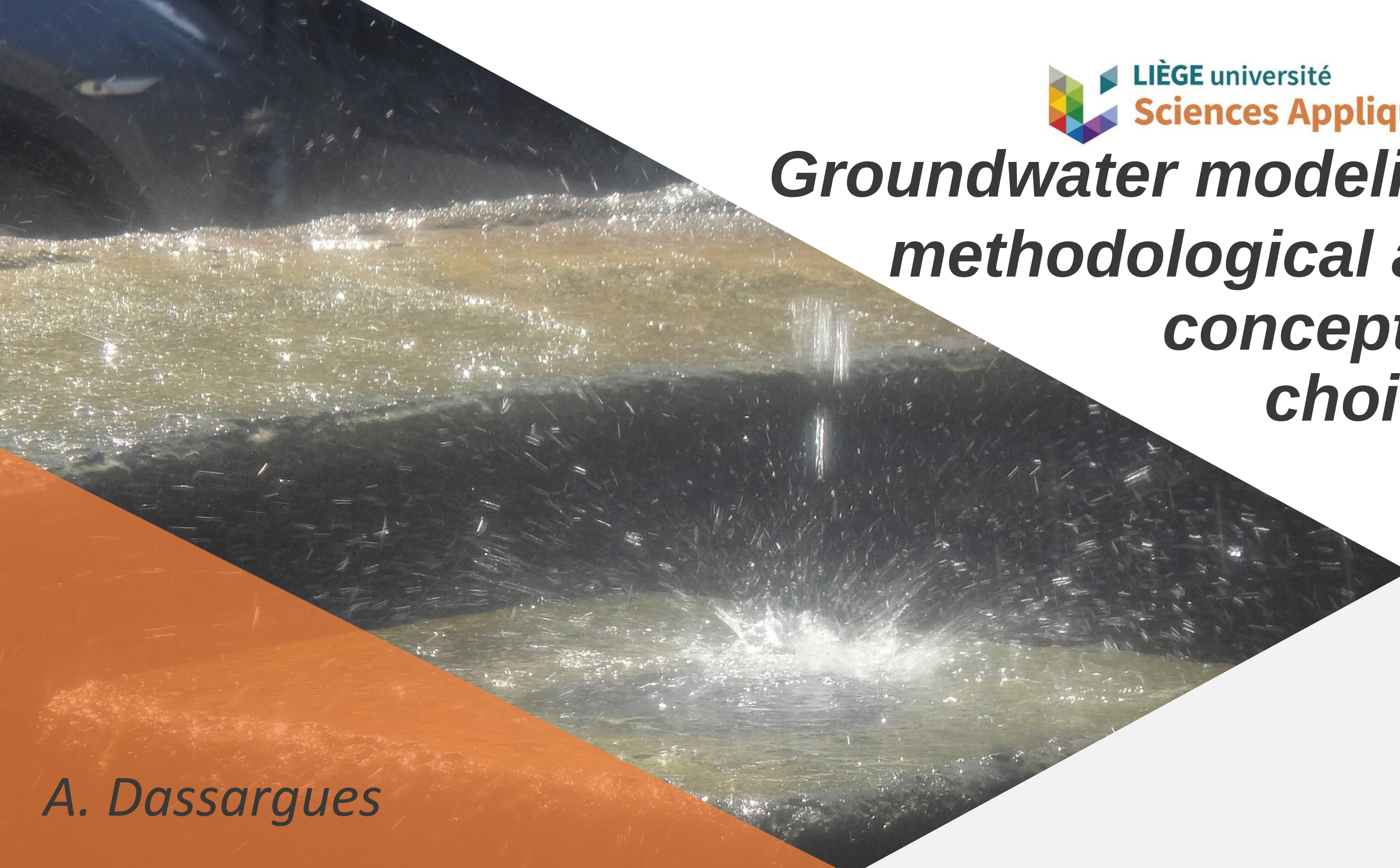

LIÈGE université
Sciences Appliquées

Groundwater modeling: methodological and conceptual choices

A. Dassargues

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Dassargues A., 2018. Hydrogeology: groundwater science and engineering, 472p. Taylor & Francis CRC press (Chapter 12)

Dassargues A. 2020. Hydrogéologie appliquée: science et ingénierie des eaux souterraines, 512p. Dunod (Chapitre 12)

Groundwater modeling: methodological and conceptual choices

- *Terminology*
- *General methodology*
- *Conceptual model*
  - *Time scale*
  - *Spatial scale, extension and dimensionality*
  - *Initial values*
  - *Boundaries*
  - *Parsimony vs complexity*
  - *Software choice and numerical model main characteristics*
  - *Modeling errors*
- *Data needs*
- *Implementation, calibration and sensitivity*
- *Evaluation/reporting*
- *References*

Terminology

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

(Brouyère et al. 2011)

the lack of precision in the representation of reality strongly depends on the scale at which the problem is considered *(Dassargues 1998)*

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

Reaction/answer

Deterministic

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

…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, Dassargues et al. 2006, Tonkin et al. 2007 and many others)

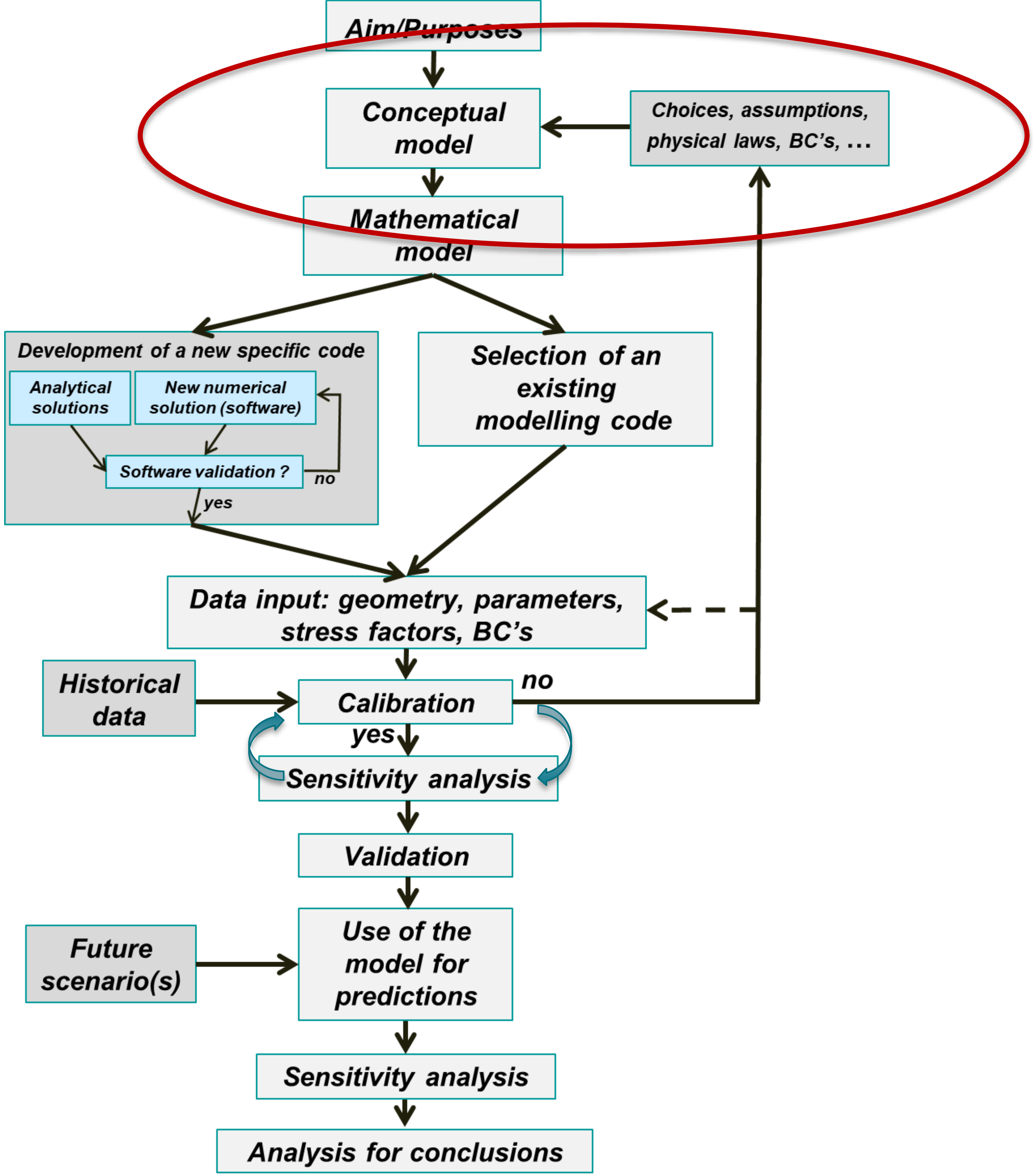
Multiple simulations ➡ multiple responses statistically treated assuming (most often) Gaussian behavior

- ➡ *results in statistical distributions*
- ➡ *probability distribution for each response based on the statistical distribution of data (including 2ary data, parameters and stress factors)* *(Huysmans et al. 2008, Huysmans and Dassargues 2009, 2011)*

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
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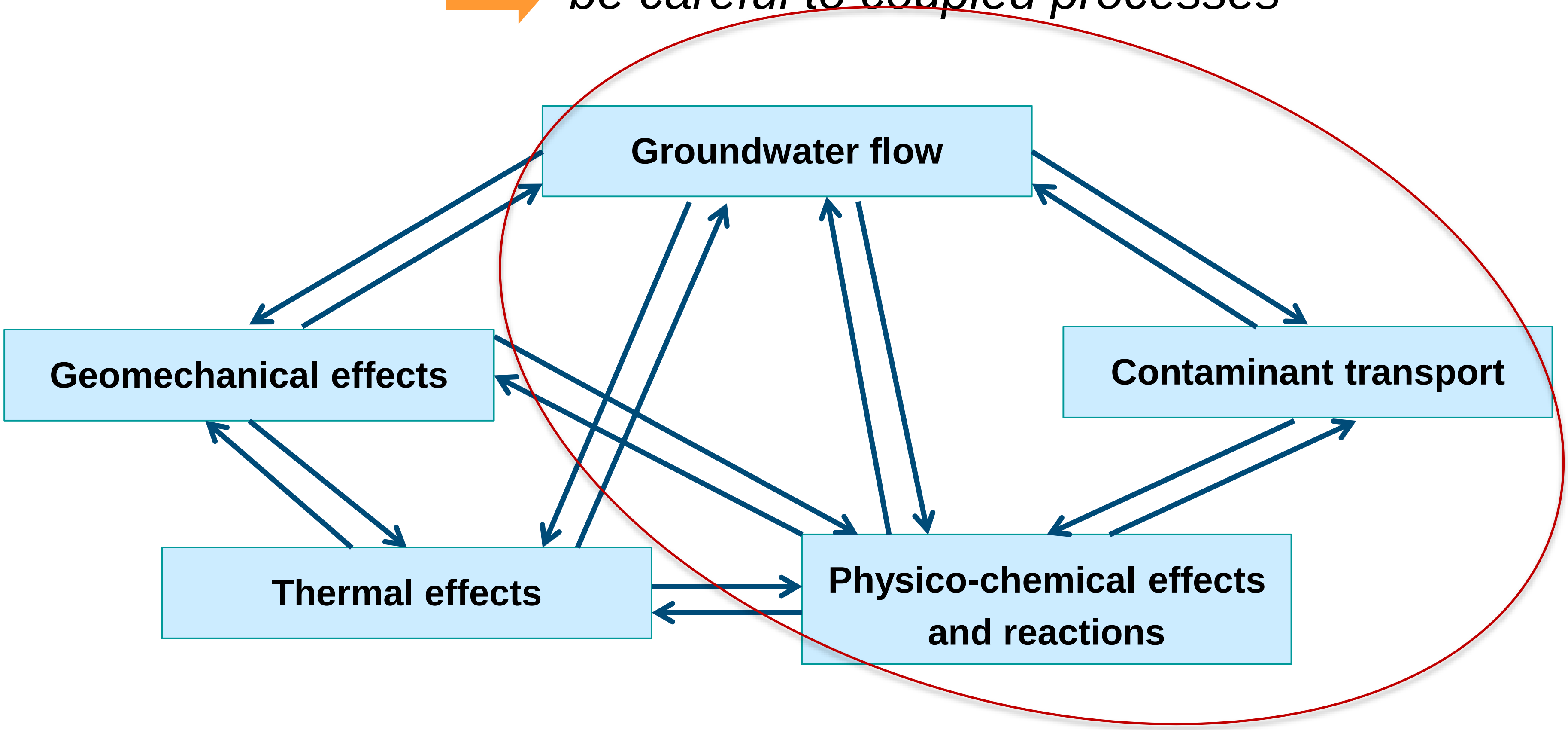
General methodology: conceptual model

(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, Dassargues 2020)

Conceptual model

fundamental step where the main assumptions of the modelling are chosen

- *steady state or transient analysis*
- *scale level*
- *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)*

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*

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*

Conceptual model

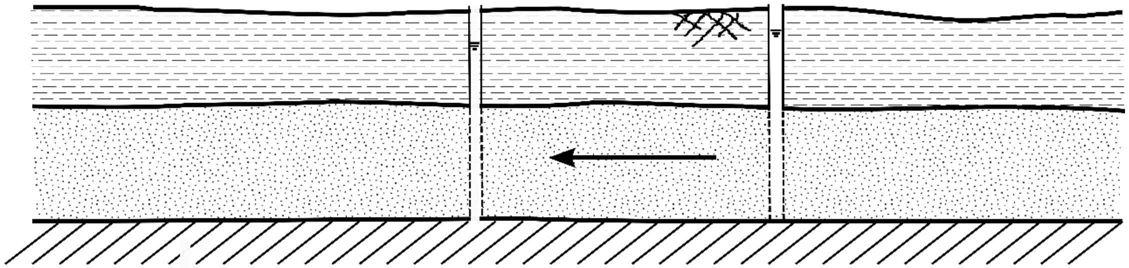
Extension and dimensionality

- *1D, … (often in the partially saturated zone)*
- *2D horizontal models:*

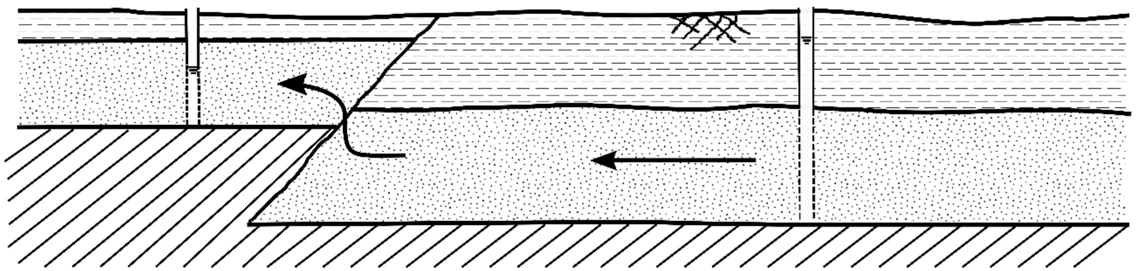
  groundwater flow considered as mostly horizontal

Is it realistic ?

OK



here a 3D approach is needed



Conceptual model

Extension and dimensionality

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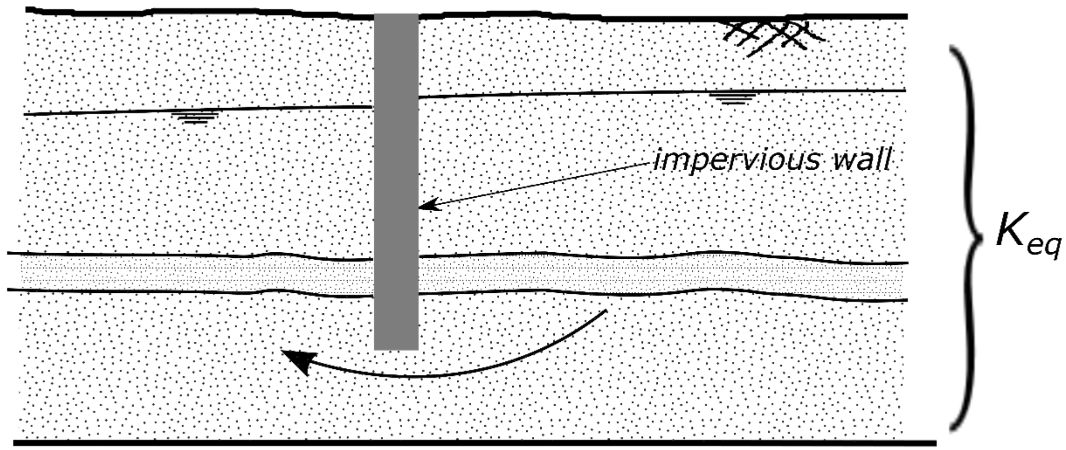

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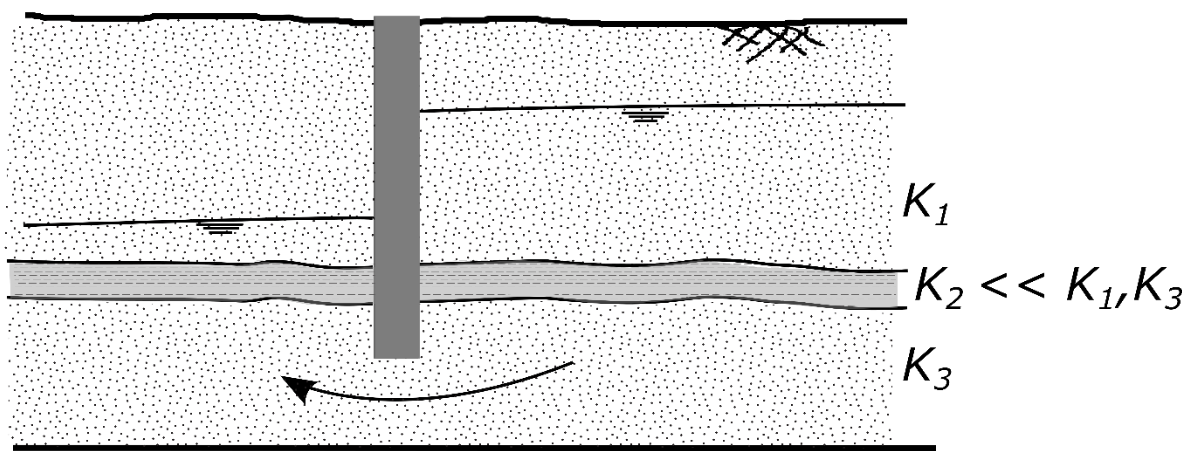
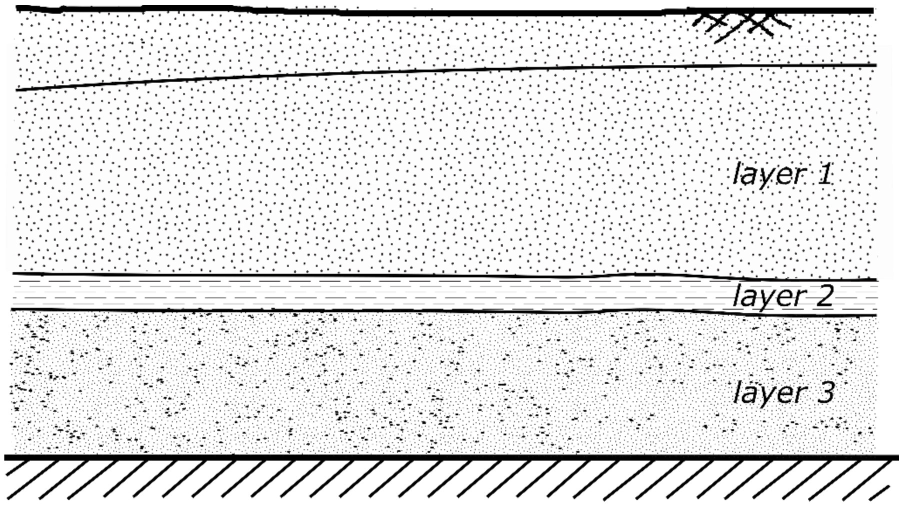
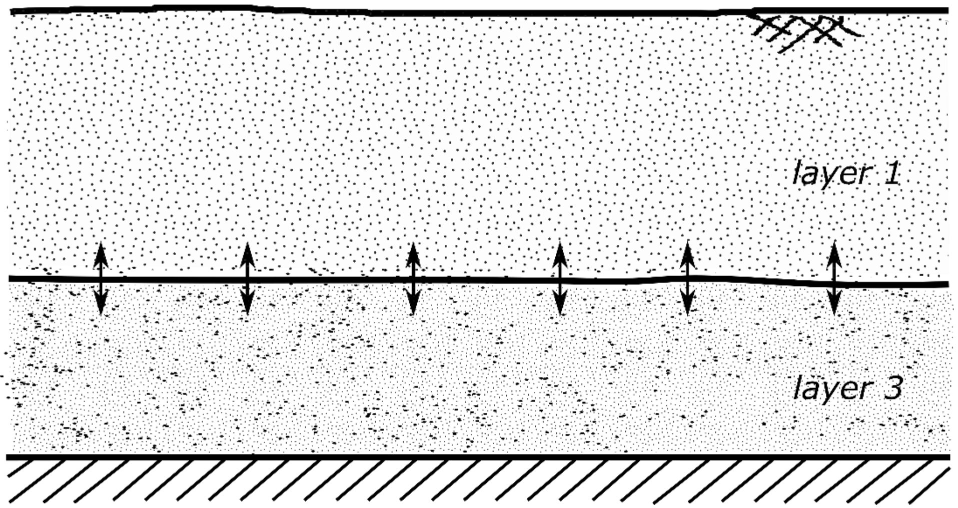


Conceptual model

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*

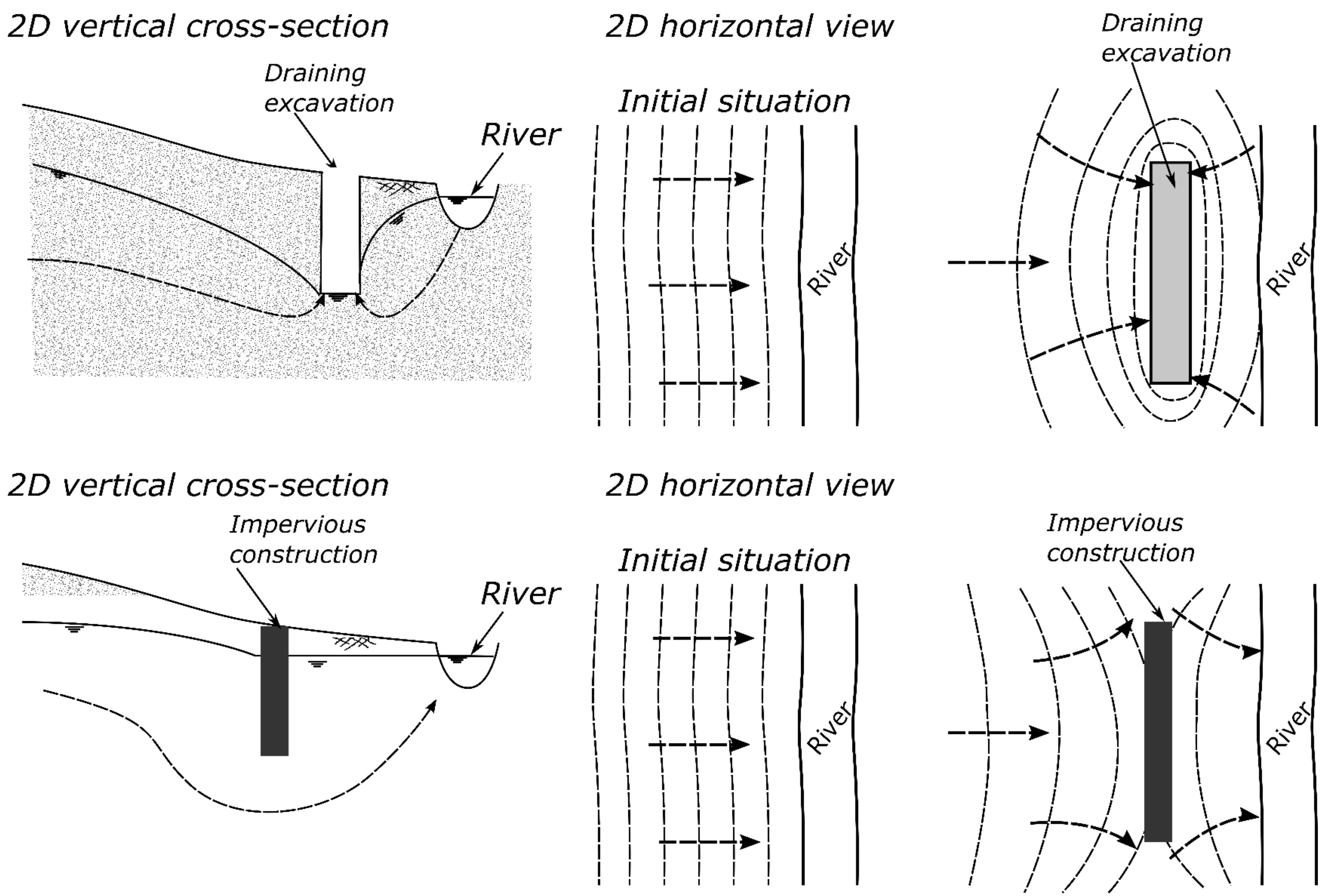




Conceptual model

Extension and dimensionality

- *2D vertical models: OK but gw flow not in the considered plane is neglected*



Conceptual model

- ***Initial conditions**: initial values of the main variable (generally piezometric head h) in each node of the mesh*
  - *1[st] used values for a steady state computation (1[st] 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 system 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*

Conceptual model

***Boundary conditions**: to be discussed*

see next chapters about groundwater flow simulations and solute transport simulations including various interactions

(e.g. river groundwater interactions)

(Goderniaux et al. 2009)

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

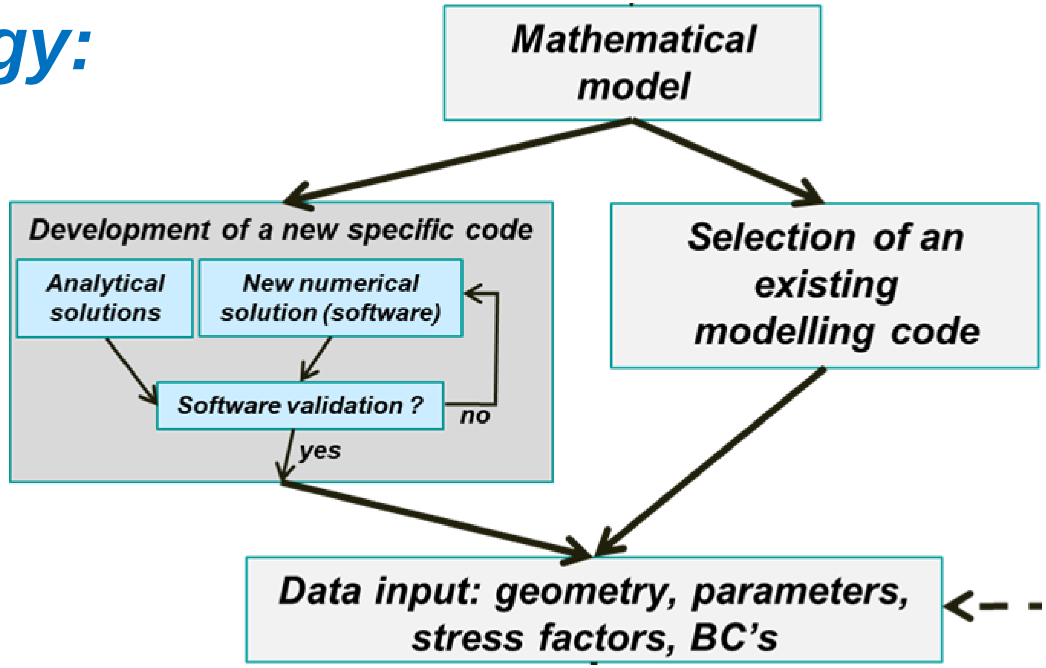
modelled processes remain understandable

(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)

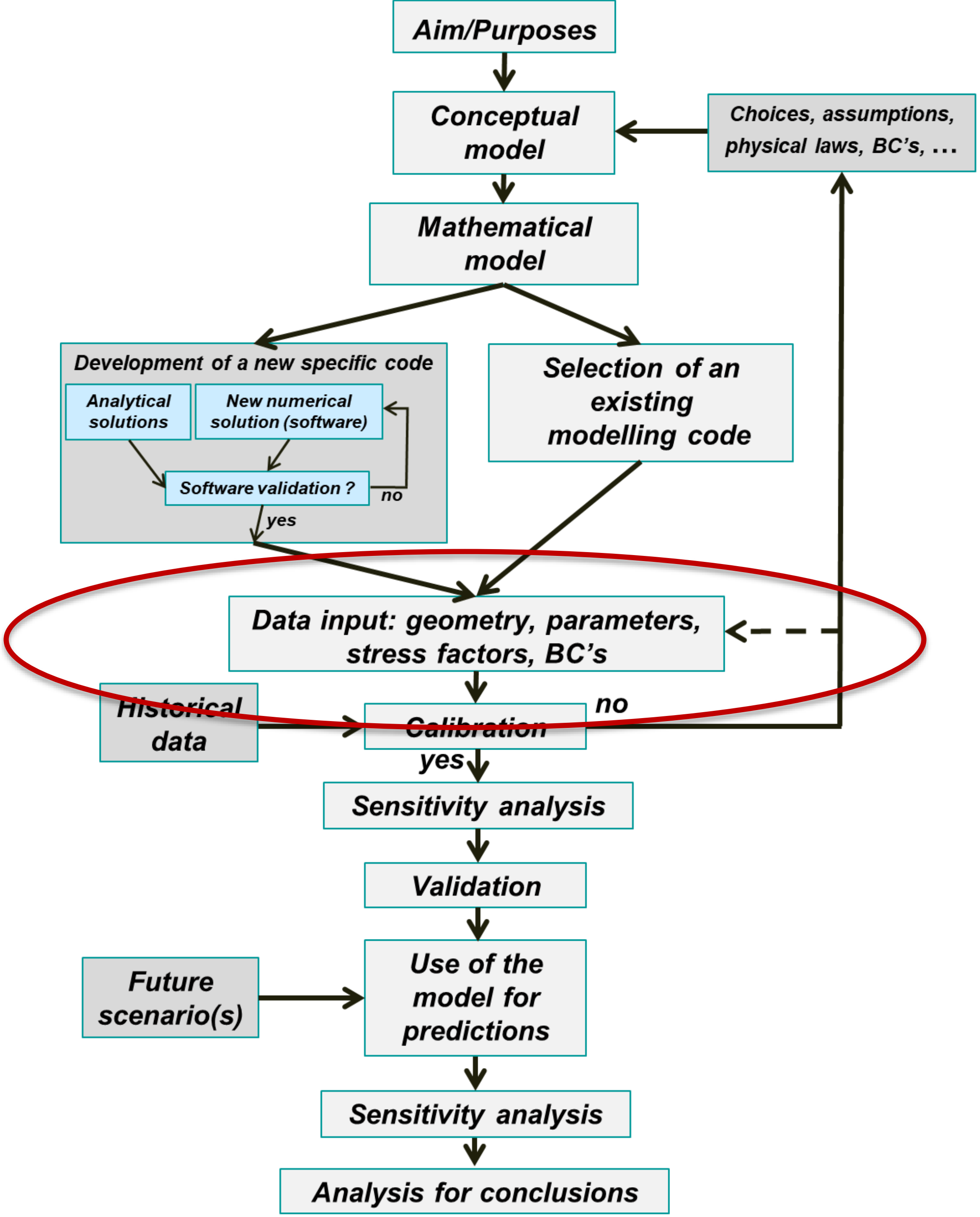
a very useful concept that implicitly assumes a continuum and a porous medium *(Molz 2017)*

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 than model scale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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
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Sensitivity analysis
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Data needs

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*

(Dassargues et al. 1988, Dassargues 2018, Dassargues 2020)

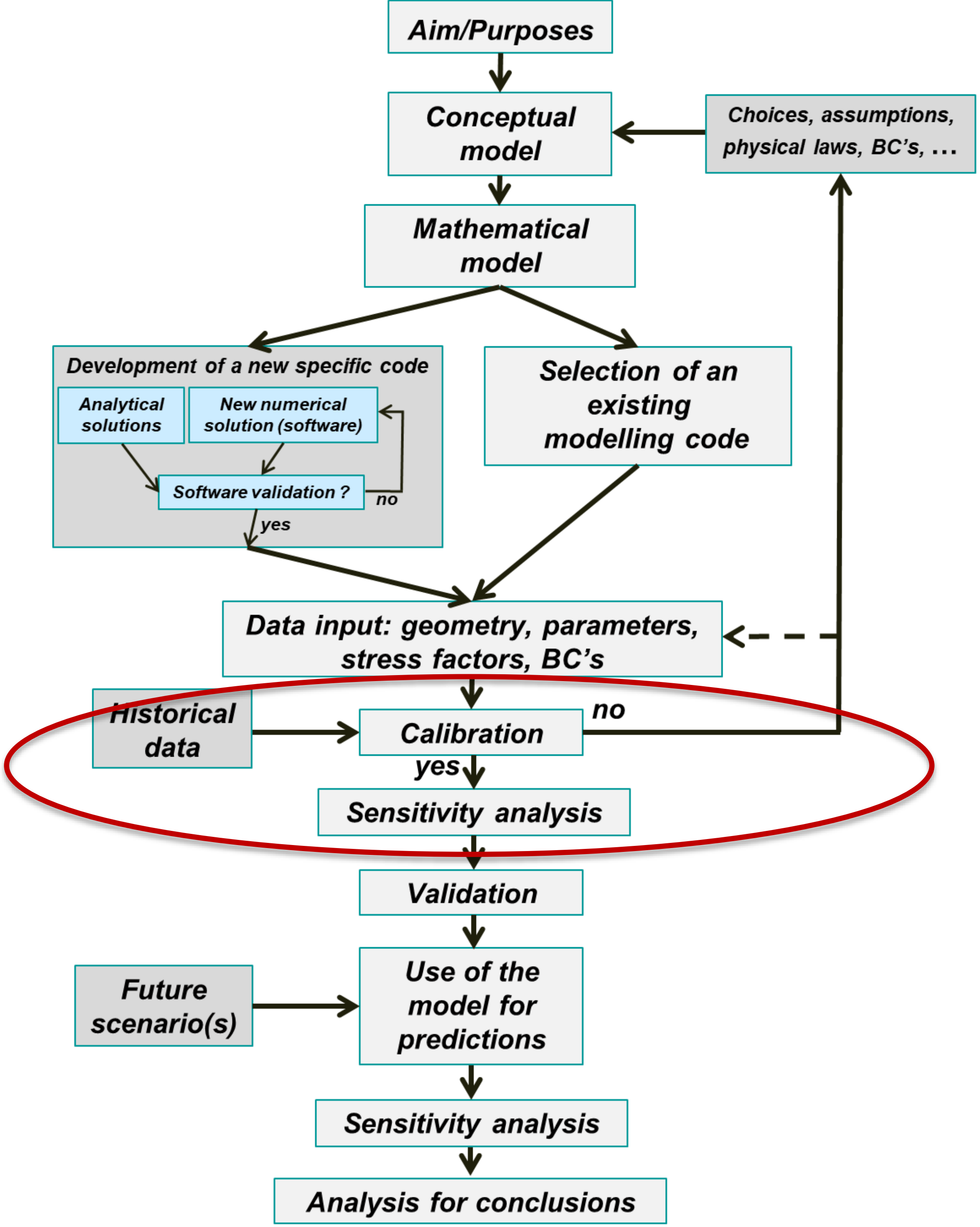
General methodology:

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*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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

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

the importance of observations as a whole to a single parameter

(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*
- *+ possible use of pilote points*

  (Doherty 2005, Skahill and Doherty 2003 & 2005, Poeter et al. 2005)
- *+ parameter correlation coefficients*

  (example in Batlle Aguilar et al. 2009)
- *+ use of other data (e.g. temperature, geophysical data)*

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

(Klepikova et al. 2016)

(Rentier et al. 2002)

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*

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