NUMERICAL SIMULATION OF HEAT- AND MOISTURE TRANSPORT IN CAPILLARY-POROUS BUILDING MATERIALS

Prof. Dr.-Ing. John Grunewald Dipl.-Ing. Heiko Fechner, Dr. Andreas Nicolai

The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° 260162

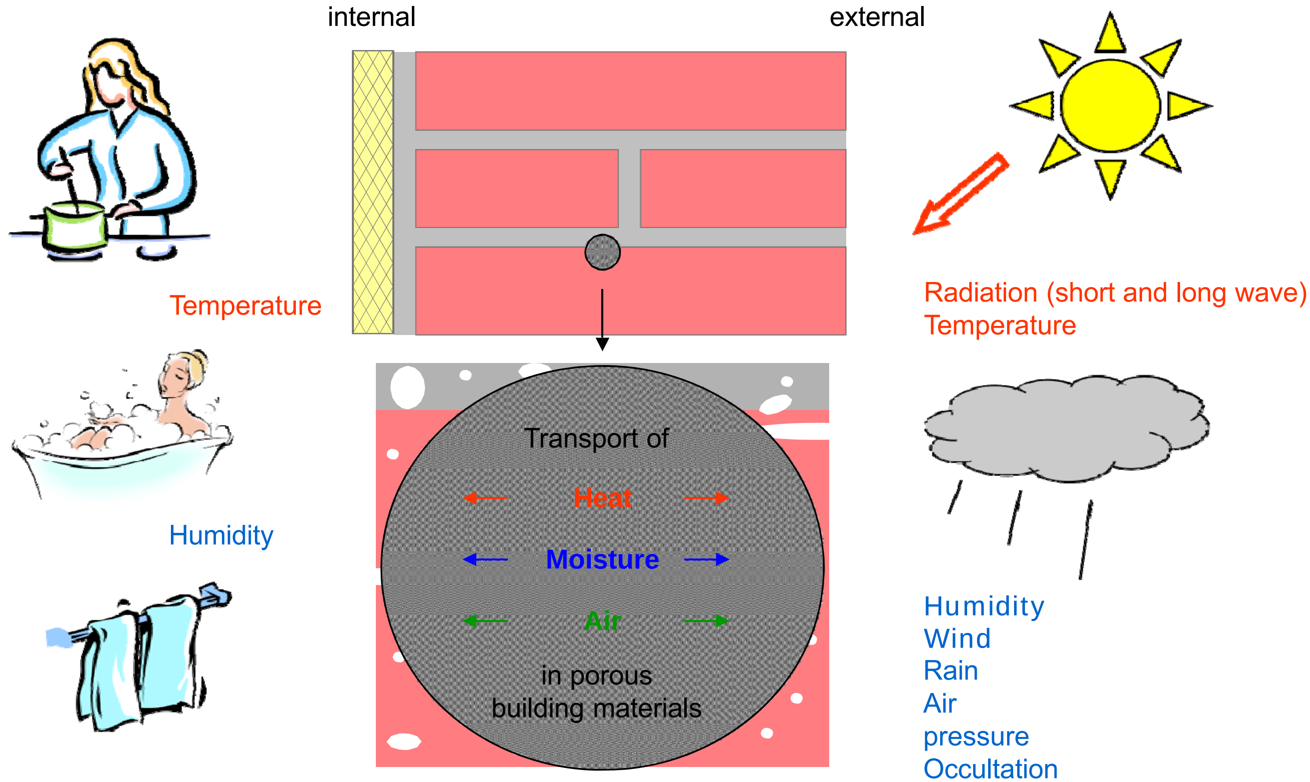
Basics of simulation software DELPHIN

Basic of simulation

- Transient
  - Usage of dynamical boundary conditions (external und internal climate)
  - Thermal and hygric inertia of construction is considered
- Hygro-thermal
  - Heat conductivity and storage
  - Moisture transport (vapour and capillary conductivity) and moisture storage
- Building elements
  - Materials and systems/constructions
  - Constructional details
- Simulation
  - For analysis (expertises) and prediction (feasibility study/optimisation)

Basic of simulation

Transient transport processes in capillary-porous building materials



Basic of simulation

Basic knowledge for the use of simulation software

- Material properties
- Conserved quantity
- Transport processes
- Initial conditions
- Boundary conditions

} Physical state equations

- Mathematical method
- Space discretisation
- Time steps Precision

} Numerical solving method

Part 1

Physical basic equations and models

Physical basic equations and models

Mathematical basics and nomenclature

Einsteins' summation rule:

$$j_k = \sum_k j_k$$

Usage of direction index implicates sigma sign

For cartesian coordinate systems:

$$k = x, y, z$$

Usage for partial derivative:

$$\frac{\partial}{\partial x_k} = \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$$

Example:

$$m = m(t, x_k)$$

Conserved quantity is defined in dependency of time and space

$$\frac{\partial m}{\partial x_k} = \frac{\partial m}{\partial x} + \frac{\partial m}{\partial y} + \frac{\partial m}{\partial z}$$

Partial derivatives are summed

Physical basic equations and models

$$\frac{\partial Q}{\partial t} = \frac{\partial}{\partial x_k}\left(\lambda \frac{\partial \theta}{\partial x_k}\right)$$

with $Q = Q(t, x_k)$ and $\theta = \theta(t, x_k)$

Q	J/m^3	Internal energy density
θ	$°C$	Temperature

Change of internal energy in time (only heat storage):

$$\frac{\partial Q}{\partial t} = \rho_{dry} c_T \frac{\partial \theta}{\partial t}$$

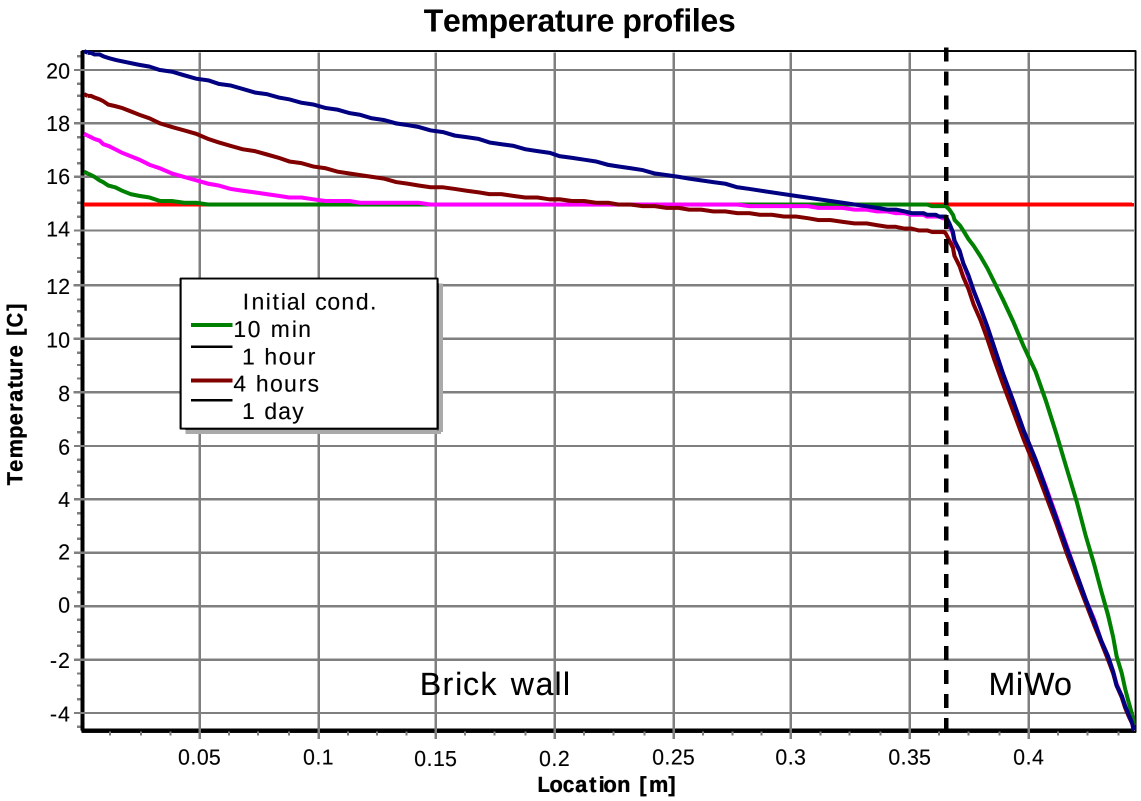
Important material parameter:

ρ_{dry}	kg/m^3	Density of dry materials
c_T	$J/$	Specific heat capacity
λ	kgK	Heat conductivity

$J/smK = W/mK$

Physical basic equations and models

Transient heat conductivity – till achievement of steady-state conditions



Physical basic equations and models

Transient heat conductivity – till achievement of steady-state conditions

Steady-state conditions = no change of conservation quantities in time anymore

$$\frac{\partial Q}{\partial t} = 0 = \frac{\partial}{\partial x_k}\left(\lambda \frac{\partial \theta}{\partial x_k}\right)$$

Heat fluxes constant: $q = -\lambda \frac{\partial \theta}{\partial x} = const$

Storage term and heat capacity are irrelevant for stationary state

At transient processes the storage term controls how quick the system responses to boundary conditions:

- high heat capacity – slow achievement of stationary conditions
- low heat capacity – quick response

Physical basic equations and models

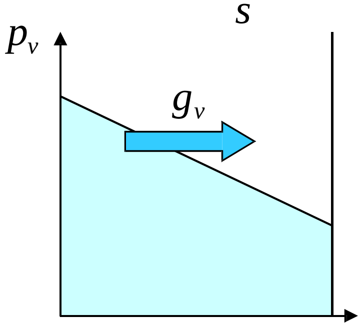
Water mass balance (transient conservation equation for moisture in building components):

$$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial x_k}\left(g_{v,k} + g_{w,k}\right) \quad \text{with} \quad w = w\left(t, x_k\right)$$

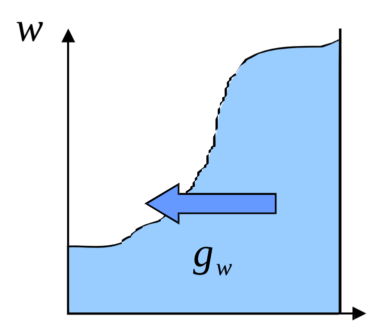
w kg/m^3 Water mass density

g_v $kg/m^2 s$ Vapour flux density

g_w $kg/m^2 s$ Capillary water flux density



Vapour pressure gradient Vapour diffusion



Water content difference capillary conductivity

Physical basic equations and models

Gas mass balance (transient conservation equation for gaseous phase in building components):

$$\frac{\partial \rho_g}{\partial t} = -\frac{\partial}{\partial x_k}\left(g_{gc,k} + g_{gg,k}\right)$$

with $\rho_g = \rho_g\left(t, x_k\right)$ and $\rho_g = \rho_g\left(T, w, p_g\right)$

ρ_g	kg/m^3	Gas density
g_{gc}	$kg/m^2 s$	Convective gas flux density
g_{gg}	$kg/m^2 s$	Gas flux density due to gravity

Physical basic equations and models

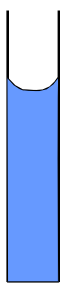
Transport processes and models

Heat flux density: $q = -\lambda \frac{\partial \theta}{\partial x}$

Vapour diffusion: $g_v = -\frac{\delta_{v,air}}{\mu} \frac{\partial p_v}{\partial x} = -\frac{D_v}{R_v T} \frac{\partial p_v}{\partial x}$

Capillary water transport: $g_w = -K_\ell \frac{\partial p_\ell}{\partial x}$

Gas transport: $g_{gc} = -\frac{K_g}{\rho_g} \frac{\partial p_g}{\partial x}$ $\quad g_{gg} = -K_g \cdot g_z \rho_g$



r

Capillary pressure: □ $p_c \quad \frac{2\gamma \cos\varphi}{r}$ → The smaller the pore radius, the bigger the traction force and therefore the water height in the capillary tube

Water pressure: $p_\ell = p_c + p_g$

Pressure gradient in liquid phase induces water transport

Physical basic equations and models

Transport processes and models

Evaporative cooling and heat of condensation

Specific enthalpy of water vapour: $h_v = c_{T,v}\left(T - T_{Ref}\right) + H_{evap}$

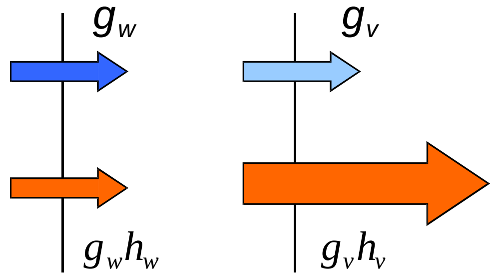
Specific enthalpy of water: $h_w = c_{T,w}\left(T - T_{Ref}\right)$

Evaporation enthalpy: $H_{evap} = 3.08 \cdot 10^6 \text{ J/kg}$

→ $h_v \gg h_w$ although $c_{T,w} \approx 2c_{T,v}$

Enthalpy transport of water vapour is much bigger than of liquid water!

Example:



Physical basic equations and models

Summary

Conservation equations

Moisture mass balance: $$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial x_k}\left(g_{v,k} + g_{w,k}\right)$$

Energy balance: $$\frac{\partial Q}{\partial t} = -\frac{\partial}{\partial x_k}\left(q_k + h_v g_{v,k} + h_w g_{w,k}\right)$$

Solution of equations

Initial conditions (one for each conservation equation), e.g.: T, φ or T, w

Boundary conditions (types):

Neumann (2nd)	Describes **fluxes** from surroundings into construction, z.B. radiation heat flux, Vapour diffusion flux
Dirichlet (1st)	Describes **boundary values**, e.g. surface temperature
Cauchy (3rd)	Describes **fluxes** and **boundary values**

Physical basic equations and models

Summary

Material parameters and material functions

General parameter:		
ρ_{dry}	kg/m^3	Density of dry material
c_T	J/kgK	Specific heat conductivity
Transport parameter:		
λ	W/mK	Heat conductivity
μ	$-$	Water vapour diffusion resistance value
K_ℓ	s	Liquid water conductivity
Moisture storage parameter:		
$w(p_c)$	kg/m^3	Moisture retention curve (MRC)
$w(\varphi)$	kg/m^3	Sorption isotherm

Part 2

The numerical solving method

The numerical solving method

Control volume method

Used to transform partial differential equations into systems of ordinary differential equations

Analytic derivation using the example of heat conduction equation:

1. Transformed original equation:

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x_k}\left(q_k\right) = 0$$

2. Multiplied with function:

$$\omega \cdot \left[\frac{\partial U}{\partial t} + \frac{\partial}{\partial x_k}\left(q_k\right)\right] = 0$$

3. Integrated over a volume:

$$\int_V \omega \cdot \left[\frac{\partial U}{\partial t} + \frac{\partial}{\partial x_k}\left(q_k\right)\right] dV = 0$$

Presumptions/preconditions:

$w = const$ (= 0-order FEM) and $\int_V \frac{\partial U}{\partial t}\, dV \approx \frac{\partial U}{\partial t} V$

The numerical solving method

Control volume method

Analytic derivation using the example of heat conduction equation:

4. Equation transformed/simplified: $$\frac{\partial U}{\partial t} = -\frac{1}{V}\int_V \frac{\partial}{\partial x_k}(q_k)\, dV$$

5. Gauss-Green-Theorem: $$\frac{\partial U}{\partial t} = -\frac{1}{V}\oint_A \vec{n}_k A_k \vec{q}_k \, dA$$

6. Application for discrete areas: $$\frac{\partial U}{\partial t} = -\frac{1}{V}\sum_i \vec{n}_i \, A_i \, \vec{q}_{k,i}$$

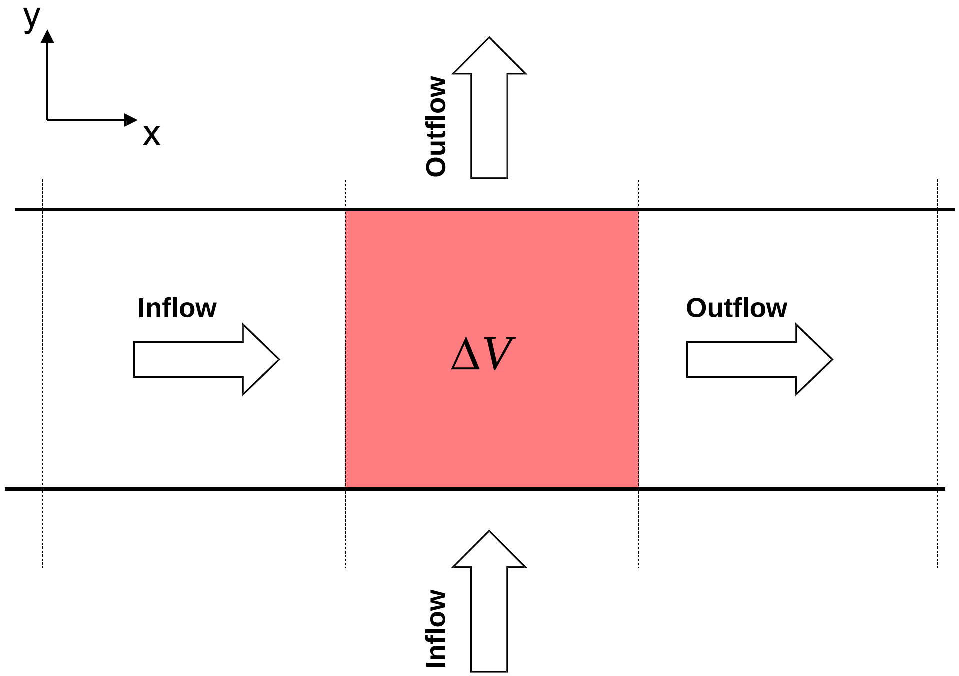
Example: 1D $$\frac{\partial U}{\partial t} = \frac{1}{V}\left[A_l q_l - A_r q_r\right]$$

$$\frac{\partial U}{\partial t} = \frac{1}{\Delta x}\left[q_l - q_r\right]$$

with the borders of the volume l = left, r = right

The numerical solving method

Balancing of conserving quantities (mass + energy)

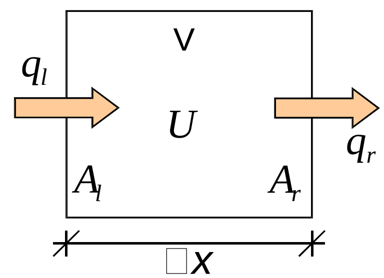


Change of density in the discrete volume = Difference between inflow and outflow

The numerical solving method

Control volume method

Derivation at concrete example:



Change of absolute conservation quantities per time = difference of fluxes

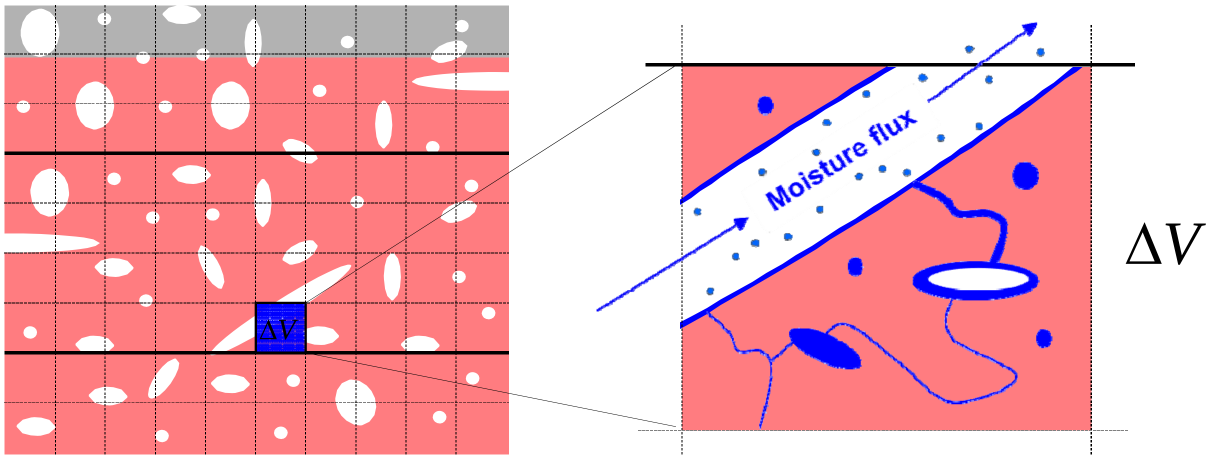
$$\Delta U \cdot V = \Delta t \left(A_l q_l - A_r q_r \right)$$ at which $A_l = A_r = A$ and $V = \Delta x\, A$

hence $$\frac{\Delta U}{\Delta t} = \frac{A}{V}(q_l - q_r)$$ and $$\frac{\Delta U}{\Delta t} = \frac{1}{\Delta x}(q_l - q_r)$$

and for infinitesimal time steps: $$\frac{\partial U}{\partial t} = \frac{A}{V}(q_l - q_r)$$

The numerical solving method

Discretisation



Discretisation for numerical solution

Material macroscopically homogenous
Isotropic transport properties
Properties of volume elements, representative for the material

Definition of local state variables

θ_l	*Water content*
T	*Temperature*
φ	*Relative humidity*
p_v	*Vapour pressure*
p_c	*Capillary pressure*

The numerical solving method

Discretisation of partial derivation

$$q_k = -\lambda \frac{\partial \theta}{\partial x_k}$$

Example: Heat fluxes between control volumes

Taylor series expansions:

$$f(x+\Delta x) = f(x) + \Delta x \frac{\partial f}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{\Delta x^3}{3!} \frac{\partial^3 f}{\partial x^3} + \dots$$

Estimation of 1. derivation of function (with fault 2nd order):

$$\frac{\partial f}{\partial x} = \frac{f(x+\Delta x) - f(x)}{\Delta x} + O(2)$$

Discrete formulation of heat flux
Density between control volumes:

$$q_k = -\lambda \frac{\Delta \theta}{\Delta x_k}$$

The numerical solving method

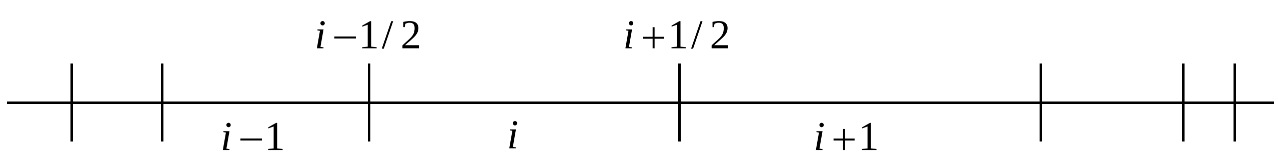
Numerical solving methods at a glance

$$\frac{\partial U}{\partial t} = -\frac{\partial}{\partial x_k}\left(\lambda \frac{\partial \theta}{\partial x_k}\right)$$

+
Control volume method
+
Discretisation of partial derivations
=
System of ordinary differential equation
(one equation per control volume and conserving quantity)

e.g. 1D heat cond-
ductivity equation

$$\frac{\partial U_i}{\partial t} = \frac{1}{\Delta x_i}\left(\lambda_{i-1/2}\frac{\theta_{i-1}-\theta_i}{\Delta x_{i-1/2}} - \lambda_{i+1/2}\frac{\theta_i-\theta_{i+1}}{\Delta x_{i+1/2}}\right)$$



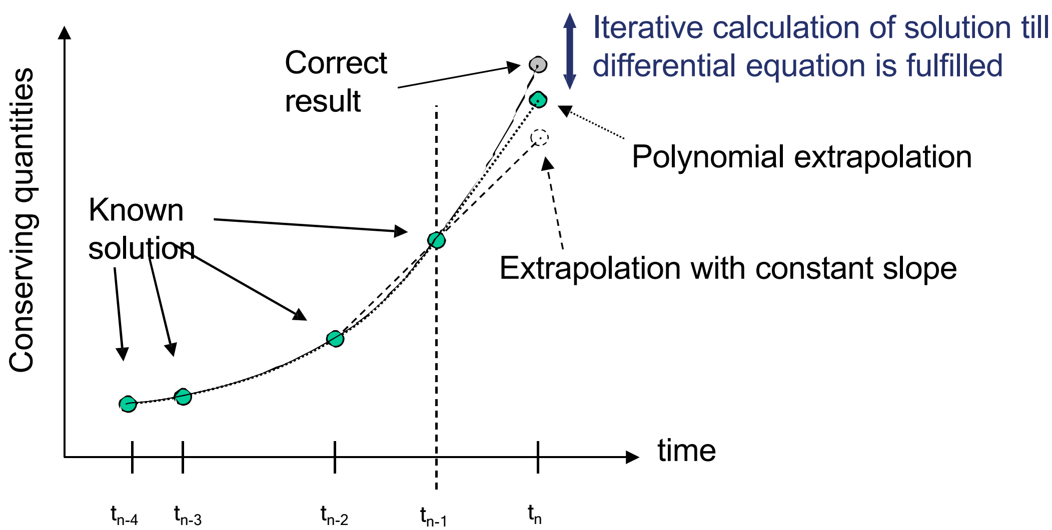
The numerical solving method

Numerical solution

Discretised differential equation (example: moisture mass balance)

$$\frac{\partial w}{\partial t} = -\frac{1}{\Delta V}\left[\sum_A \left(g_{vapour} + g_{liquid}\right)_A\right]$$

Numerical Integration



The numerical solving method

Numerical solving methods at a glance

2 balance equations * n elements = number of equations & unknowns

Vector with unknowns: $\mathbf{y} = \{Q_i, w_i\}$

System of differential equations: $\frac{\partial \mathbf{y}}{\partial t} = \mathbf{f}(t, \mathbf{y})$

Solution of equation systems by time integration:

$$\mathbf{y}(t) = \mathbf{y}_0 + \int_t \mathbf{f}(t, \mathbf{y})\, dt$$

→ Simulation software DELPHIN

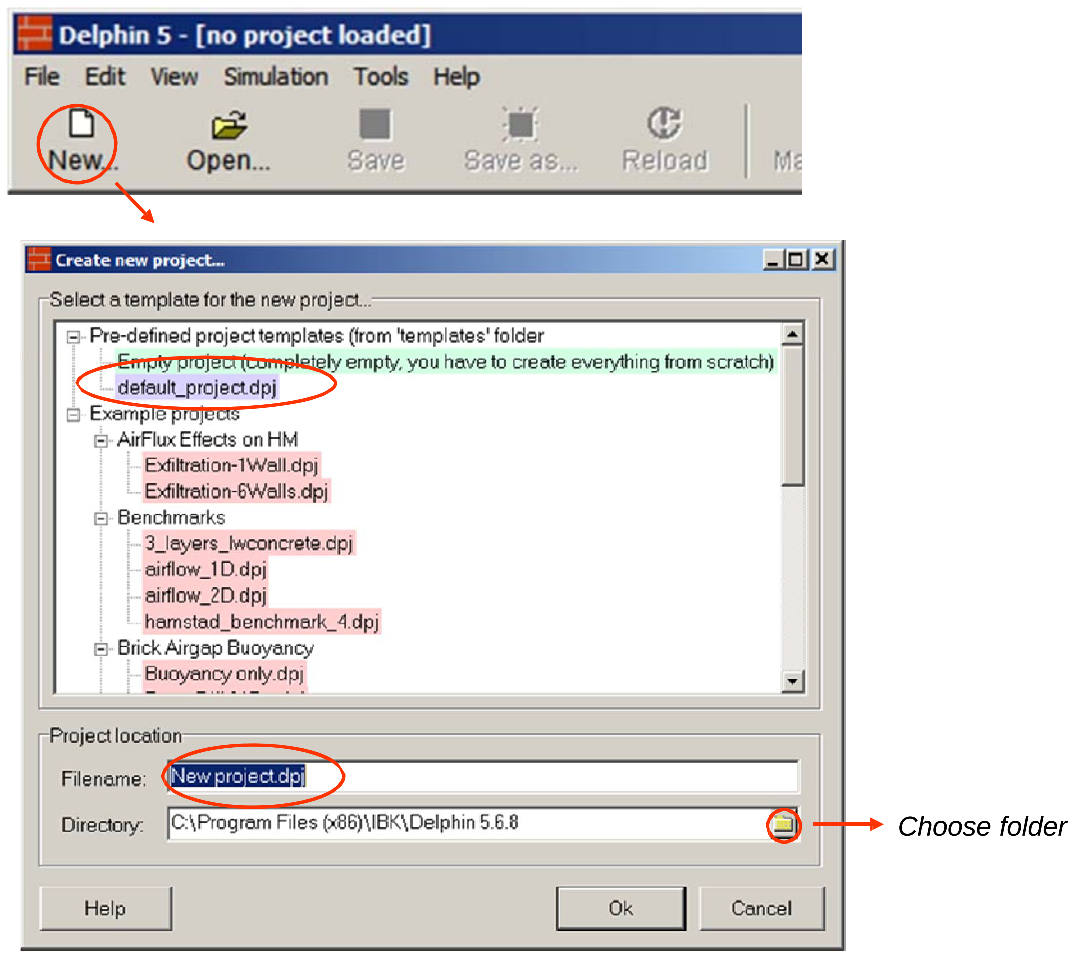
Application of Delphin

DELPHIN: Program operation

Steps - New Project

- Open new project template
- Choose memory location of the project
- Delphin project name

DELPHIN opens a standard template (.dpj).*



DELPHIN: Program operation

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

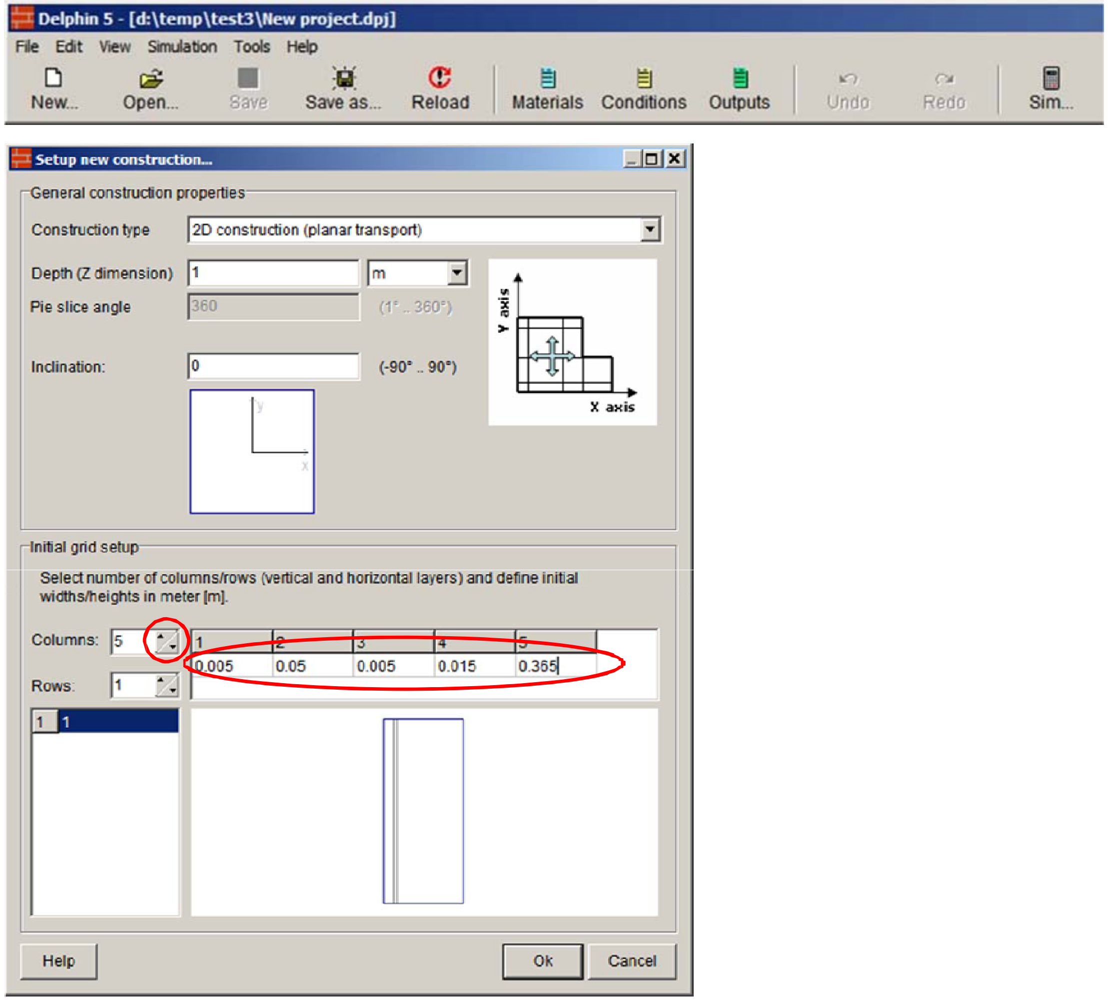
Steps - Construction

- Define type of construction, here: 1D horizontal
- Adjust number of material layers in x-direction
- Adjust thickness of different layer in [m]

Only transport in x-direction:

The height (y-direction) und depth (z-direction) should be 1 m to calculate a wall area of 1m².

DELPHIN then opens the construction view and shows the succession of layers – initially without materials.



TECHNISCHE UNIVERSITÄT DRESDEN

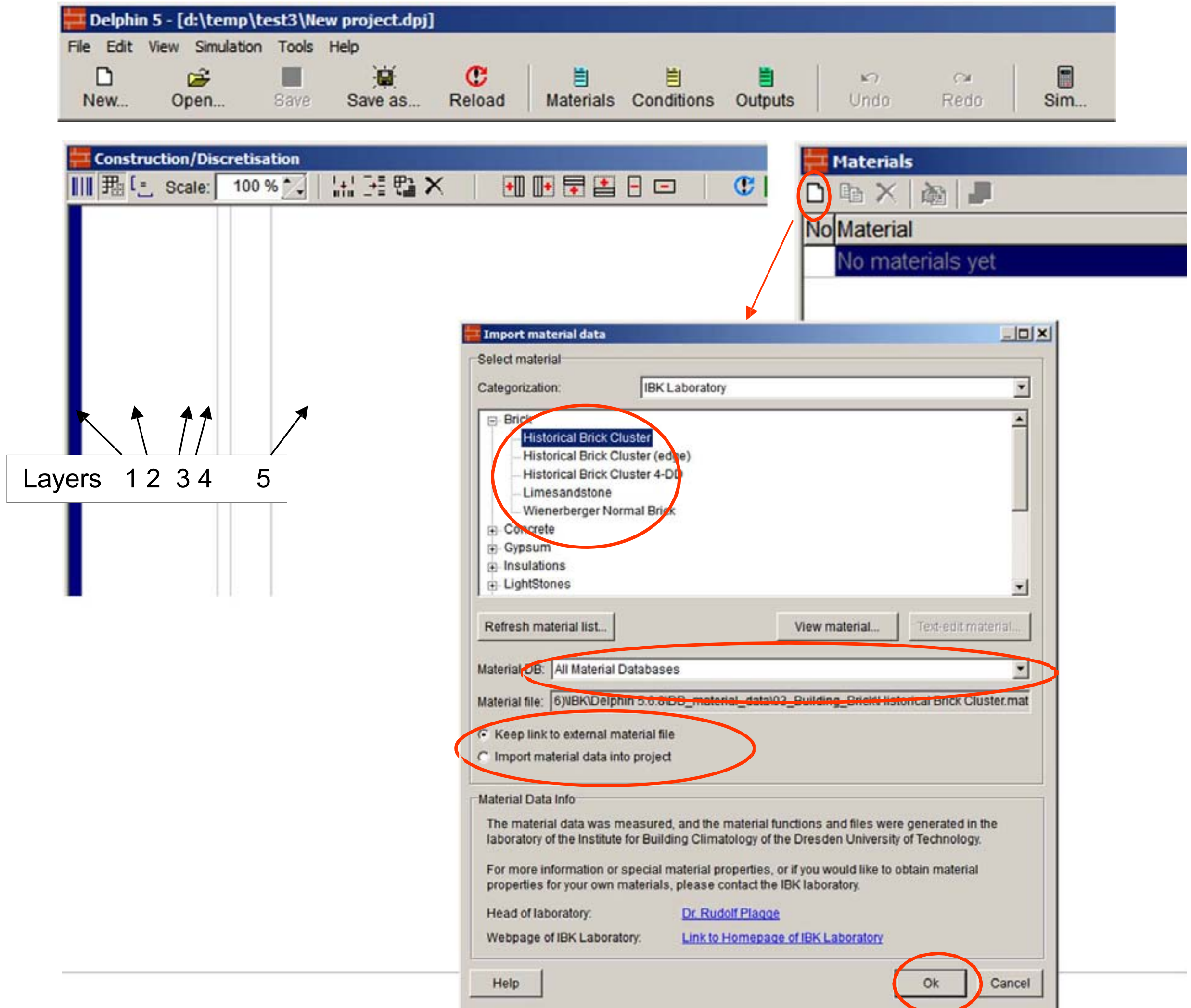
EURAC research

DELPHIN: Program operation

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

Steps - Material

- Import material
- Choose program or user data base
- Choose import modus
- Choose material and import it



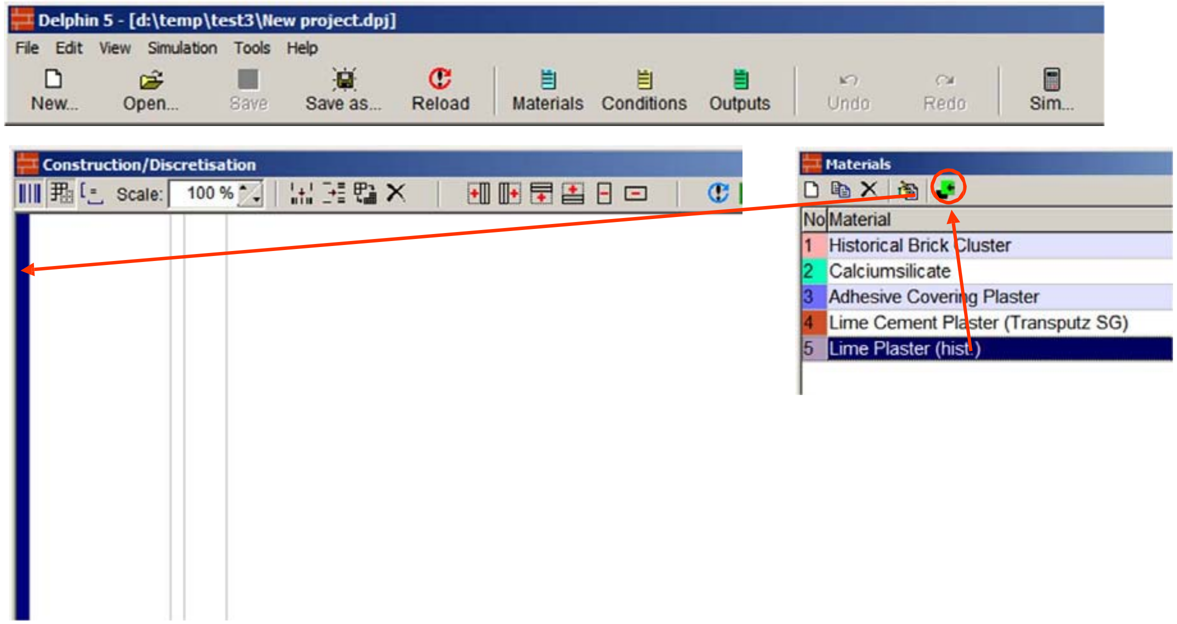
DELPHIN shows the imported materials in the material list.

TECHNISCHE UNIVERSITÄT DRESDEN
EURAC research

DELPHIN: Program operation

Steps

- Mark material and favoured layer
- Click on green assign button



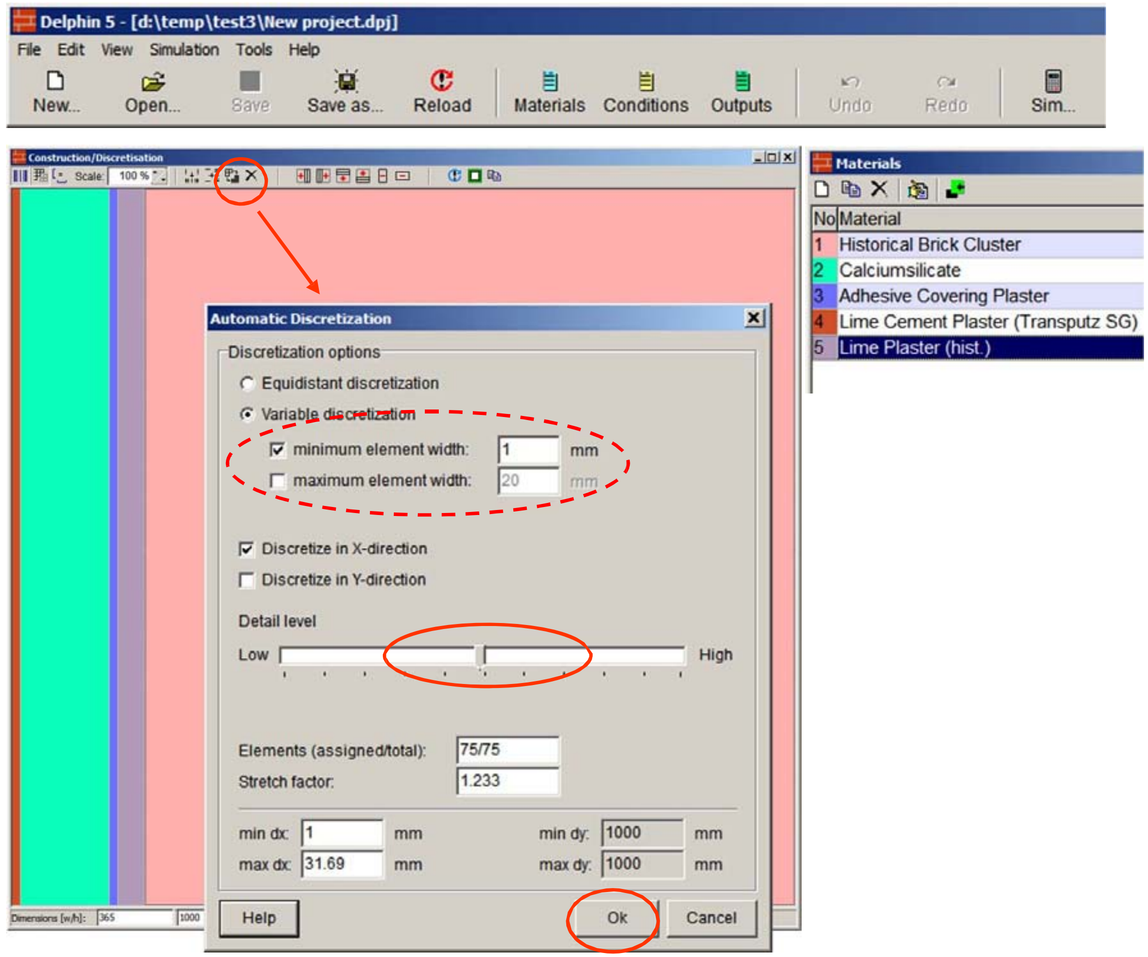
DELPHIN generates a material assignment data set and colours layers with material assignment corresponding to the colour of the material.

DELPHIN: Program operation

Steps

- Call discretisation dialogue
- Set grade of refinement (higher = more refined discretisation)
- Set minimal/maximal element thickness eventually
- Start discretisation (>> Ok)

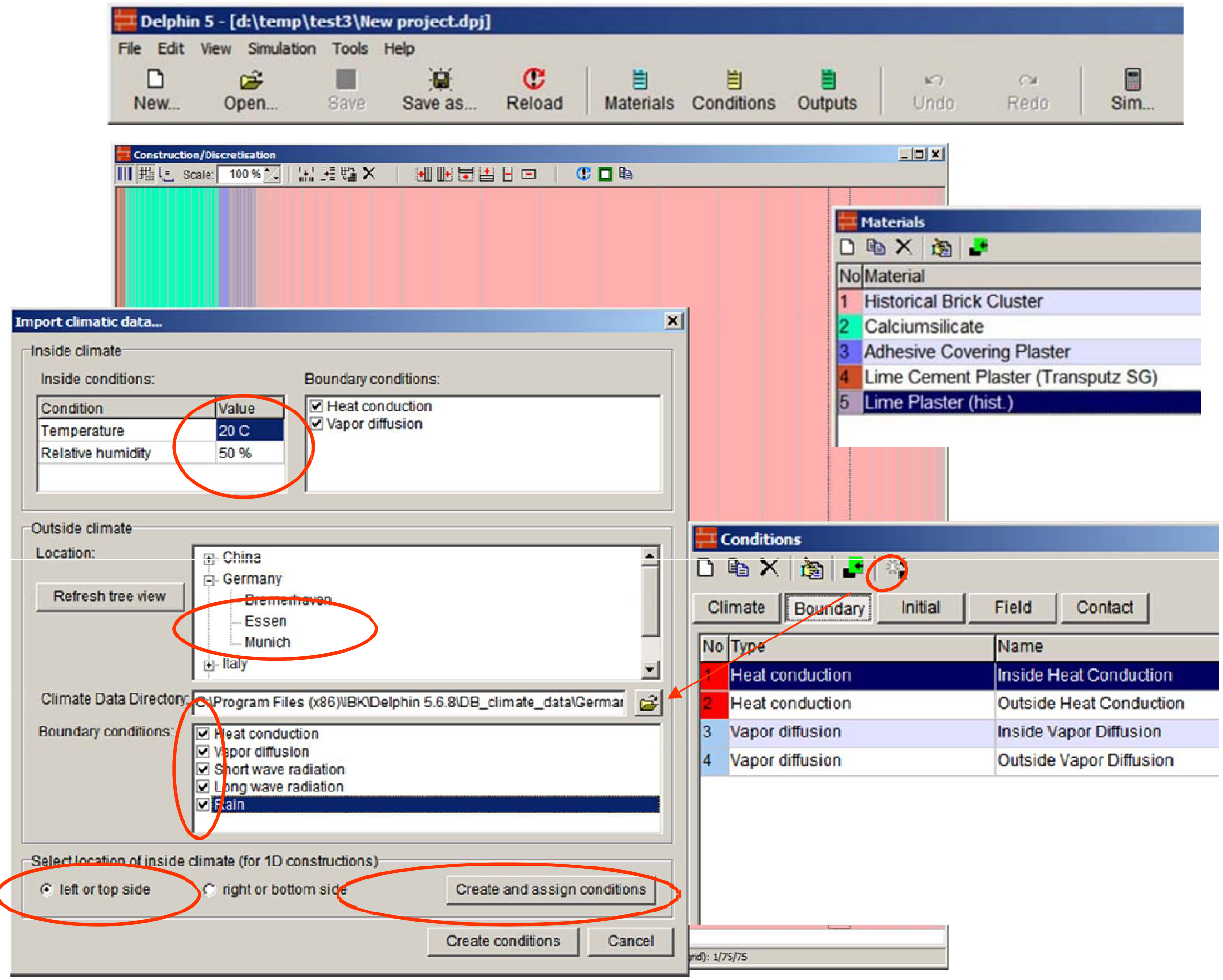
DELPHIN divides material layers in discrete volume elements.



DELPHIN: Program operation

Steps - Climate

- Import climate conditions
- Adjust internal and external climate data
- Import and assign boundary conditions data sets



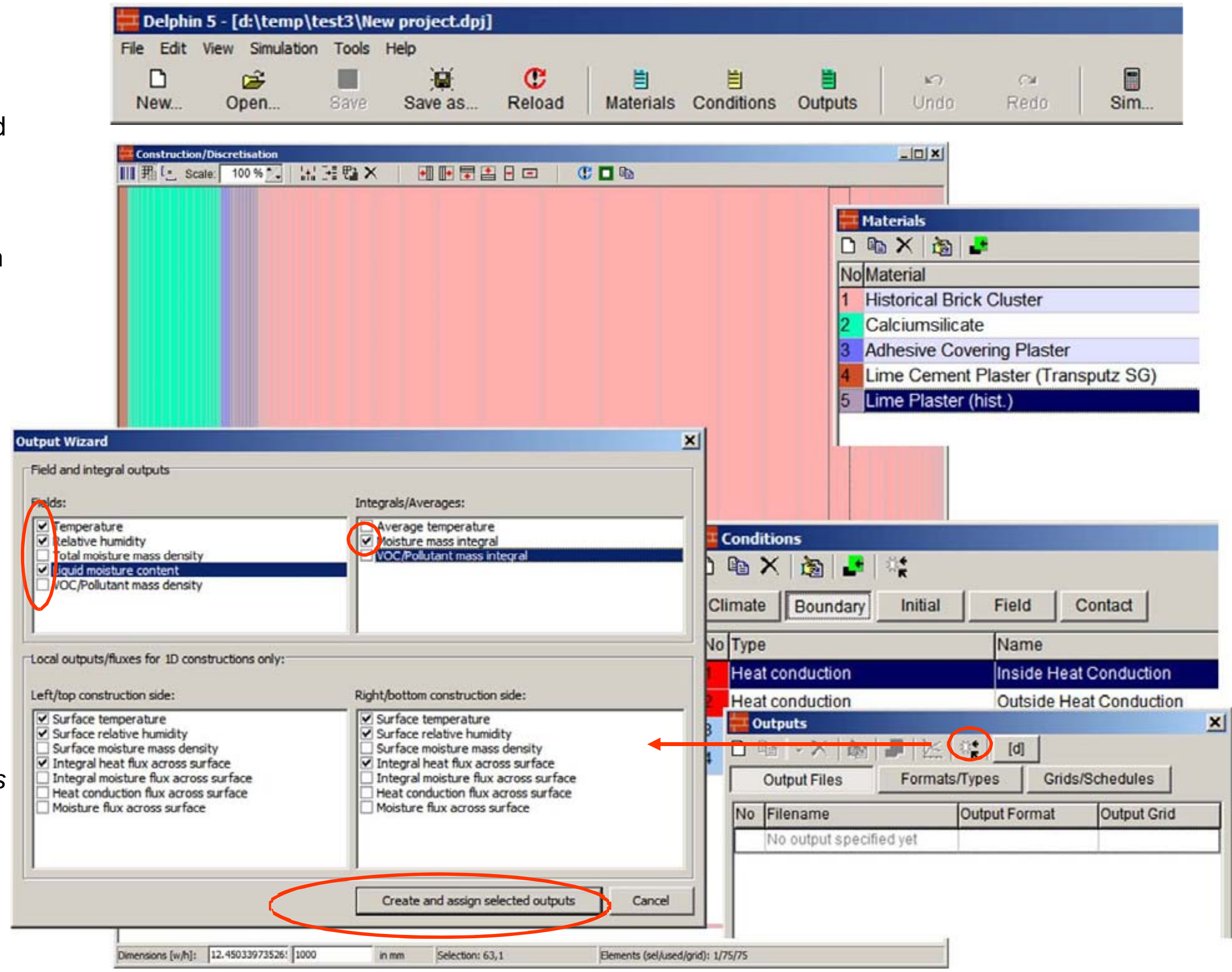
DELPHIN shows the imported climate and boundary conditions in the conditions windows and enables the assignment to the construction.

DELPHIN: Program operation

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

Steps - Outputs

- Start Outputs-Wizard
- Deactivate VOC-outputs, activate water content
- Generate and assign output files



DELPHIN generates output files and enables the assignment to the geometry.

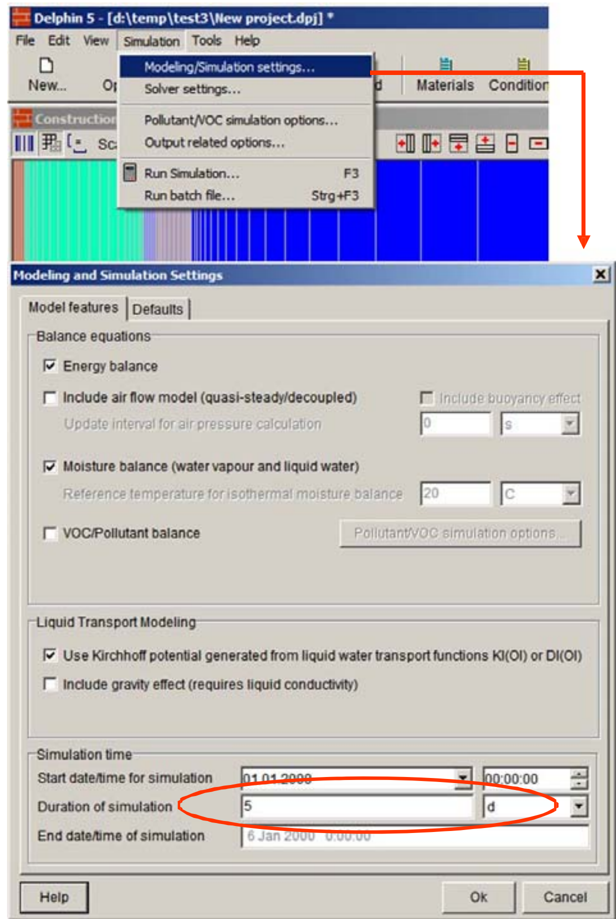
TECHNISCHE UNIVERSITÄT DRESDEN
EURAC research

DELPHIN: Program operation

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

Steps - Simulation

- Open modelling and simulation properties
- Define starting point and total duration of simulation



TECHNISCHE UNIVERSITÄT DRESDEN

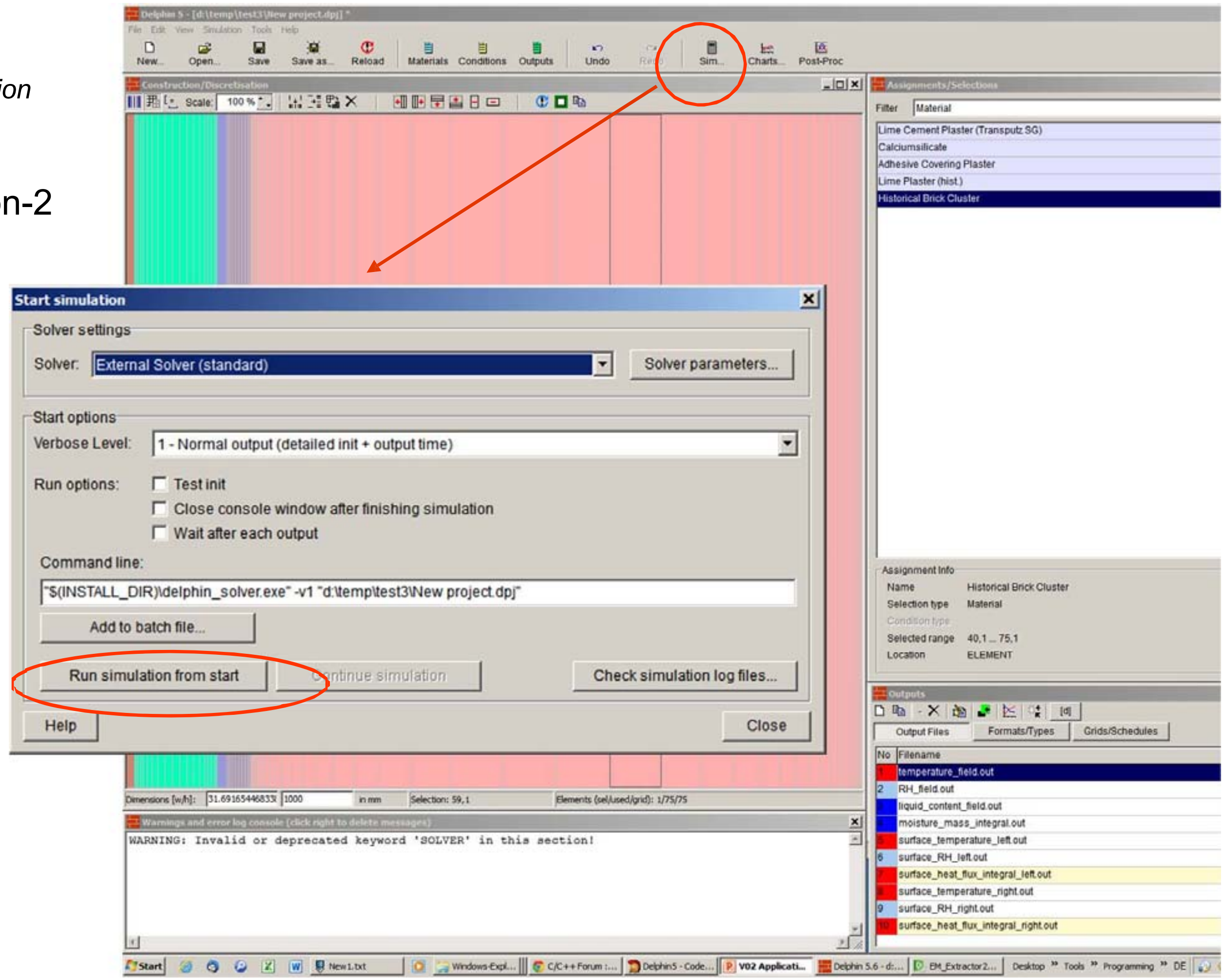
EURAC research

DELPHIN: Program operation

Start DELPHIN simulation

Steps – Simulation-2

- Start solver dialogue
- Start simulation



DELPHIN starts the numeric solver in a separate windox.

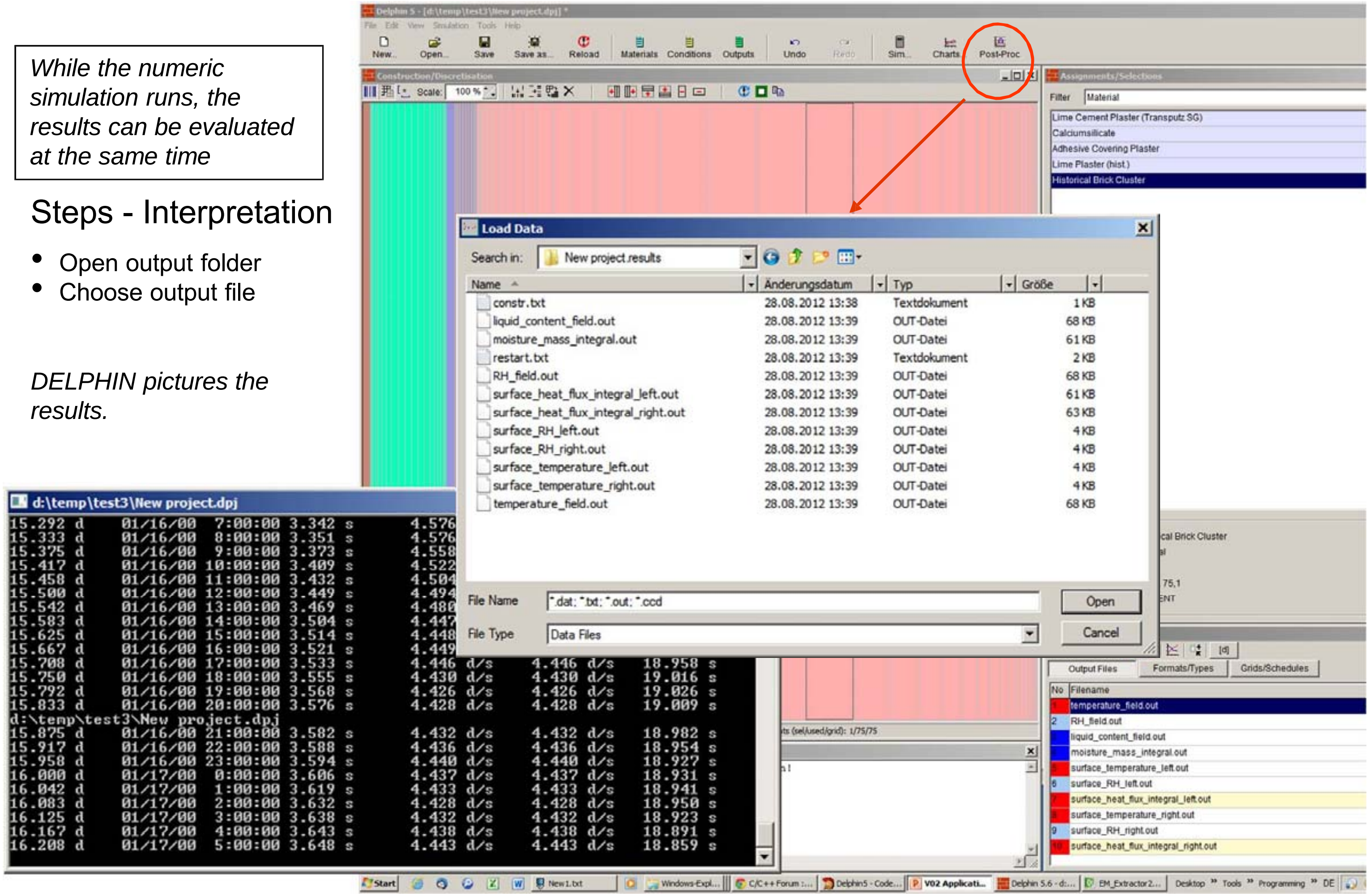
DELPHIN: Program operation

While the numeric simulation runs, the results can be evaluated at the same time

Steps - Interpretation

- Open output folder
- Choose output file

DELPHIN pictures the results.

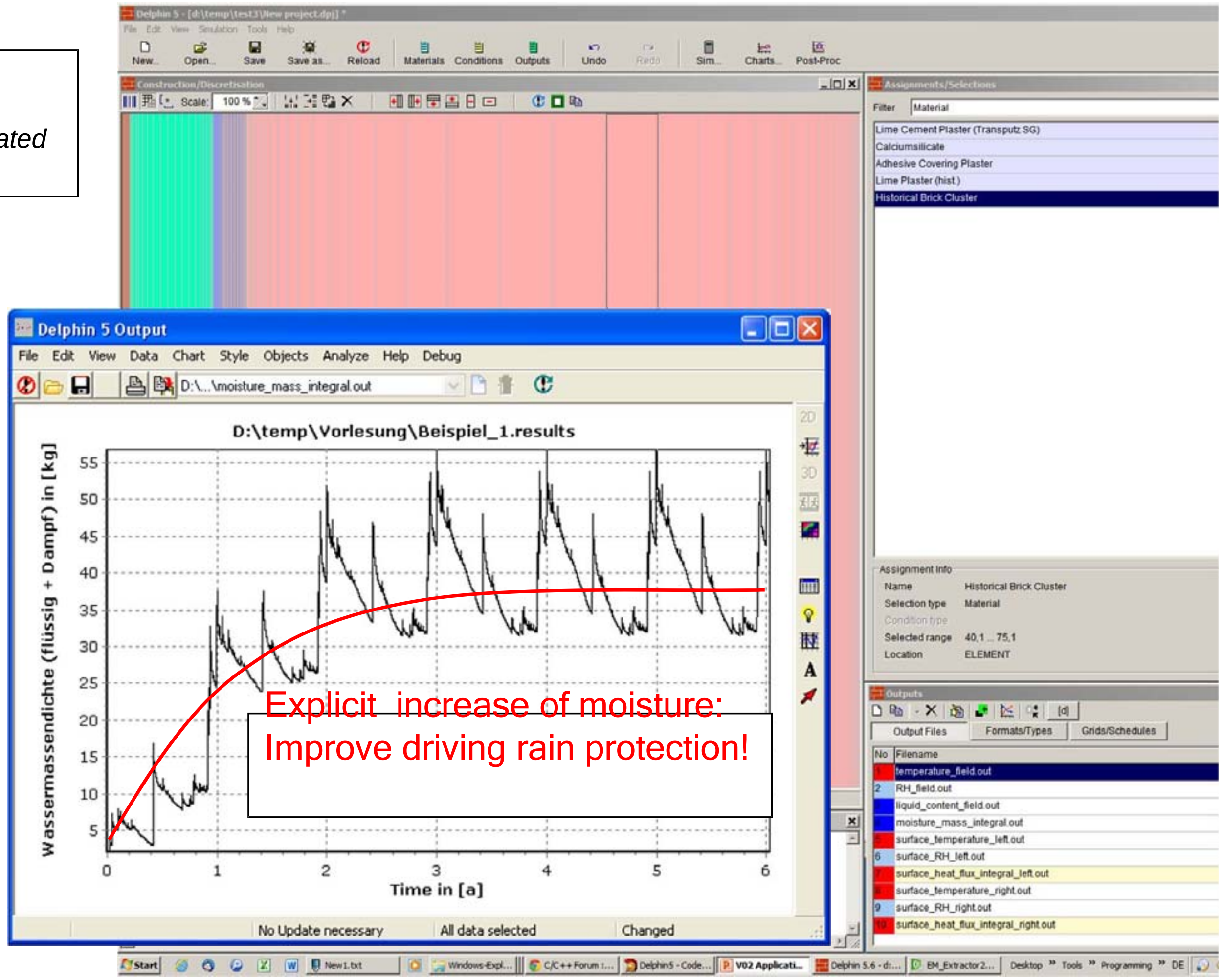


DELPHIN: Program operation

While the numeric simulation runs, the results can be evaluated at the same time

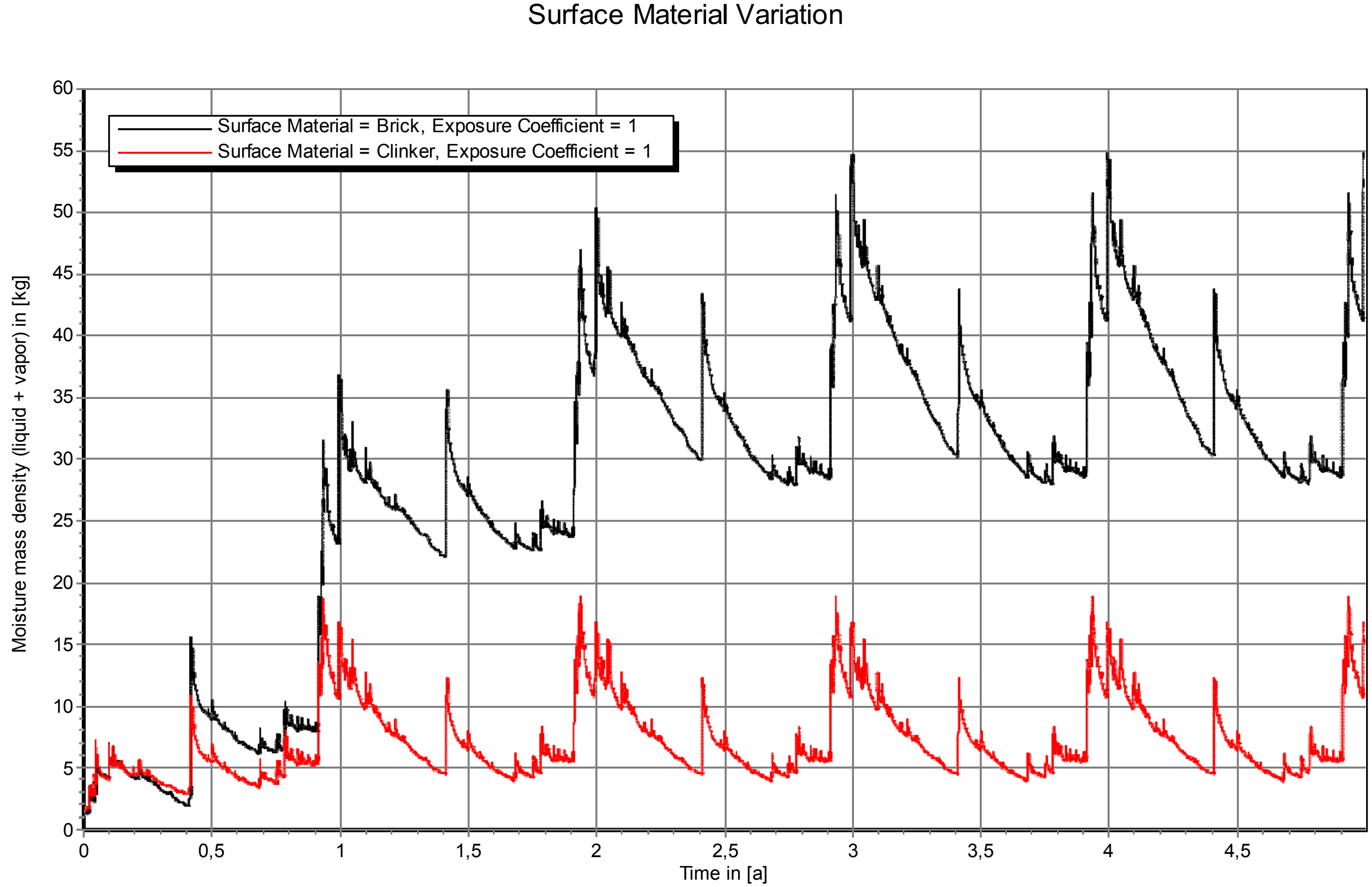
Steps - interpretation

- Updating while calculation possible
- Manifold adjustment of the charts
- Export into other software via clipboard



DELPHIN: results

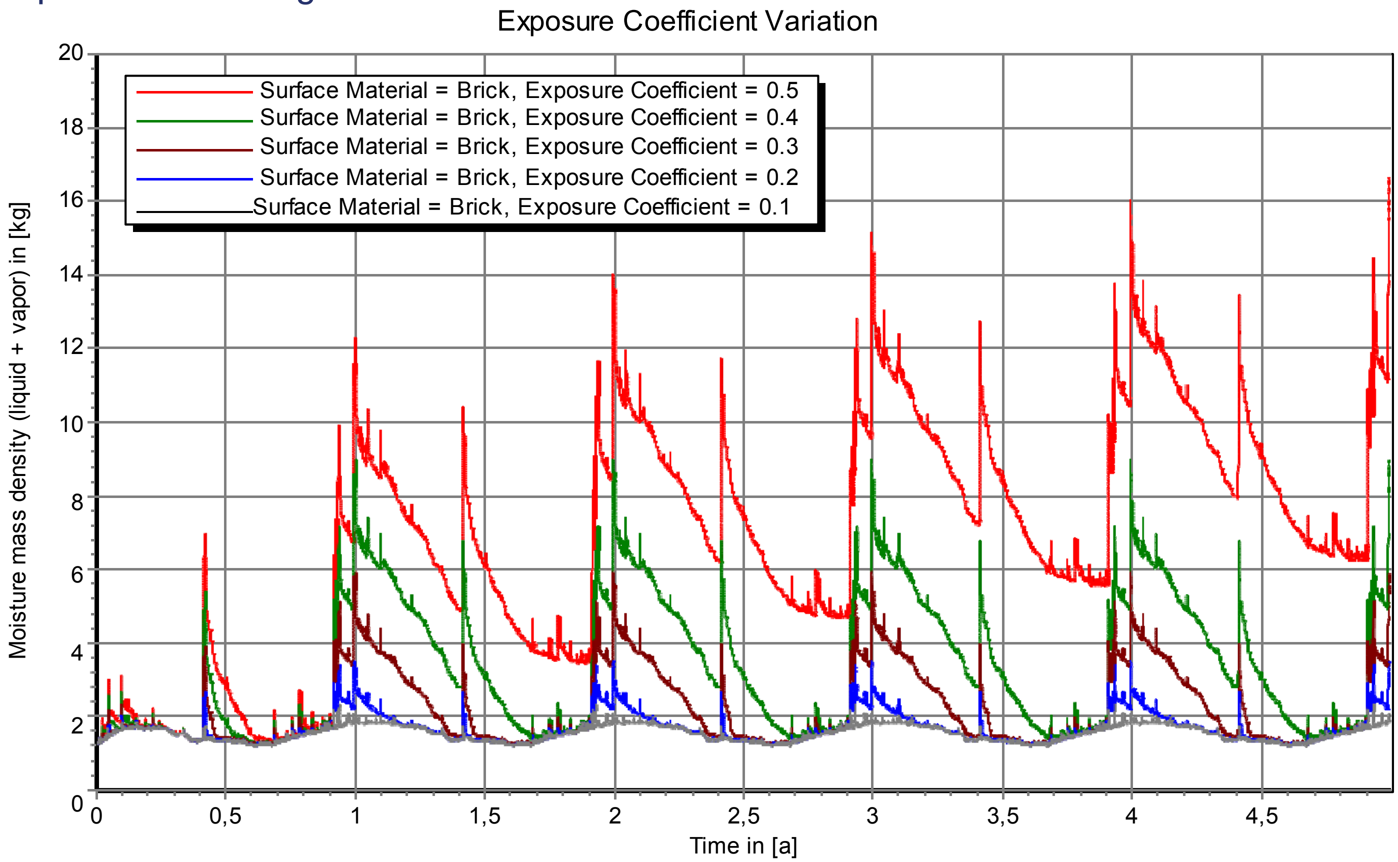
Different materials



DELPHIN: results

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

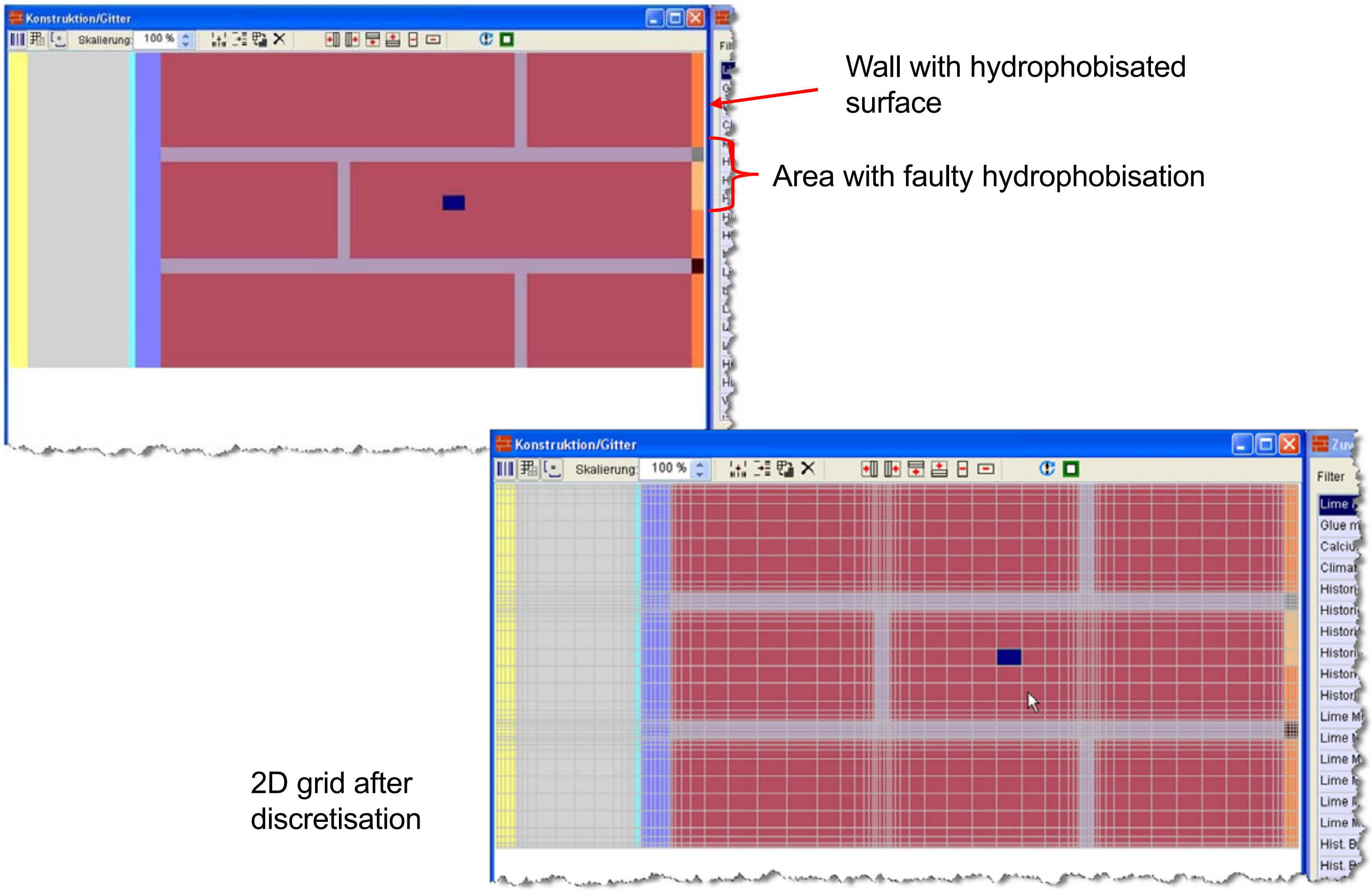
Rain protection/roofing:



TECHNISCHE UNIVERSITÄT DRESDEN

EURAC research

DELPHIN – Analysis of 2D problems

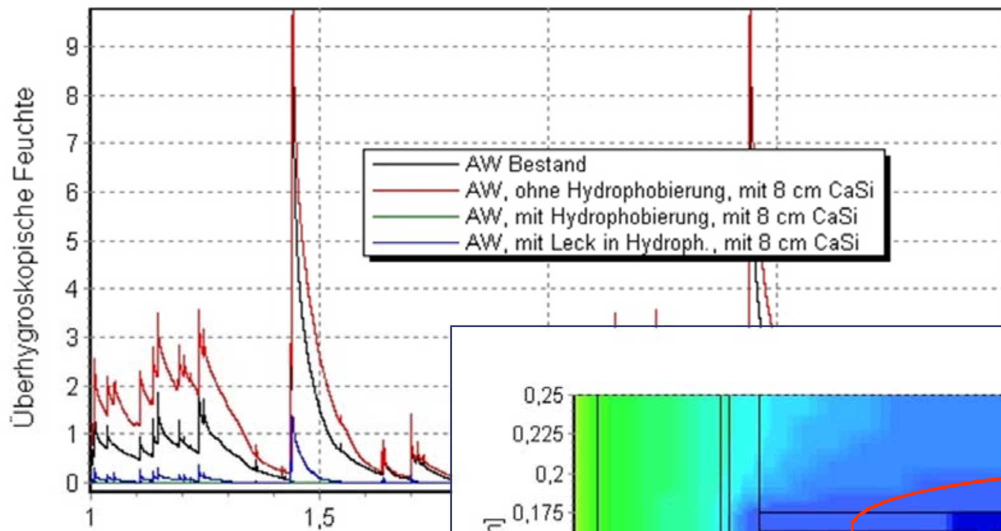


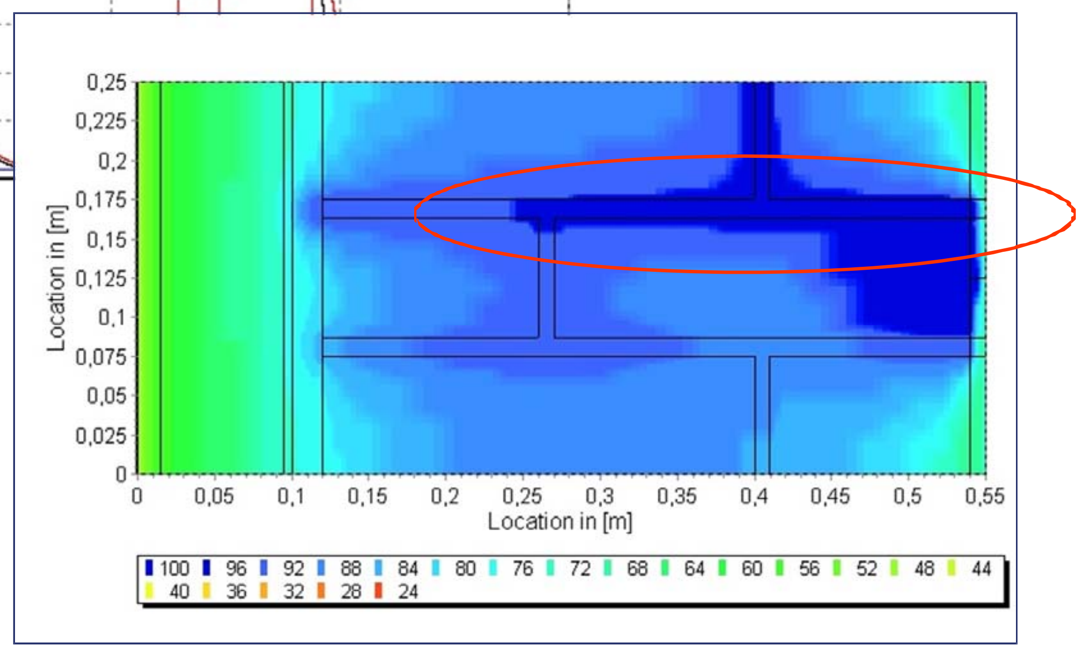
Wall with hydrophobisated surface

Area with faulty hydrophobisation

2D grid after discretisation

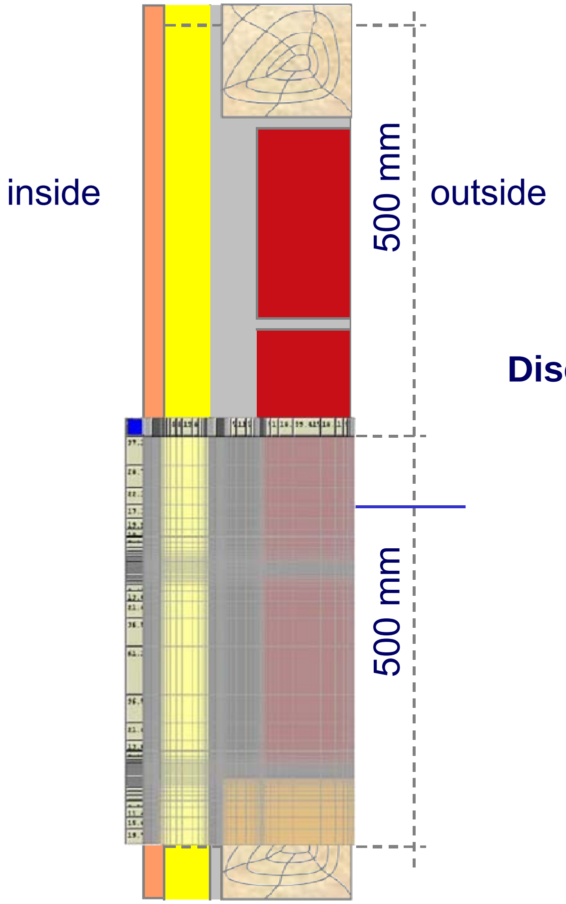
DELPHIN – Analysis of 2D problems



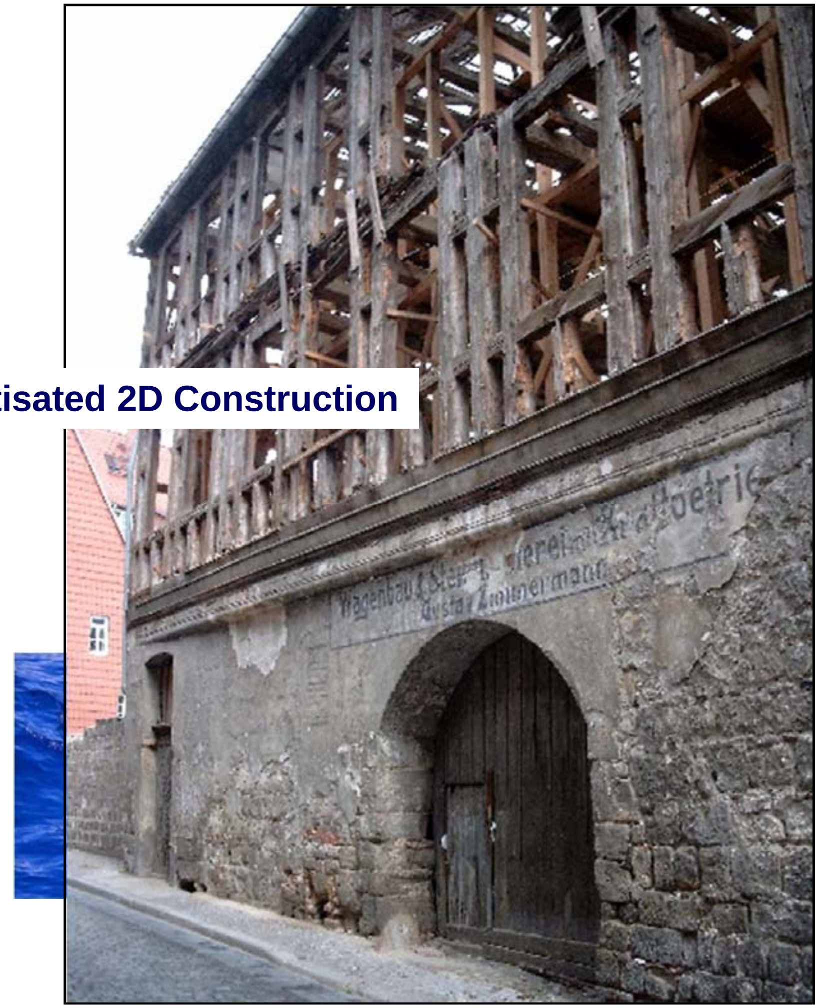


Field of humidity with faulty hydrophobisation

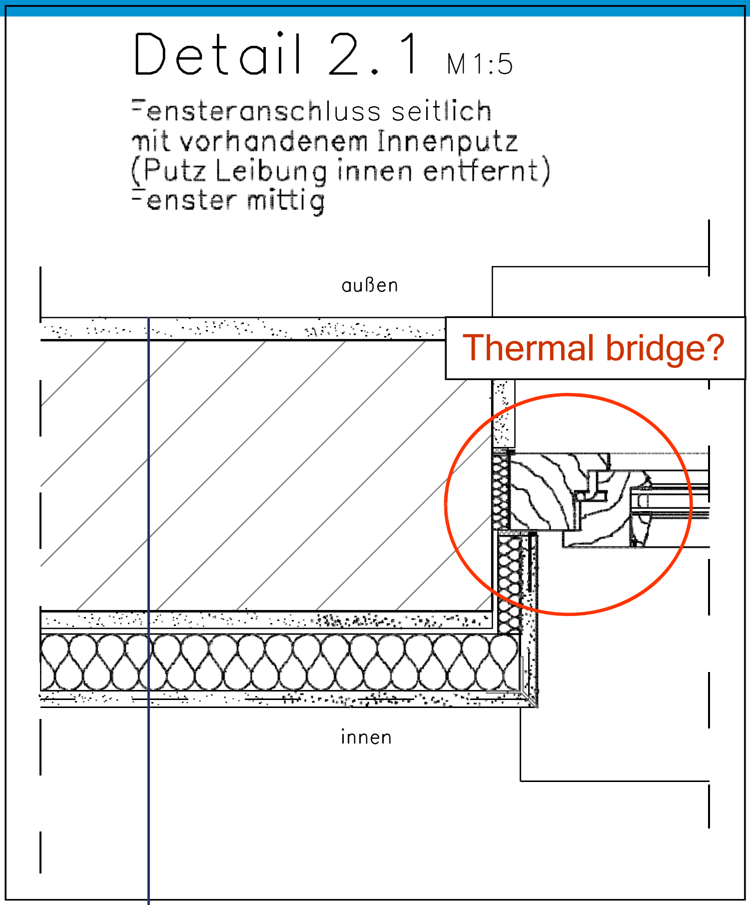
Rehabilitation and Building in older housing stock

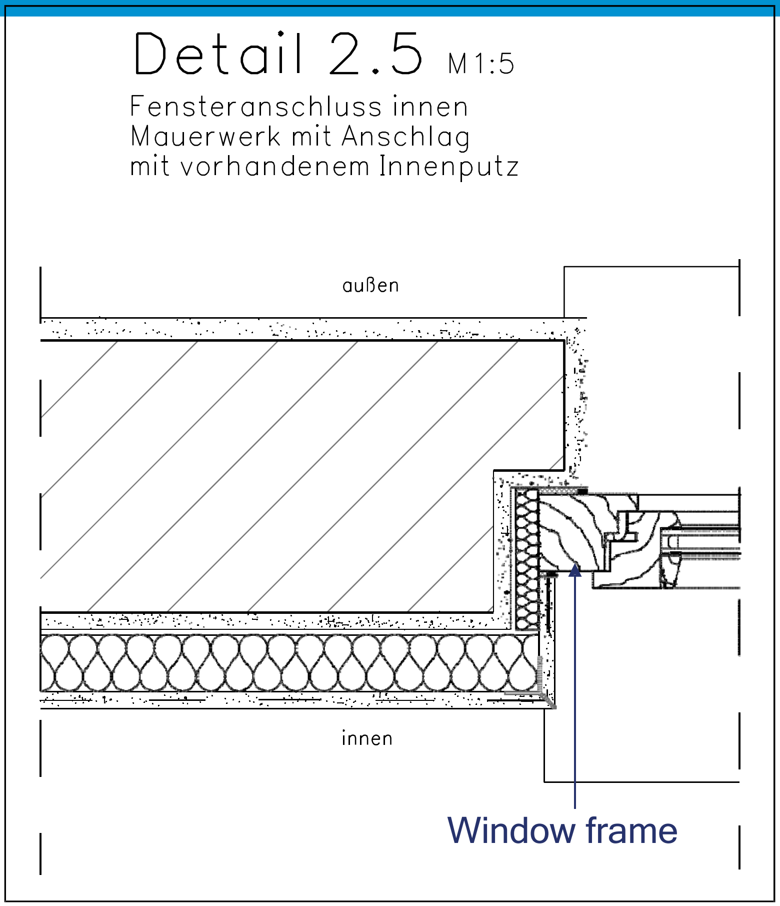


Discretisated 2D Construction



DELPHIN – Analysis of constructional details



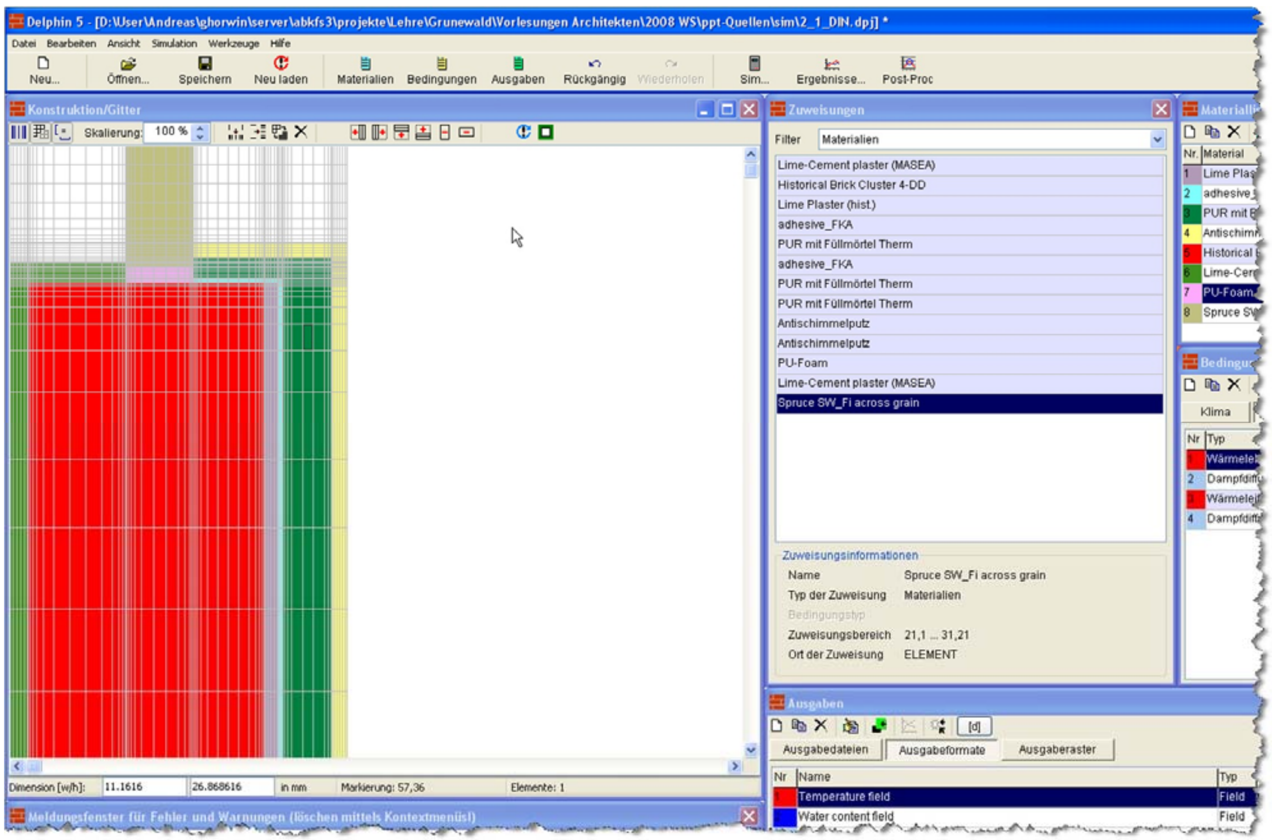


Plaster, Brick, Plaster, Glue mortar, Insulation, Plaster

DELPHIN – Analysis of constructional details

3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

- Analysis with DELPHIN



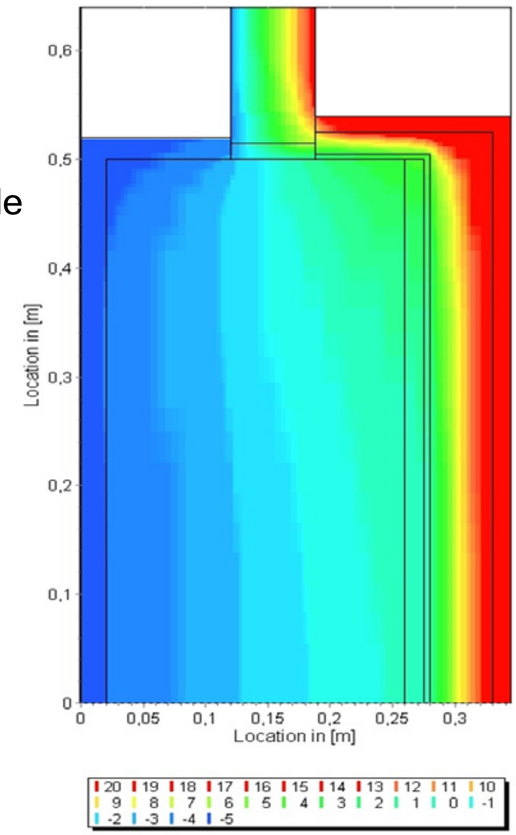
TECHNISCHE UNIVERSITÄT DRESDEN

EURAC research

DELPHIN – Analysis of constructional details

- Detail 2.1 - with window rabbet

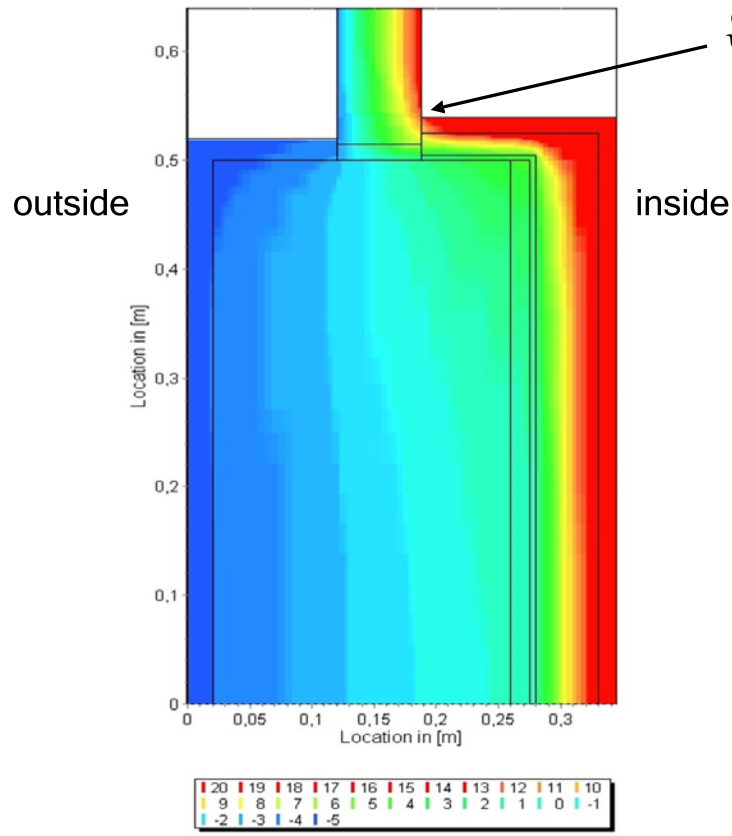
outside



inside

DELPHIN – Analysis of constructional details

- Detail 2.1 - without window rabbet



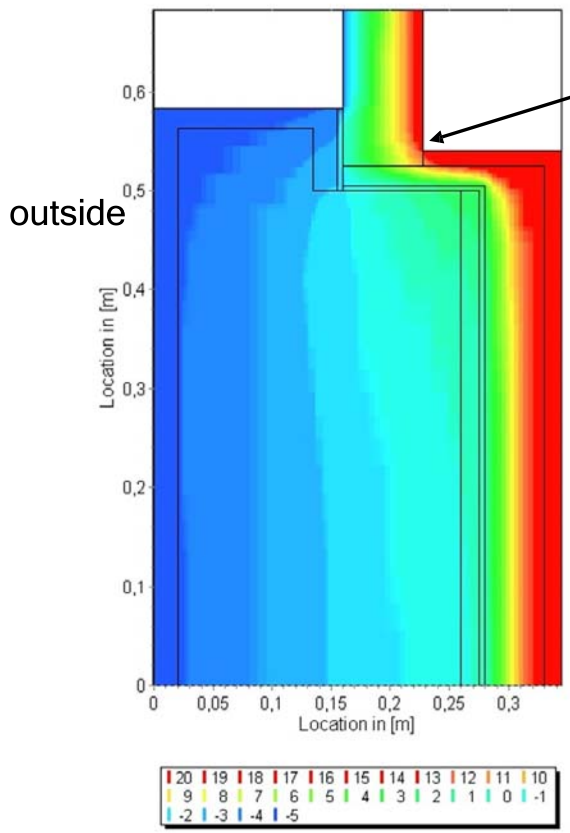
$\vartheta_{oi} = 12{,}1°C$

Incorrect! DIN 4108-2 demands:

$\vartheta_{oi} > 12{,}6°C$

DELPHIN – Analysis of constructional details

- Detail 2.5 - with window rabbet



$$\vartheta_{oi} = 13,8°C$$

Ok, thermal protection fulfilled.

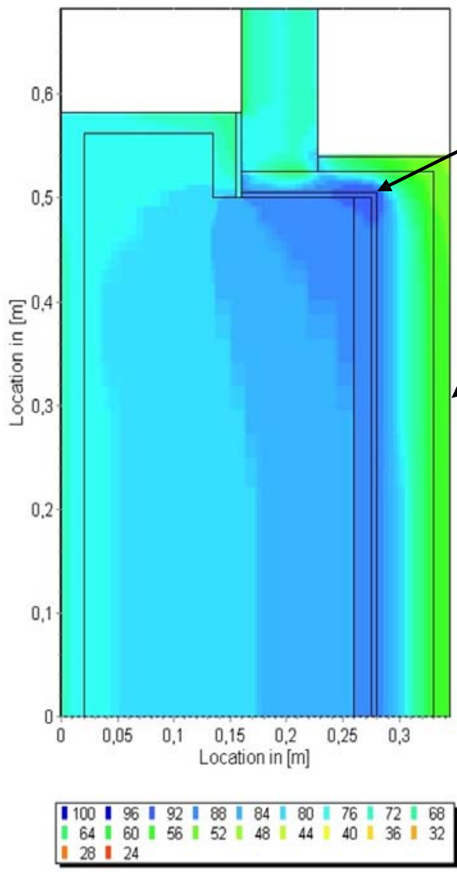
Minimum thermal protection of the guideline ensures, that the dew point temperature resp. minimum pretensions for mould are not reached or exceeded (e.g. on wallpaper).

What about the internal condensate?

DELPHIN – Analysis of constructional details

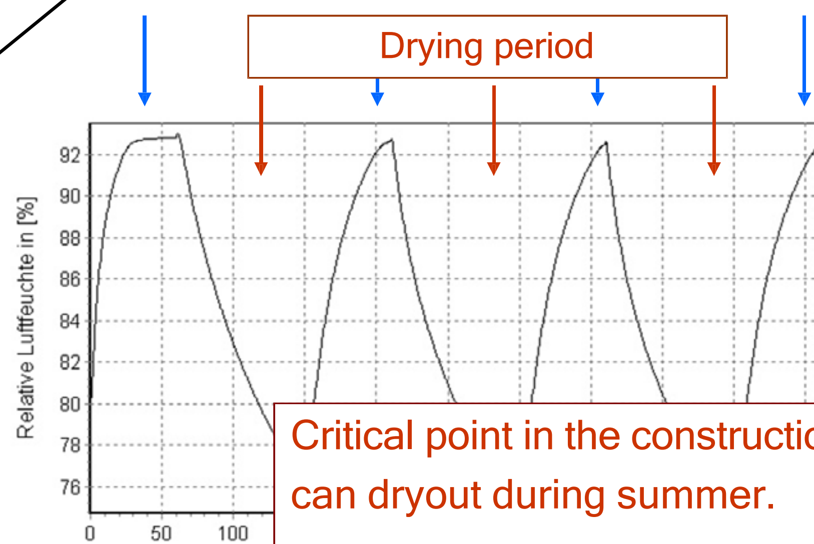
3encult
EFFICIENT ENERGY FOR EU CULTURAL HERITAGE

- Critical moisture content: Condensation and drying behaviour



$\varphi = 92,7\%$

$\varphi = 56,6\%$



Critical point in the construction can dryout during summer.

No moisture accumulation!

TECHNISCHE UNIVERSITÄT DRESDEN

EURAC research