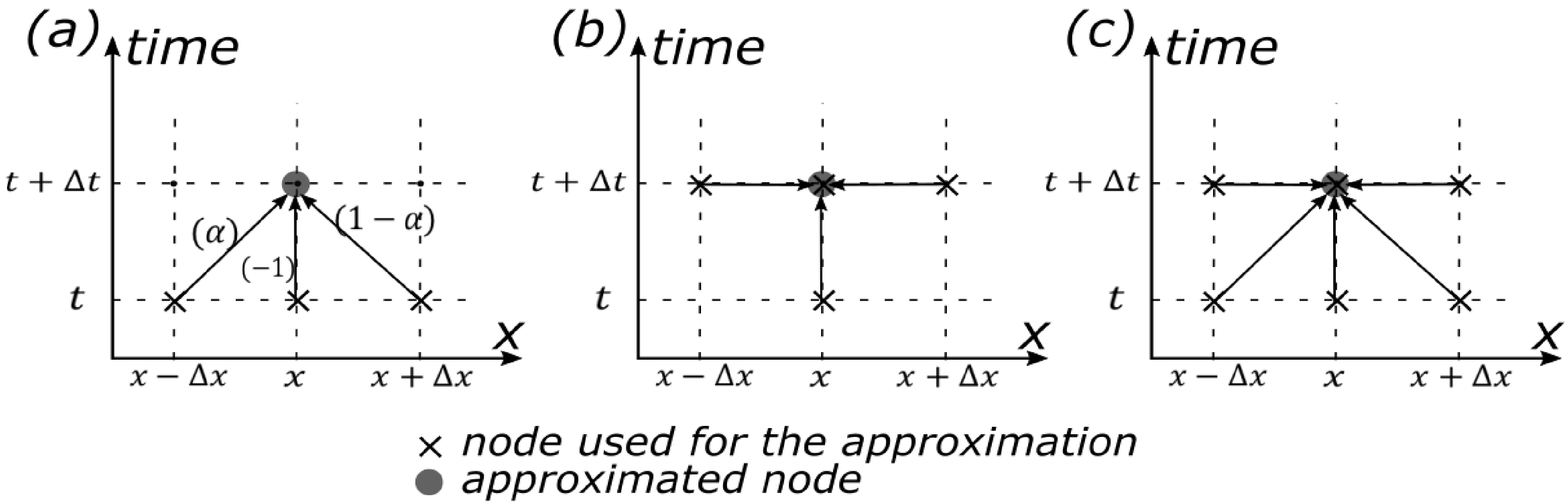
$$\frac{\partial C}{\partial x} \approx \frac{(1-\alpha)C(x+\Delta x)-C(x)+\alpha C(x-\Delta x)}{\Delta x}$$

α *must be chosen larger than 0.5 to create an upwind weighting*

Introduction to solute transport solving methods

Eulerian methods: *combined with different time integration schemes*

central-in-space



nodal contributions to the approximated C(x,t+Δt) with a central-in-space upwind weighting combined with

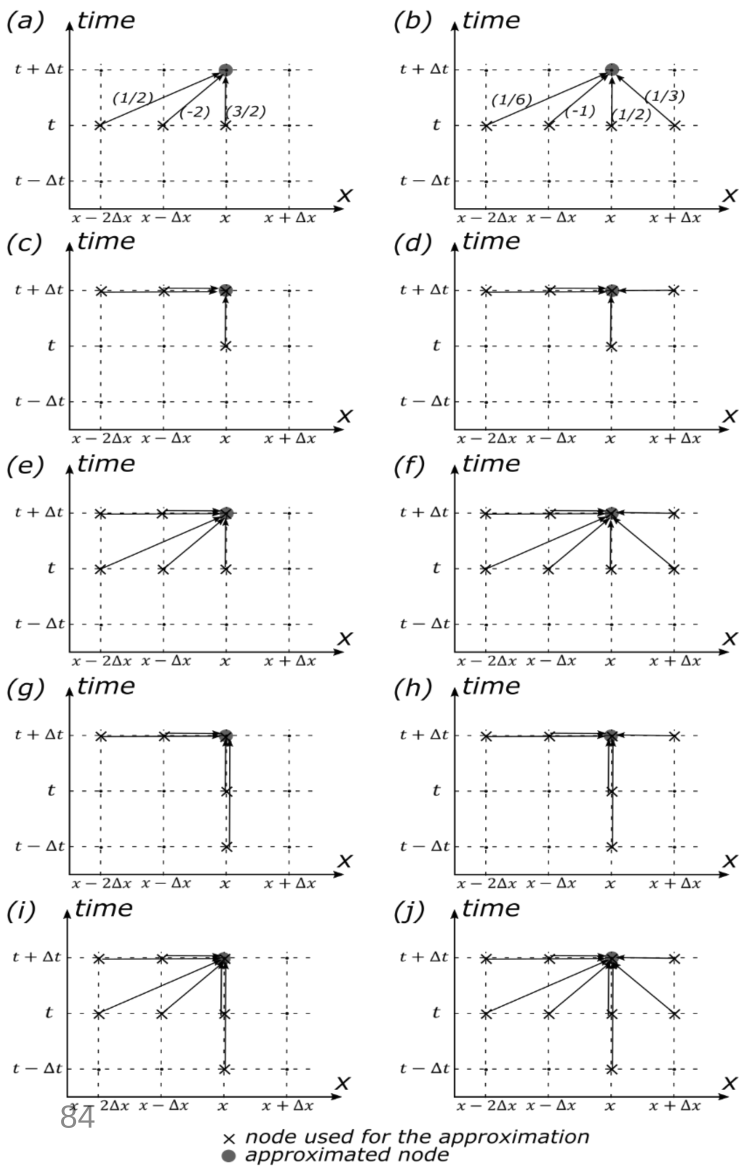
- *(a) an explicit*
- *(b) an implicit*
- *(c) a Crank-Nicolson time integration scheme*

The weight of each nodal contribution is not mentioned for implicit schemes as it depends on the combination of the spatial with the temporal weighting.

Eulerian methods: *higher order upstream weighting*

Spatial weighting

2^{nd} order | *3^{rd} order*



Time scheme

Explicit $\theta = 0$

Implicit $\theta = 1$

Crank-Nicolson $\theta = 0.5$

1st order BDF implicit $\theta = 1$

BDF = Backward Differentiation Formula (family of implicit methods

3^{rd} order BDF partially explicit $\theta = \frac{1}{3}$

Eulerian methods: *higher order upstream weighting*

- *these upstream techniques reduce oscillations but create numerical dispersion*
- *wise to apply them only if Pe < 2 and Cr < 1*
- *an additional check about sensitivity to changes in longitudinal and transverse dispersivities*

  ➡ *good way to assess the relative parts of numerical and physical dispersion in the simulated results*

Introduction to solute transport solving methods

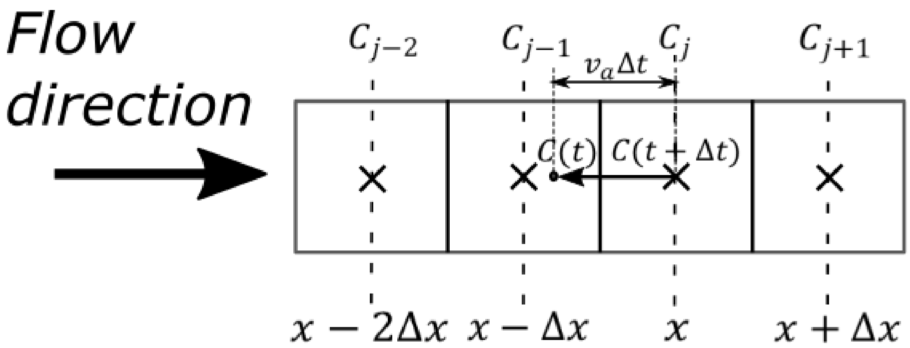
***Eulerian methods: TVD method** (Total Variation Diminishing)*

(Cox and Nishikawa 1991, Zheng 1990, Zheng and Bennet 1995, Zheng and Wang 1999)

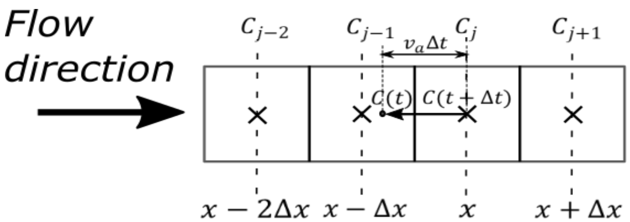
- *can be implemented in FDM-, FVM- and FEM-based models to solve advection dominated transport*
- *known as more accurate than standard central-in-space weighting and upstream methods for simulating sharp concentration variations*
- *wise to apply them only if Pe < 2 and Cr < 1*
- *in a FD regular grid, considering only 1D advection:*

$$\Rightarrow C(x, t+\Delta t) = C(x - v_a t, t)$$

- *point found by interpolation from the concentrations at the 4 neighboring nodes: a 3rd order polynomial is used*



Eulerian methods: TVD method *(Total Variation Diminishing)*



$$C_j(t+\Delta t) = C_j(t) - Cr\Bigg[\left(\frac{C_{j+1}(t)}{3} + \frac{C_j(t)}{2} - C_{j-1}(t) + \frac{C_{j-2}(t)}{6}\right) - Cr\left(\frac{C_{j+1}(t) - 2C_j(t) + C_{j-1}(t)}{2}\right) + Cr^2\left(\frac{C_{j+1}(t) - 3C_j(t) + 3C_{j-1}(t) - C_{j-2}(t)}{6}\right)\Bigg]$$

$$\boxed{Cr = \frac{v_a \Delta t}{\Delta x}}$$

- *may lead to oscillations in advection dominated problems*
- *a 'flux limiter' is activated when the spatial concentration profile does not show a monotonic evolution* *(Leonard and Niknafs 1990 and 1991, Zheng and Wang 1999)*

- *TVD scheme is explicit, subject to stability constraints*
- *other terms of the solute transport equation solved by an explicit or an implicit procedure*
- *mostly mass conservative !*

Eulerian Lagrangian methods

PDE

$$\frac{\partial C^v}{\partial t} = -\frac{\boldsymbol{v_a}}{R} \cdot \nabla C^v + \frac{1}{R}\nabla \cdot (\boldsymbol{D_h} \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R\, n_m}\left(C^v - C_s^v\right)$$

in a Lagrangian approach:

ODE

$$\frac{dC^v}{dt} = \frac{1}{R}\nabla \cdot (\boldsymbol{D_h} \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R\, n_m}\left(C^v - C_s^v\right)$$

$$\frac{dC^v}{dt} = \frac{\partial C^v}{\partial t} + \frac{\boldsymbol{v_a}}{R} \cdot \nabla C^v$$

(Zheng 1990, Bear and Cheng 2010)

the left hand side is Lagrangian while the right hand side remains Eulerian

Eulerian Lagrangian methods

$$\frac{dC^v}{dt} \approx \frac{C^v(t+\Delta t) - C^{v*}(t+\Delta t)}{\Delta t}$$

$$C^v(t+\Delta t) \approx C^{v*}(t+\Delta t) + \Delta t\left[\frac{1}{R}\nabla\cdot(\boldsymbol{D_h}\cdot\nabla C^v) - \lambda C^v - \frac{q_s}{R\,n_m}\left(C^v - C_s^v\right)\right]$$

C^{v*} = 'intermediate' concentration at time $(t+\Delta t)$

(Zheng 1990)

1) Solving advection by a 'characteristic' method

2) Solving the 2nd term by classical method with explicit, implicit, Crank-Nicolson or Galerkin time integration

Introduction to solute transport solving methods

Eulerian Lagrangian methods

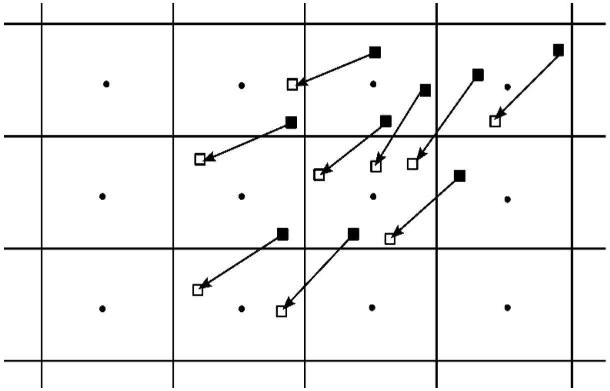
C^{v*} = *'intermediate' concentration at time* $(t + \Delta t)$

… can be calculated by a particle tracking or a method of characteristics

- *'Method Of Characteristics' MOC*
- *'Modified Method Of Characteristics' MMOC*
- *'Hybrid Method Of Characteristics' HMOC*

Eulerian Lagrangian methods

‘Method Of Characteristics’ MOC (Garder et al. 1964, Konikow and Bredehoeft 1978, Zheng 1990)



- cell centered node
- particle at time t
- particle at time $t+\Delta t$

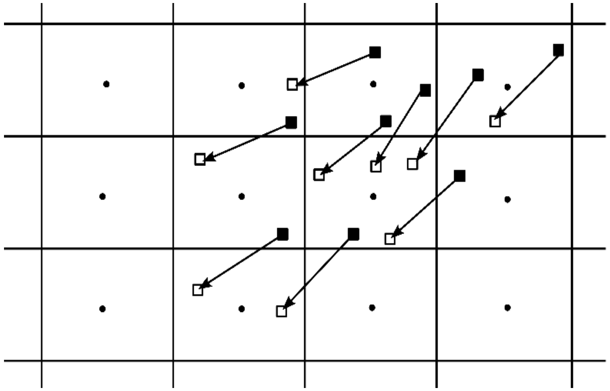
$$\tilde{C}_i^{v*}(t+\Delta t) = \frac{1}{np_i}\sum_{k=1}^{np_i} C_k^{v}(t)$$

$$C_i^{v*}(t+\Delta t) = \omega \tilde{C}_i^{v*}(t+\Delta t) + (1-\omega)\, C_i^{v}(t)$$

- *initial ‘set’ of particles: an initial position and a concentration given to each of them*
- *small time step, particles moving along streamlines*
- *at the end of the time step, concentration computed by counting the arrived particles in the concerned cell*
- *nearly no numerical dispersion but time consuming and memory consuming with many particles*
- *if too few particles: mass conservation problems*

Eulerian Lagrangian methods

'Method Of Characteristics' MOC *(Garder et al. 1964, Konikow and Bredehoeft 1978, Zheng 1990)*



$$\tilde{C}_i^{v*}(t+\Delta t) = \frac{1}{np_i}\sum_{k=1}^{np_i} C_k^v(t)$$

$$C_i^{v*}(t+\Delta t) = \omega \tilde{C}_i^{v*}(t+\Delta t) + (1-\omega)\, C_i^v(t)$$

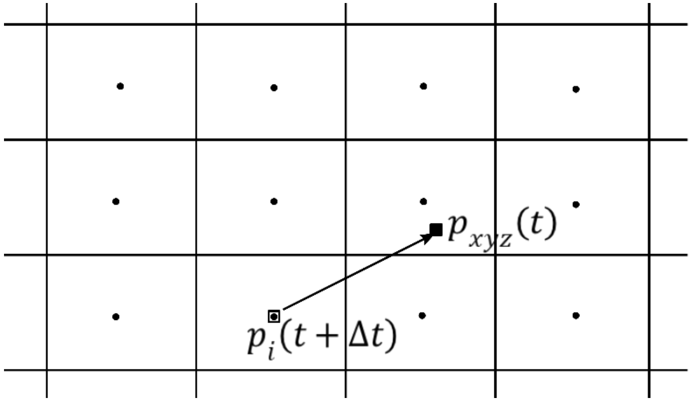
(Zheng and Wang 1999, Rausch et al. 2005)

- *no numerical dispersion even for large Pe number*
- *errors coming from the interpolation of the velocity field from the groundwater flow model*
- *discrete nature of the particles (and counting of them in each cell/element after each time step) induces local mass conservation problems*
- *more particles* ➡ *increasing rapidly the computing load and memory storage*
- *too heavy for highly heterogeneous and complex non linear problems*

Eulerian Lagrangian methods

MMOC

(Ewing et al. 1983, Cheng et al. 1984, Molz et al. 1986, Zheng and Wang 1999)



- *cell centered node*
- *particle at time t*
- *particle at time t+ Δt*

Backward unique particle tracking

$$p_{xyz}(t) = p_i(t+\Delta t) - v_a(p_i(t+\Delta t))\Delta t$$

$$C_i^{v*}(t+\Delta t) = C^v(p_{xyz}(t), t)$$

- $C^v(p_{xyz}(t), t)$ *is calculated using a linear (bilinear in 2D or trilinear in 3D) interpolation of neighboring nodal values at time* t
- *reduced memory requirements if lower order interpolation scheme*
- *faster than MOC but same mass conservation problem than MOC*
- *main issue = numerical dispersion with lower order interpolations*
- *higher order interpolation schemes lead to better results but induce oscillations when simulating sharp concentration gradients*

Eulerian Lagrangian methods

HMOC

(Neuman 1981 and 1984, Zheng and Wang 1999)

- *optimizing the choice between MOC and MMOC*
- *an automatic change of the technique as function of the local concentration gradients*
- *MOC applied in regions of the domain with steep concentration gradients*
- *MMOC applied elsewhere*

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