Optimization of open-loop shallow geothermal systems

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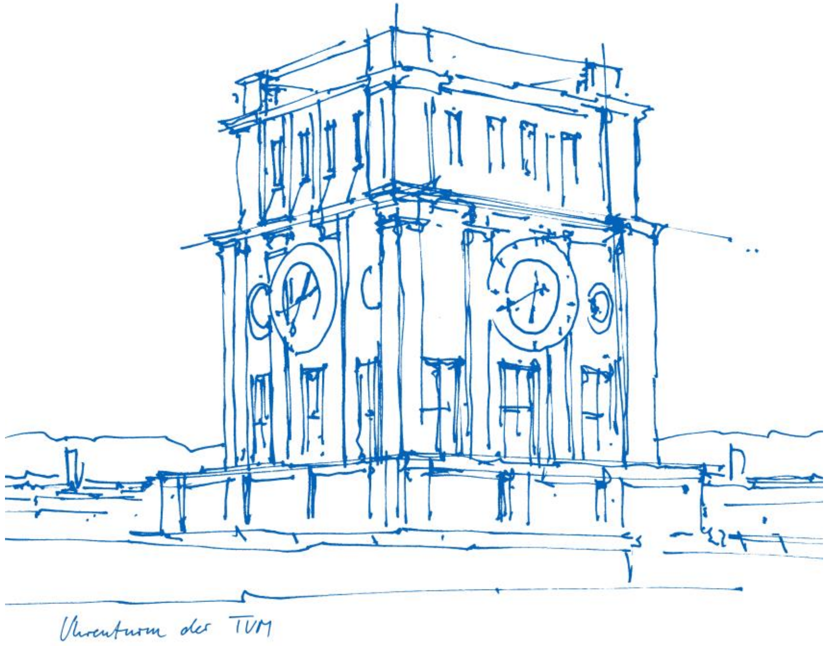
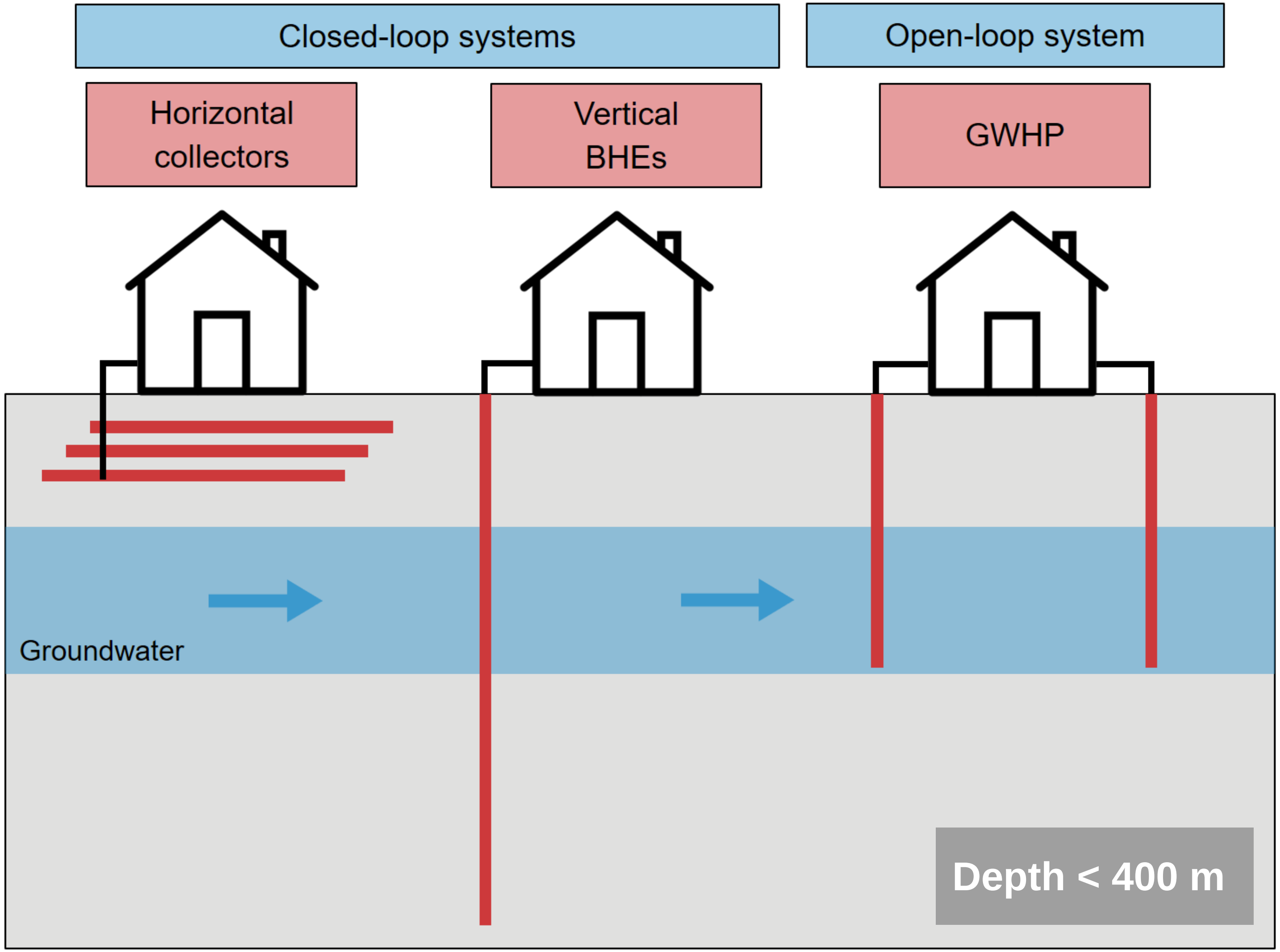
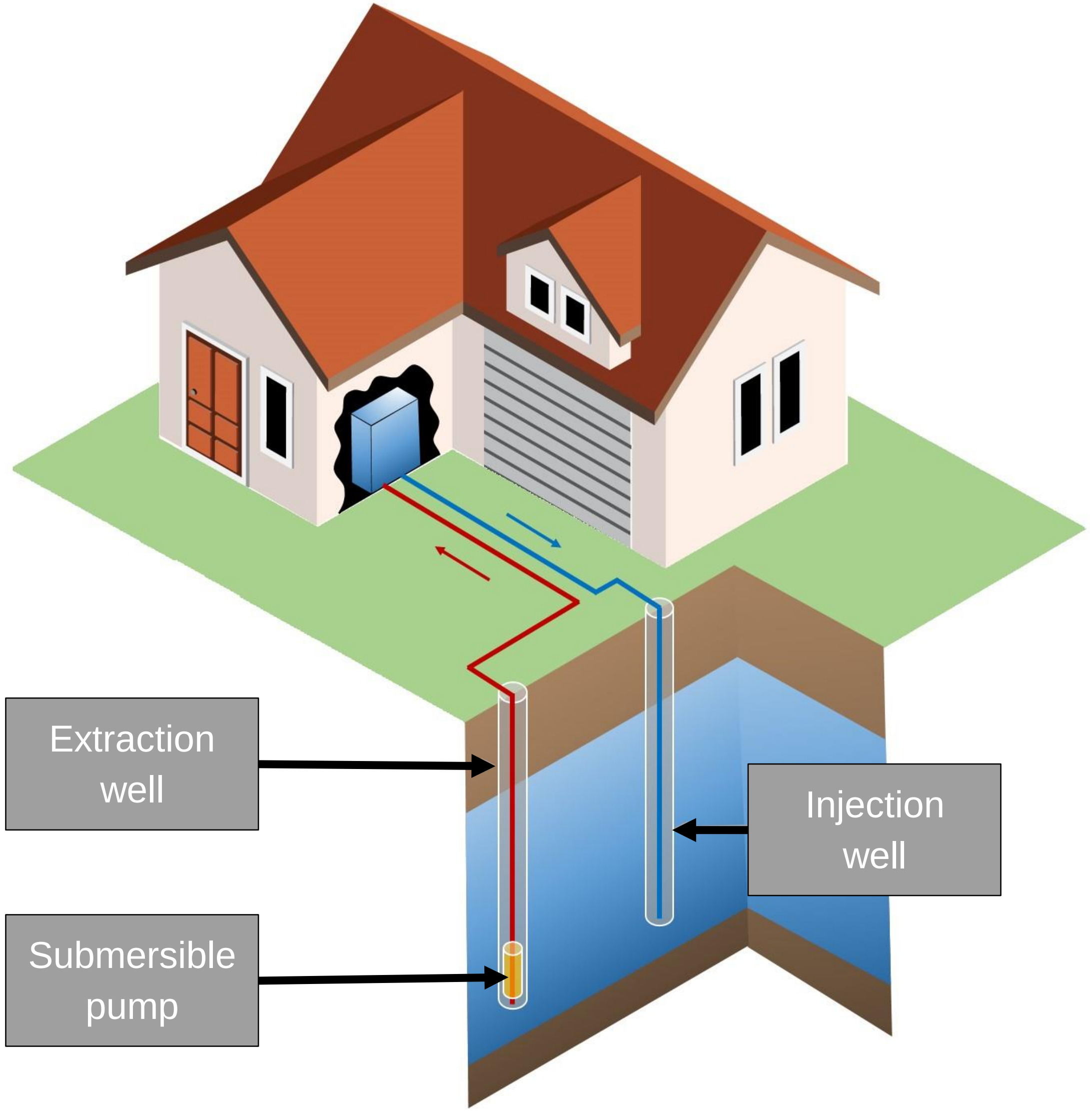
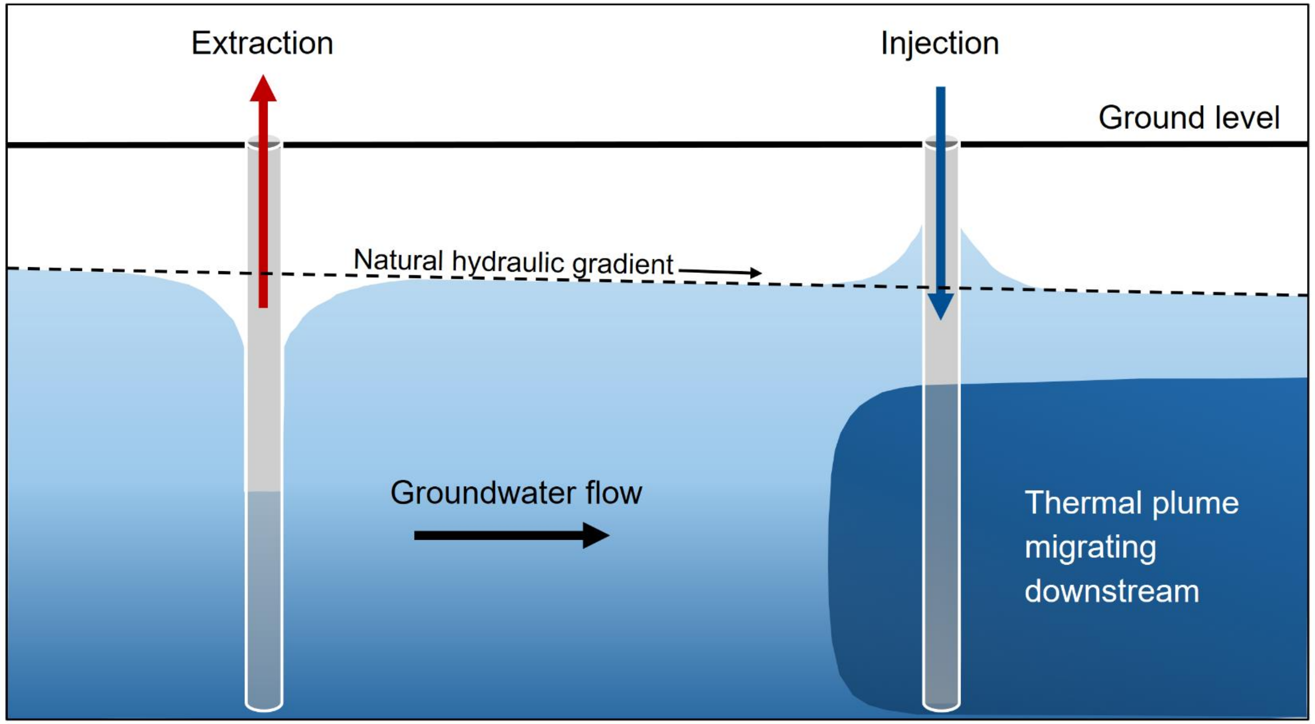


Shallow geothermal energy (SGE) systems



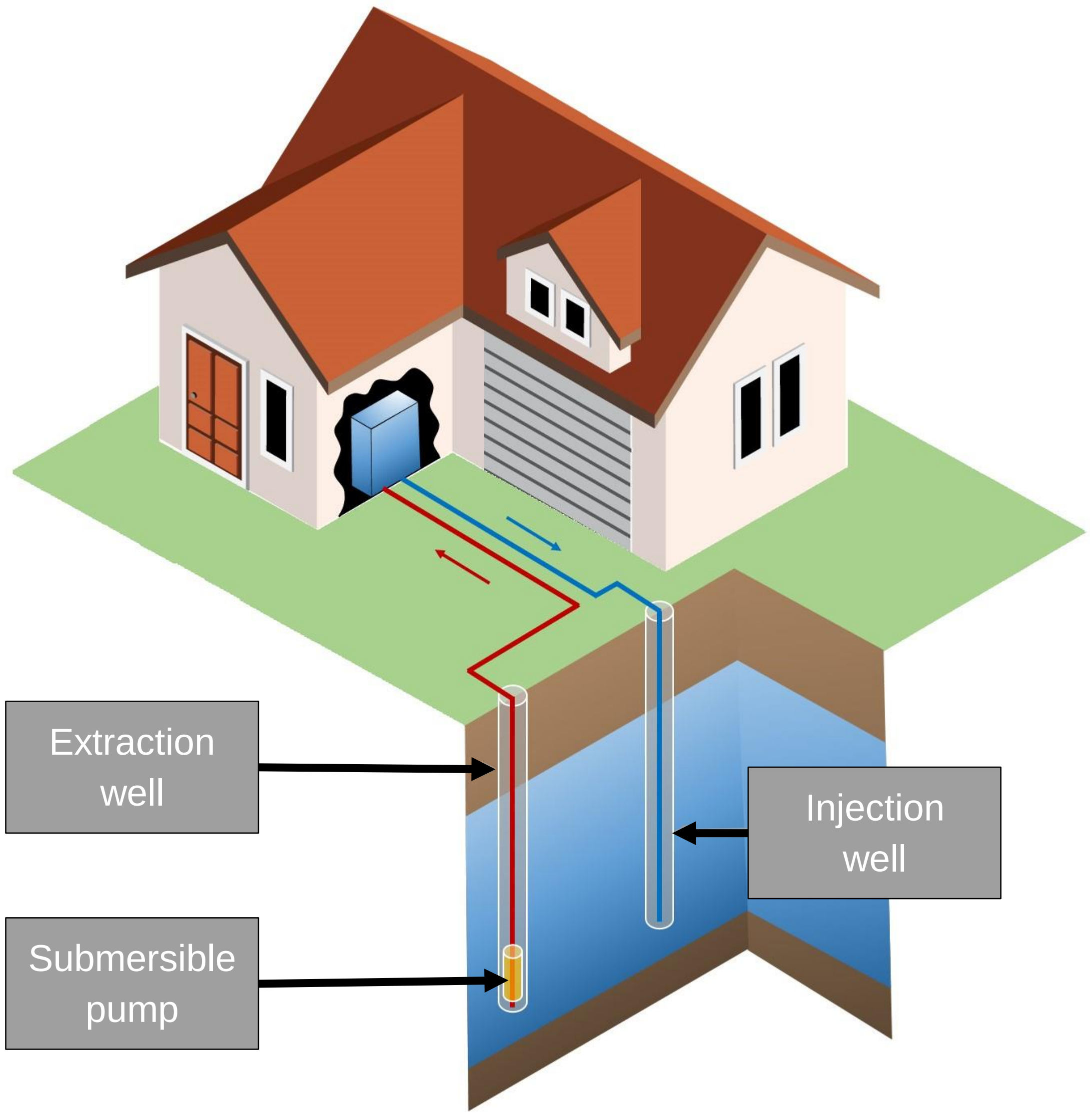
Groundwater heat pumps (GWHPs)

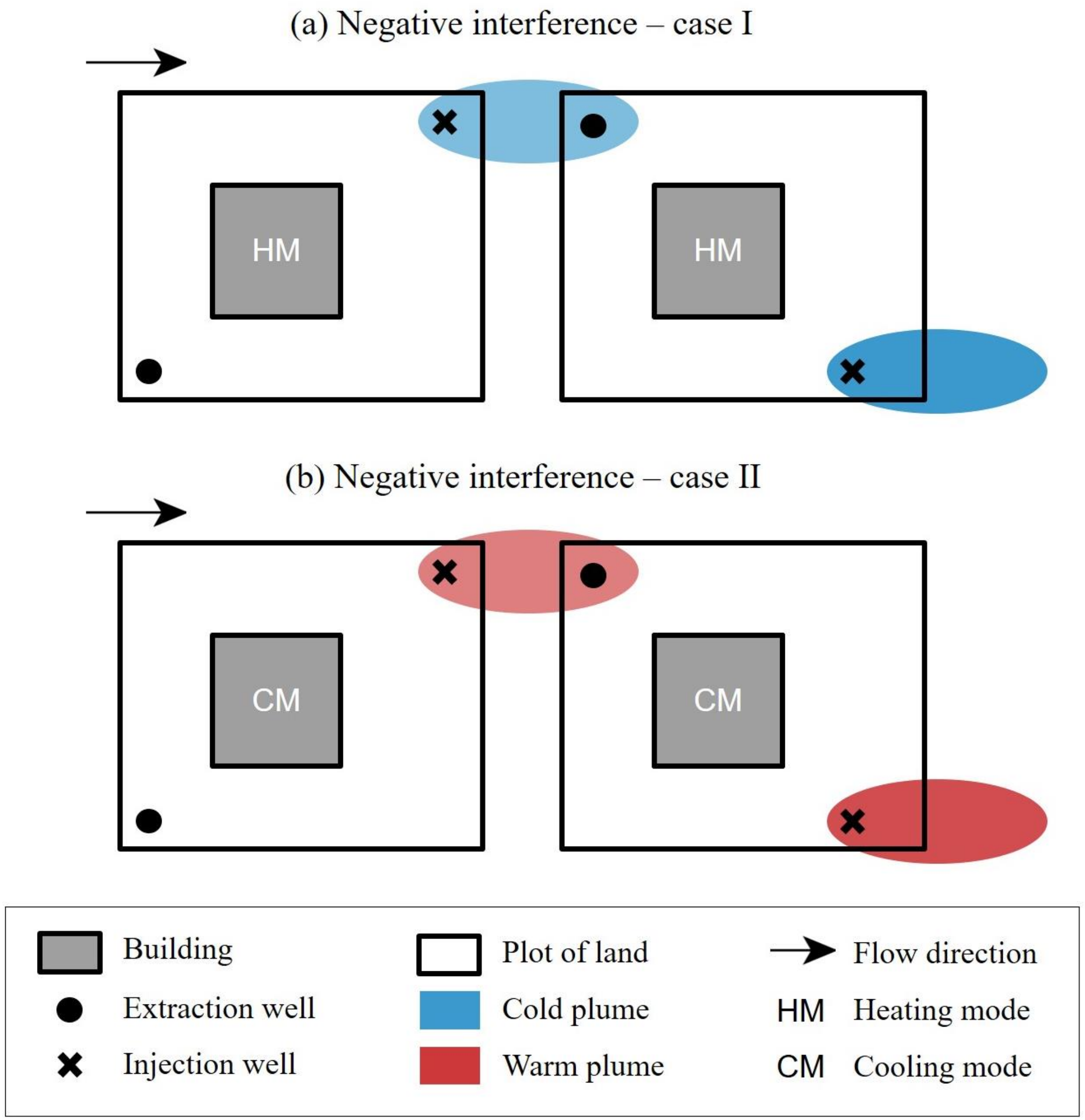




Impacts of GWHP systems [6]

Groundwater heat pumps (GWHPs)





[2]

Research topic

Research objective

Develop and evaluate novel approaches for the optimization of open-loop shallow geothermal systems, i.e. GWHP systems

Research questions

1. <u>What</u> are the viable approaches for the optimization of GWHP systems, and <u>how</u> do they compare in terms of efficiency and applicability?
2. <u>How</u> to optimize the design and operation of GWHP systems?
   a) well locations?
   b) number of GWHP wells?
   c) sizing (pumping rates) of GWHP wells?
3. <u>How</u> to effectively integrate GWHPs into energy system optimization models?

Thesis structure

Relevance of GWHPs

Publication 1: GWHPs in energy system optimization models	Q3

Optimization of GWHPs

Publication 2: Comparison of optimization approaches	Q1

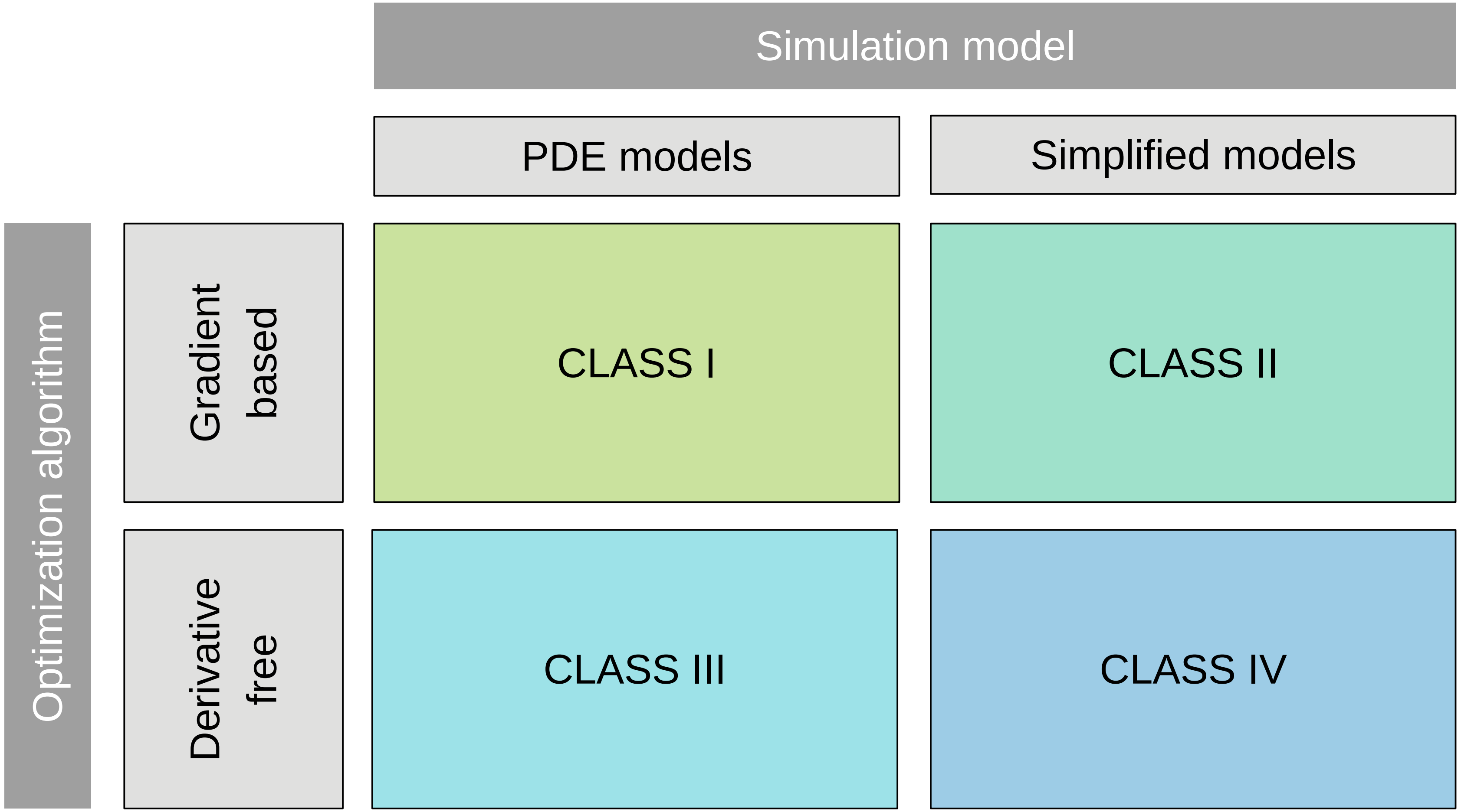
with analytical models

Publication 3: Optimization based on thermal GW conditions	Q2 a,b
Publication 4: Optimization based on hydraulic GW conditions	Q2 a,b,c

with PDE models

Publication 5: Adjoint-based optimization	Q2 a

Optimization approaches - overview



Comparison of optimization approaches (Publication [2])

Developed optimization approaches

		Simulation model	
		PDE models	Simplified models
Optimization algorithm	Gradient based	PDECO	Analytical I (thermal) Analytical II (hydraulic)
	Derivative free		

Newly developed optimization approaches (Publications [3],[4],[5])

Optimization approaches

Well placement optimization for multiple GWHP systems

Maximize spatial potential (extracted heat) or efficiency of GWHP systems
while meeting regulatory and technical conditions

PDECO approach

- PDE system for groundwater flow and heat transport
- FEM numerical simulation in Firedrake
- Gradient-based optimization using adjoints
- Optimal well locations
  - efficiency maximized
  - regulations satisfied
  - sizing predefined

Analytical approach (thermal)

- Analytic formulas for thermal plumes
- Linear advective heat transport model (LAHM)
- Integer linear programming (ILP)
- Optimal locations and number of wells
  - potential (extracted heat) maximized
  - regulations satisfied
  - sizing predefined

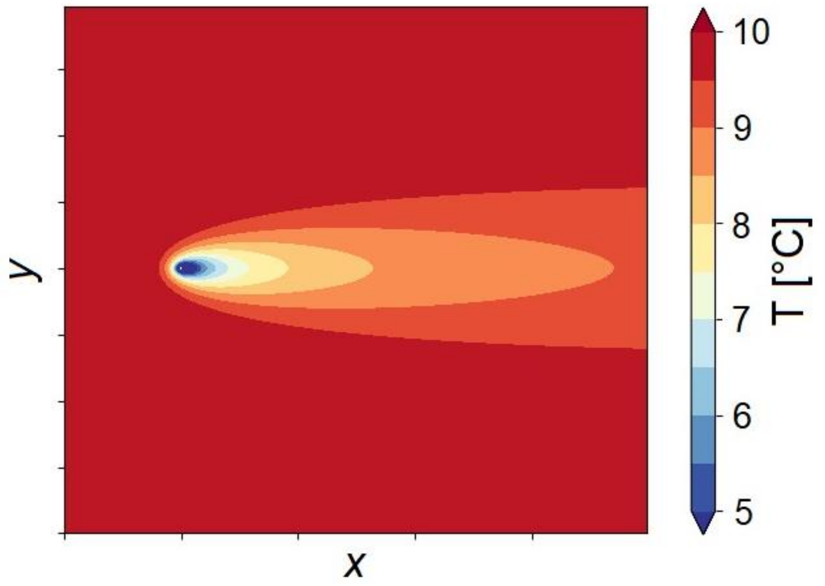
Linear advective heat transport model (LAHM)

$$\Delta T(\Delta x, \Delta y, t) = \frac{q \cdot \Delta T_{\text{inj}}}{4\varepsilon\, B\, v_a \sqrt{\pi \beta_{\text{T}}}} \exp\left(\frac{\Delta x - r}{2\,\beta_{\text{L}}}\right) \frac{1}{\sqrt{r}} \text{erfc}\left(\frac{r - v_a t/R}{2\sqrt{v_a \beta_{\text{L}} t/R}}\right)$$

[7]

$$r = \sqrt{\Delta x^2 + \Delta y^2 \frac{\beta_{\text{L}}}{\beta_{\text{T}}}}$$

ΔT	Groundwater temperature change/difference [K]
Δx, Δy	Spatial distance in x and y direction [m]
t	Time [s]
q	Pumping rate [m^3/s]
ΔT_{inj}	Difference between inlet and natural GW temperature [K]
ε	Porosity [-]
v_a	Seepage velocity [m/s]
B	Aquifer thickness [m]
β_{T}, β_{L}	Transverse/Longitudinal dispersivity [m]
r	Radial distance factor [m]
R	Retardation factor [-]



Thermal plume based on LAHM [3]

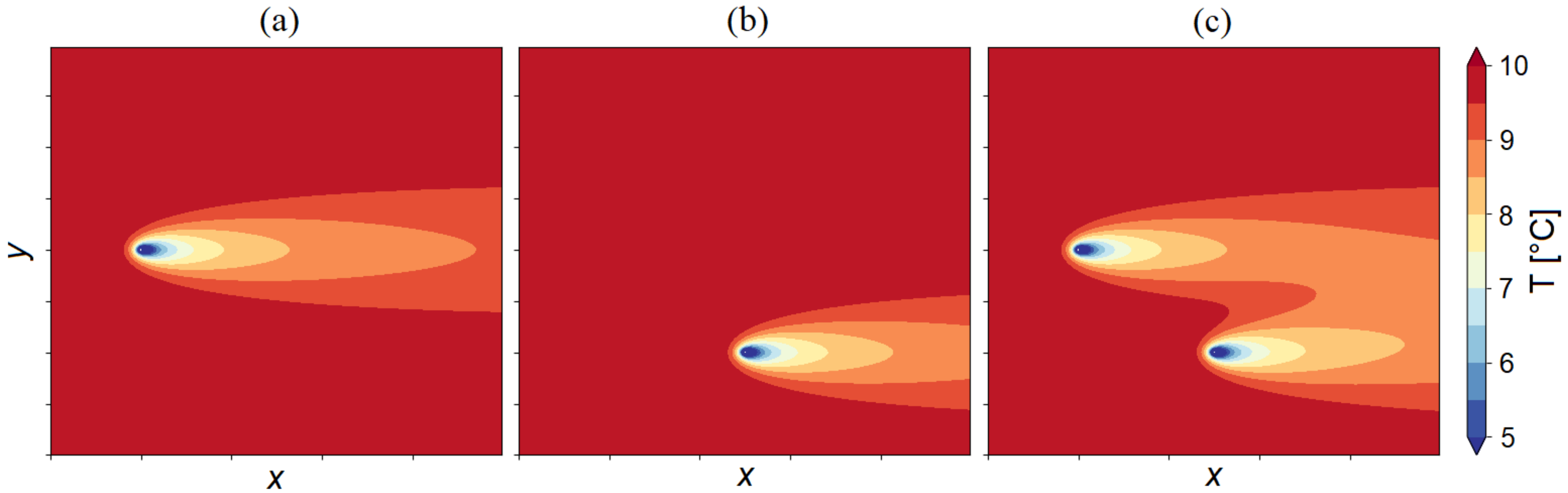
Extended LAHM

- Spatial superposition

$$\Delta T_{x,y}(t, q_{k=1\dots N}) = \sum_{k=1}^{N} \Delta T_k(x - x_k, y - y_k, t, q_k)$$

- Temporal superposition

$$\Delta T(\Delta x, \Delta y, t, q_{l=1\dots M}) = \sum_{l=1}^{M} \frac{(q_l - q_{l-1}) \cdot \Delta T_{\text{inj}}}{4\varepsilon\, B\, v_a \sqrt{\pi \beta_{\text{T}}}} \exp\left(\frac{\Delta x - r}{2\,\beta_{\text{L}}}\right) \frac{1}{\sqrt{r}} \text{erfc}\left(\frac{r - v_a(t_M - t_l)/R}{2\sqrt{v_a \beta_{\text{L}} (t_M - t_l)/R}}\right)$$



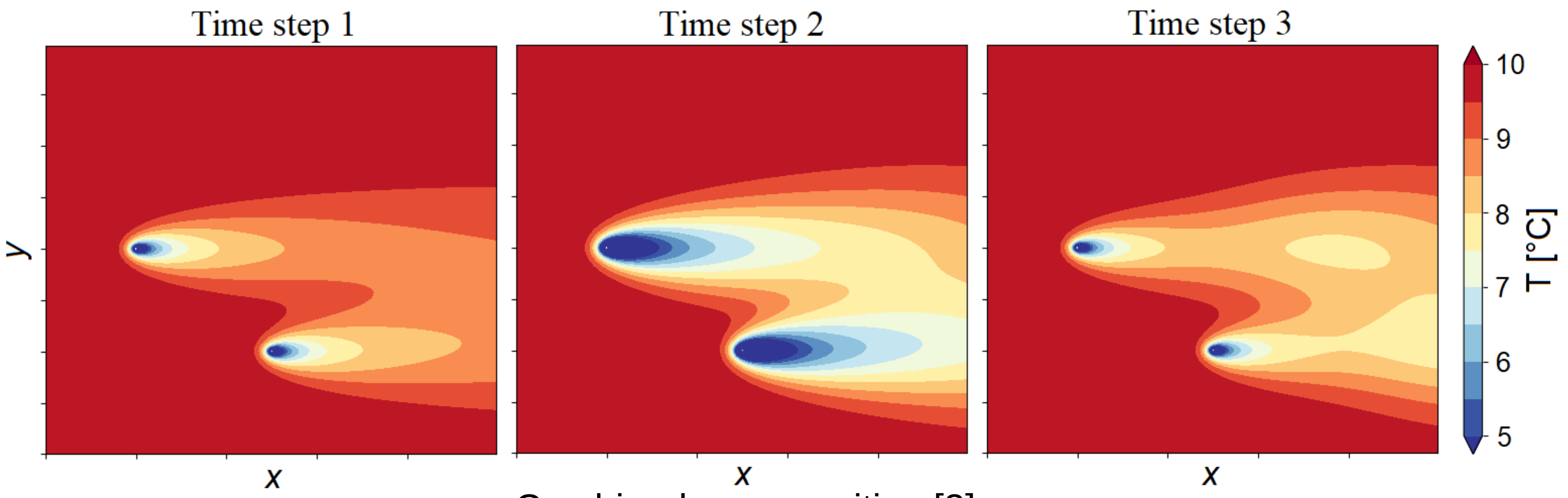
Spatial superposition [3]

Extended LAHM

- Combined superposition

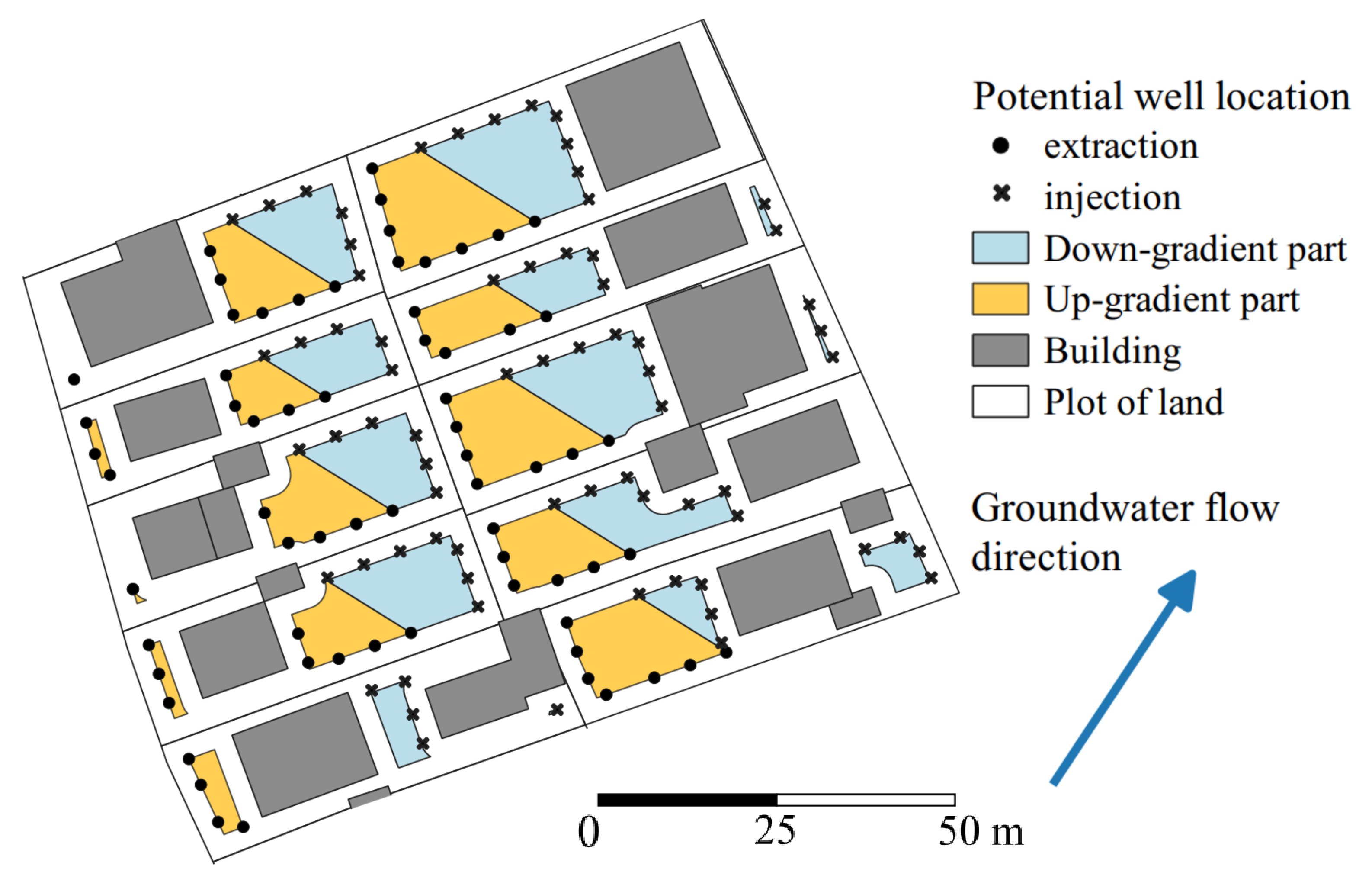
$$\Delta T_{x,y}(t, q_{1\dots N,1\dots M}) = \sum_{l=1}^{M}\sum_{k=1}^{N} q_{k,l}\,\omega_{k,l}^{t,x,y}(x - x_k, y - y_k)$$

$$\omega_{k,l}^{t,x,y}(x - x_k, y - y_k) = \frac{\Delta T_{\mathrm{inj}}}{4\varepsilon\, B\, v_a\sqrt{\pi\beta_{\mathrm{T}}}} \exp\left(\frac{\Delta x - r}{2\,\beta_{\mathrm{L}}}\right)\frac{1}{\sqrt{r}} \times\left[\mathrm{erfc}\left(\frac{r - v_a(t - t_{l-1})/R}{2\sqrt{v_a\beta_{\mathrm{L}}(t - t_{l-1})/R}}\right) - \mathrm{erfc}\left(\frac{r - v_a(t - t_l)/R}{2\sqrt{v_a\beta_{\mathrm{L}}(t - t_l)/R}}\right)\right]$$

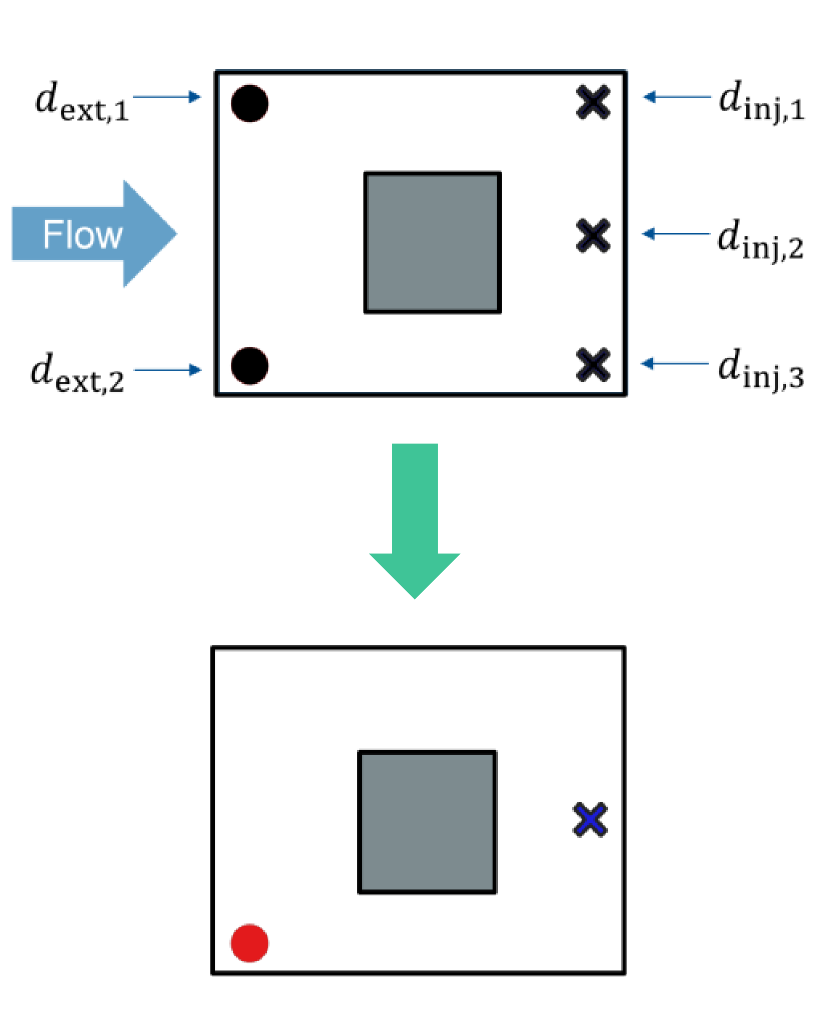


Combined superposition [3]

Analytical approach – well placement (selection)



Definition of potential well locations [3]



Well selection [3]

Analytical approach – optimization concept

- Pumping rate of each GWHP system (parcel p)

$$q_p = \sum_{i=1}^{N_{\text{inj}}^p} d_{\text{inj},i}\, q_i$$

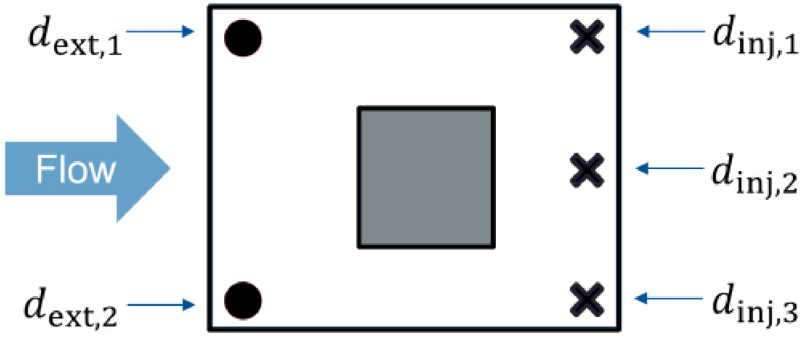
- Change of groundwater temperature (LAHM)

$$\Delta T_{x,y}(t, q_{1\ldots N,1\ldots M}) = \sum_{l=1}^{M} \sum_{k=1}^{N} d_{\text{inj},k}\, q_{k,l}\, \omega_{k,l}^{t,x,y}(x - x_k, y - y_k)$$

$$N = \sum_{p=1}^{N_p} N_{\text{inj}}^p$$

- Objective function

$$E_{\text{ext}} = \sum_{l=1}^{M} \sum_{k=1}^{N} d_{\text{inj},k}\, q_{k,l} \cdot \Delta T_{\text{inj}} \cdot C_{\text{w}} \cdot \Delta t$$



[3]

d_{inj}	Decision variables for injection wells
k	Counter for inj. wells
l	Counter for time steps
p	Counter for parcels
N	Total nr. of injection wells
N_p	Number of parcels
M	Number of time steps
E_{ext}	Heat extracted from groundwater [J]
C_{w}	Volumetric heat capacity of water [J/m^{3}K]
Δt	Time step length [s]

Analytical approach – optimization constraints

- Constraints about the number of installed wells in each plot

$$\sum_{i=1}^{N^p_{\text{inj}}} d_{\text{inj},i} \leq 1 \quad \forall p \in P$$

$$\sum_{j=1}^{N^p_{\text{ext}}} d_{\text{ext},j} \leq 1 \quad \forall p \in P$$

$$\sum_{i=1}^{N^p_{\text{inj}}} d_{\text{inj},i} = \sum_{j=1}^{N^p_{\text{ext}}} d_{\text{ext},j} \quad \forall p \in P$$

- Constraint about minimum distance between two installed wells

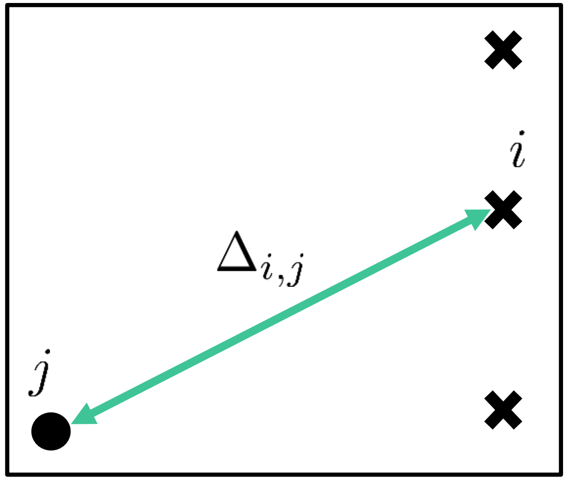
$$d_{\text{inj},i} + d_{\text{ext},j} \leq 1 \quad \text{if} \quad \Delta_{i,j} < \Delta_{\min} \quad \forall i \in \{1, ..., N^p_{\text{inj}}\}, \forall j \in \{1, ..., N^p_{\text{ext}}\}, \forall p \in P$$

- Constraint about negative thermal interference between wells

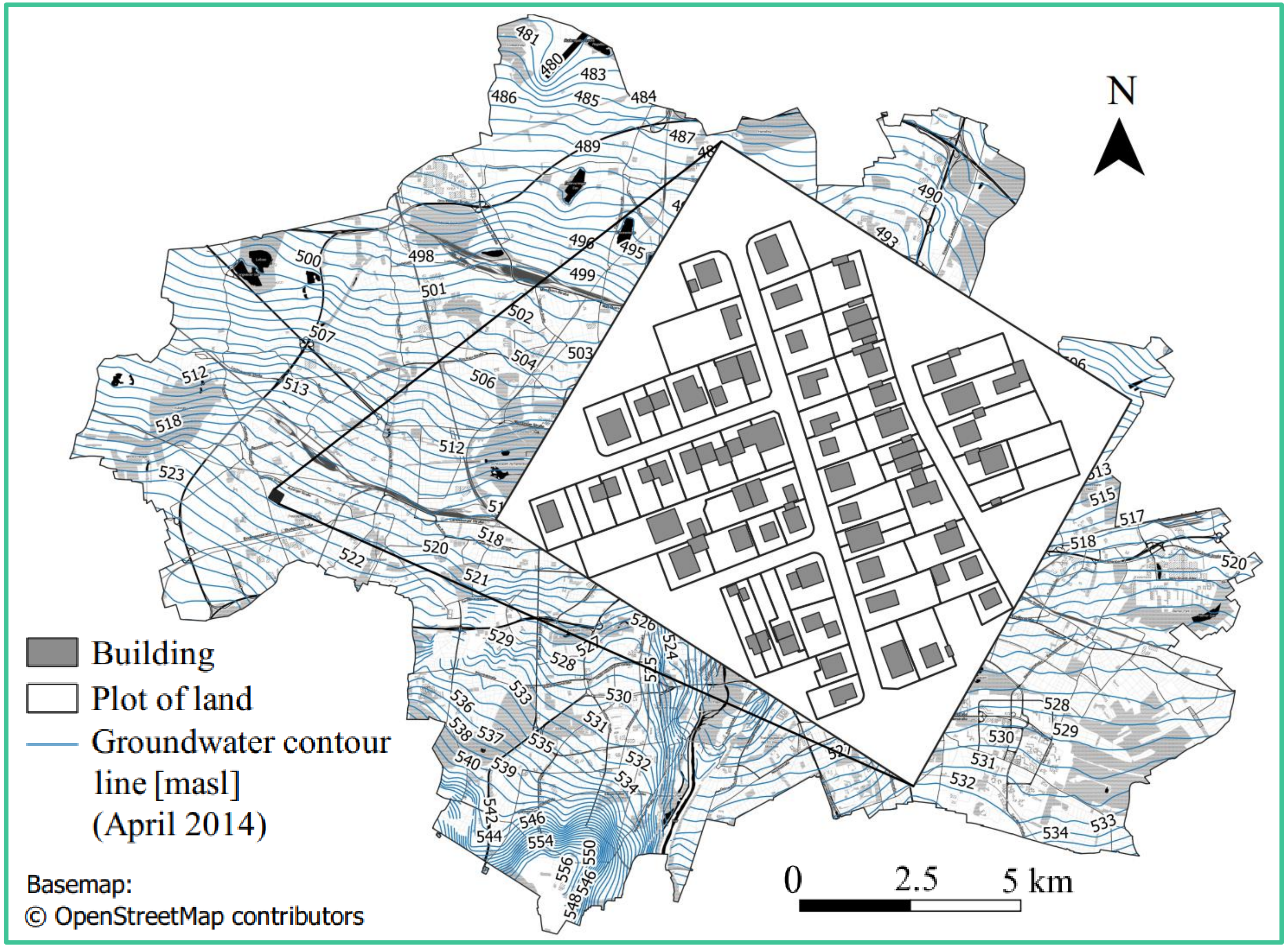
$$d_{\text{ext},j} \cdot \Delta T_{x_j,y_j}(t, \bar{q}) \leq \Delta T_{\max}$$

Linearized

$$\Delta T_{x_j,y_j}(t, \bar{q}) \leq (-m \cdot d_{\text{ext},j} + m + 1) \cdot \Delta T_{\max}$$



Analytical approach – case study

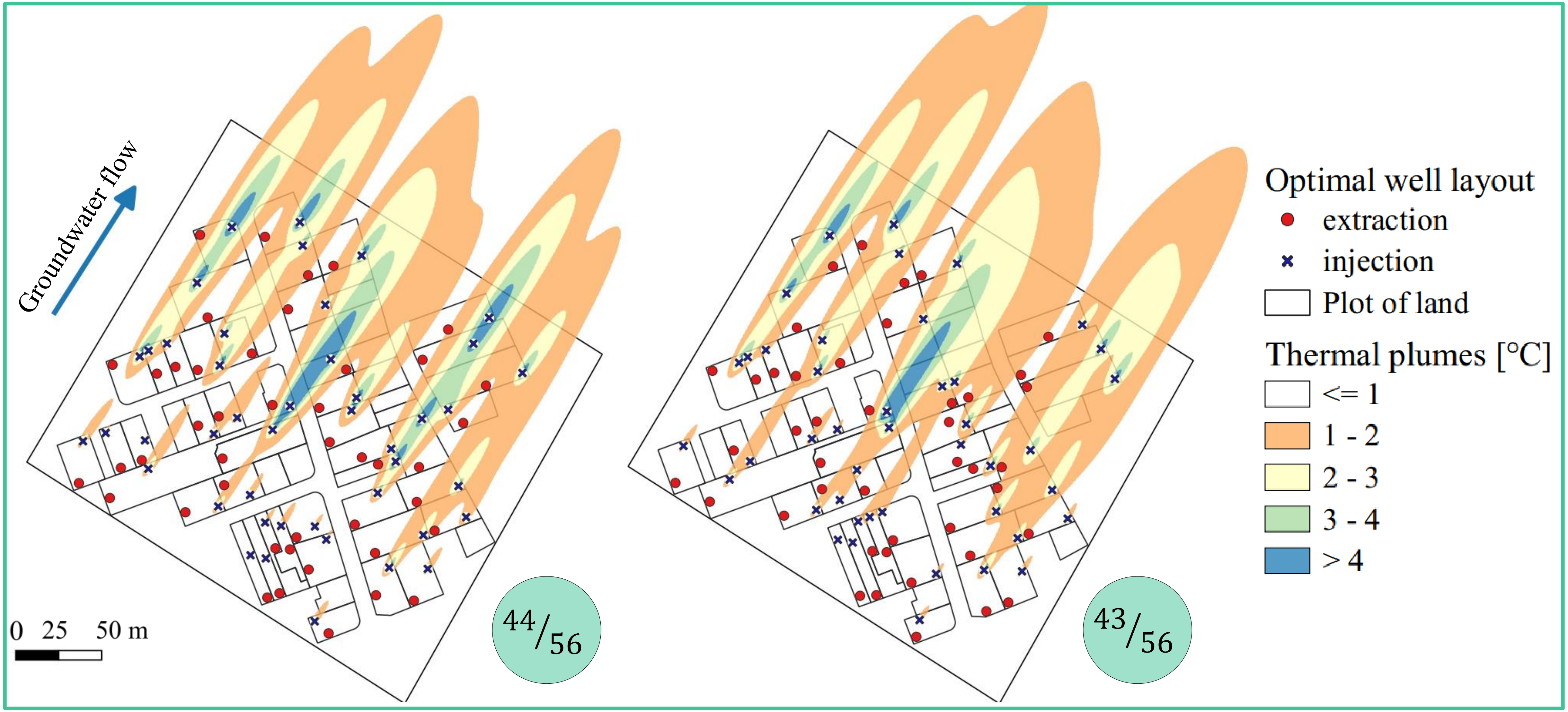


Optimization problem

- 56 plots of land
  (potential GWHP systems)
- Heating demand estimated using UrbanHeatPro [9]
- Place GWHPs and their wells
  - extracted heat maximized
  - regulations are satisfied

adapted from [3]

Analytical approach – results



‘Steady’ (winter) case [3]

Dynamic case (end of February) [3]

Optimization approaches

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PDECO – forward model (simulation)

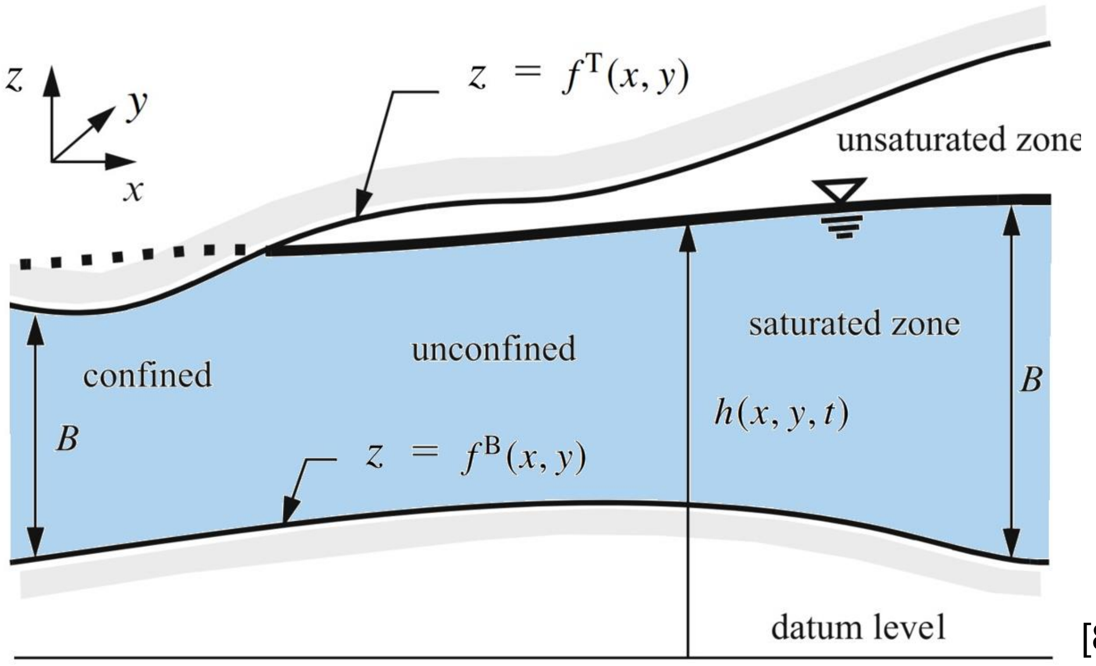
- 2D vertically averaged groundwater flow [8]:

$$(BS_0 + \varepsilon_e)\frac{\partial h}{\partial t} + \nabla \cdot (B\mathbf{q}) = \overline{Q}$$

$$\mathbf{q} = -\mathbf{K} \cdot \nabla h$$

$$B = h - f^{\mathrm{B}}$$

$$\overline{Q} = \sum_{i=1}^{N} q_i(t)\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{inj}}) - q_i(t)\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{ext}})$$



[8]

- 2D vertically averaged heat transport in aquifer [8]:

$$BC_{\mathrm{m}}\frac{\partial T}{\partial t} + BC_{\mathrm{w}}\mathbf{q} \cdot \nabla T - \nabla \cdot (B\mathbf{\Lambda} \cdot \nabla T) = \overline{P}_{\mathrm{t}}$$

$$\overline{P}_{\mathrm{t}} = \sum_{i=1}^{N} q_i(t)C_{\mathrm{w}}[T(\mathbf{x}_i^{\mathrm{inj}}, t) - T]\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{inj}})$$

h	hydraulic head $[\mathrm{m}]$
$\mathbf{q}$	Darcy velocity $[\mathrm{m/s}]$
T	groundwater temperature $[\mathrm{K}]$
$\overline{Q}$	depth integrated liquid source term $[\mathrm{m/s}]$
$\overline{P}_{\mathrm{t}}$	depth integrated heat source term $[\mathrm{W/m^2}]$

PDECO – optimization concept

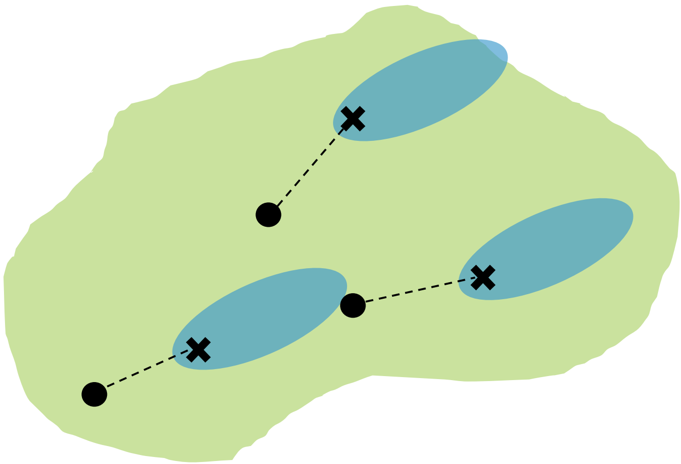
- Steady state PDE system:

$$\nabla \cdot (B\mathbf{q}) = \overline{Q}$$

$$\mathbf{q} = -\mathbf{K} \cdot \nabla h$$

$$BC_{\mathrm{w}}\mathbf{q} \cdot \nabla T - \nabla \cdot (B\mathbf{\Lambda} \cdot \nabla T) = \overline{P}_{\mathrm{t}}$$

Solved sequentially



- Control variables:

$$\boldsymbol{m} = [x_1^{\mathrm{ext}}, \dots, x_N^{\mathrm{ext}}, y_1^{\mathrm{ext}}, \dots, y_N^{\mathrm{ext}}, x_1^{\mathrm{inj}}, \dots, x_N^{\mathrm{inj}}, y_1^{\mathrm{inj}}, \dots, y_N^{\mathrm{inj}}]^T$$

- Functional of interest:

$$J_0(\boldsymbol{u}, \boldsymbol{m}) = \sum_{i=1}^{N} T(\mathbf{x}_i^{\mathrm{ext}}) = \sum_{i=1}^{N} \int_{\Omega} T(\mathbf{x}) \cdot \delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{ext}})\, \mathrm{d}\Omega$$

Optimization problem

- Heating demand / pump rates predefined
- Place GWHP wells
  - efficiency maximized
  - regulations are satisfied

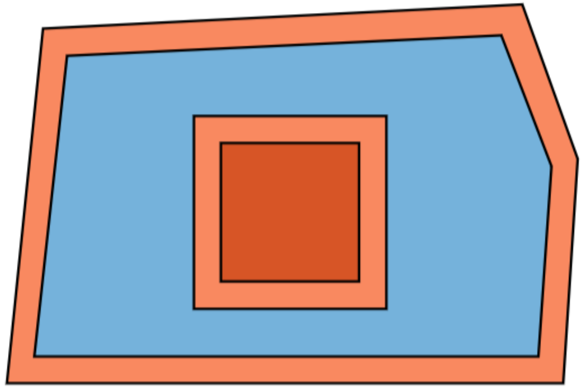
PDECO - optimization constraints

- Wells must be inside parcels

$$\mathbf{x}_i^{\text{ext}}, \mathbf{x}_i^{\text{inj}} \in D_i \quad \forall i \in \{1, ..., N\} \;\Rightarrow\; \mathbf{A}\boldsymbol{m} \leq \mathbf{b}$$

- Minimum distance between two installed wells

$$d(\mathbf{x}_i^{\text{ext}}, \mathbf{x}_i^{\text{inj}})^2 = (x_i^{\text{ext}} - x_i^{\text{inj}})^2 + (y_i^{\text{ext}} - y_i^{\text{inj}})^2 \geq d_{\text{min}}^2$$



[5]

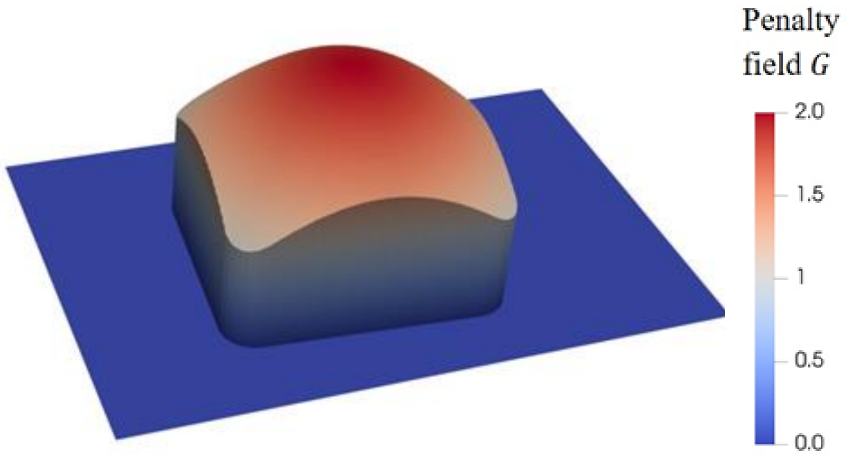
- Wells cannot be in restricted areas

$$\mathbf{x}_i^{\text{ext}}, \mathbf{x}_i^{\text{inj}} \notin R_i^j \quad \forall i \in \{1, ..., N\}, \forall j \in \{1, ..., r_i\}$$

$$P_R = \alpha \cdot \sum_{i=1}^{N} \left(p(\mathbf{x}_i^{\text{ext}}) + p(\mathbf{x}_i^{\text{inj}}) \right)$$

$$p(\mathbf{x}_i) = \int_\Omega G(\mathbf{x}) \cdot \delta(\mathbf{x} - \mathbf{x}_i) \, \mathrm{d}\Omega$$

$$G(\mathbf{x}) = \begin{cases} 0 & \text{if} \quad \mathbf{x} \notin R_i^j \quad \forall i \in \{1, ..., N\}, \forall j \in \{1, ..., r_i\} \\ 1 + \cos\left[\frac{d(\mathbf{x}, \mathbf{x}_{i,j}^{\text{P}})}{r_{i,j}^{\text{P}}} \cdot \frac{\pi}{2} \right] & \text{if} \quad \mathbf{x} \in R_i^j \end{cases}$$



[5]

PDECO - Dirac functions

Dirac delta functions problematic for gradient based optimization

→ Replace them with smooth ‘bump’ functions

- Using exponential terms

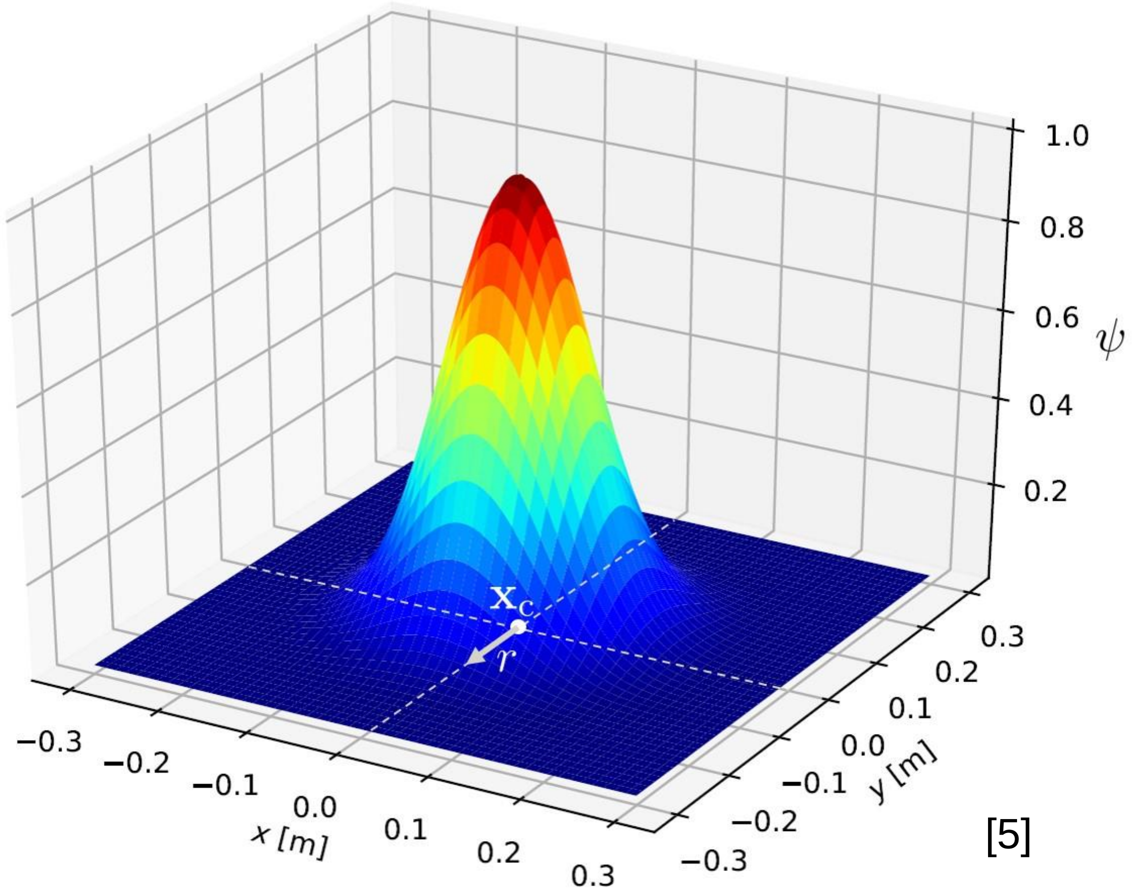
$$\delta(\mathbf{x}-\mathbf{x}_i)=\delta(x-x_i)\delta(y-y_i)$$

$$\delta(\mathbf{x}-\mathbf{x}_i)\rightarrow \mathrm{e}^{-\frac{(x-x_i)^2+(y-y_i)^2}{r^2}}=\psi(x,y,x_i,y_i)$$

- Normalize the values with the volume

$$V=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi(x,y,x_i,y_i)dxdy=r^2\pi$$

r : Radius of wells



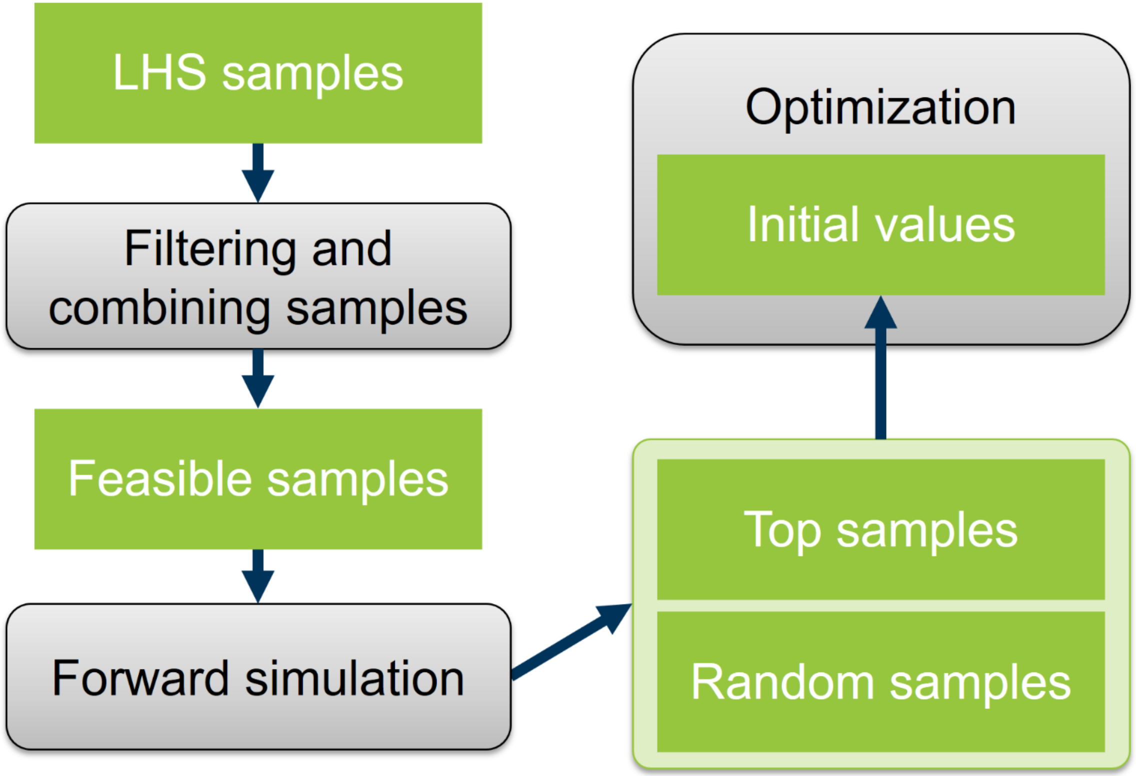
[5]

PDECO - problem formulation and initialization

- Reduced-space problem

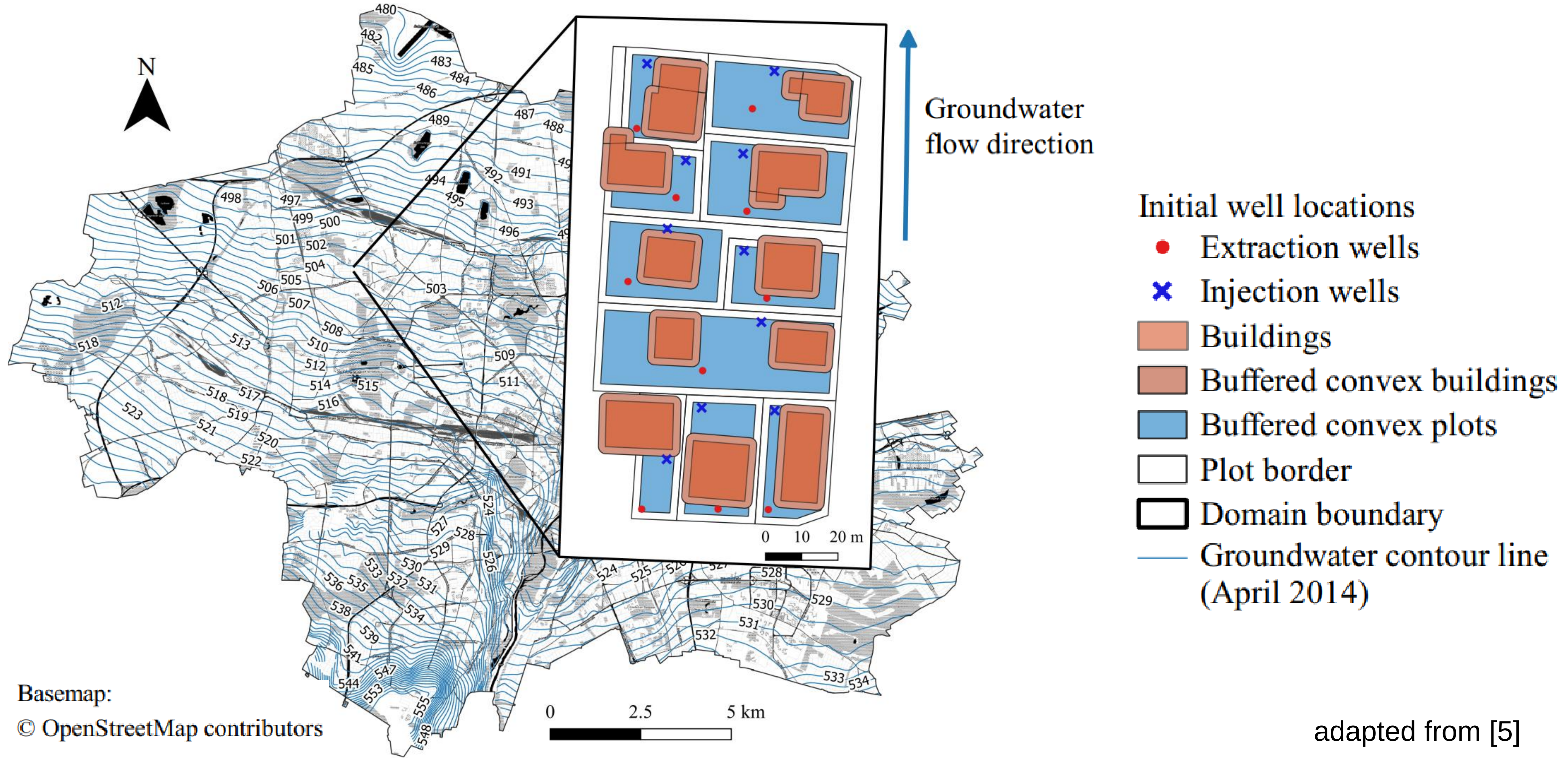
$$\begin{aligned} \min_{\boldsymbol{m}} \quad & -\hat{J}_0(\boldsymbol{m}) + P_R(\boldsymbol{m}) \\ \text{subject to} \quad & g_1(\boldsymbol{m}) \leq 0 \\ & g_2(\boldsymbol{m}) \leq 0 \end{aligned}$$

$\boldsymbol{m}$	control variables
$\hat{J}_0$	reduced functional of interest
P_R	penalty term
g_1	linear inequality constraints
g_2	minimum well distance constraints



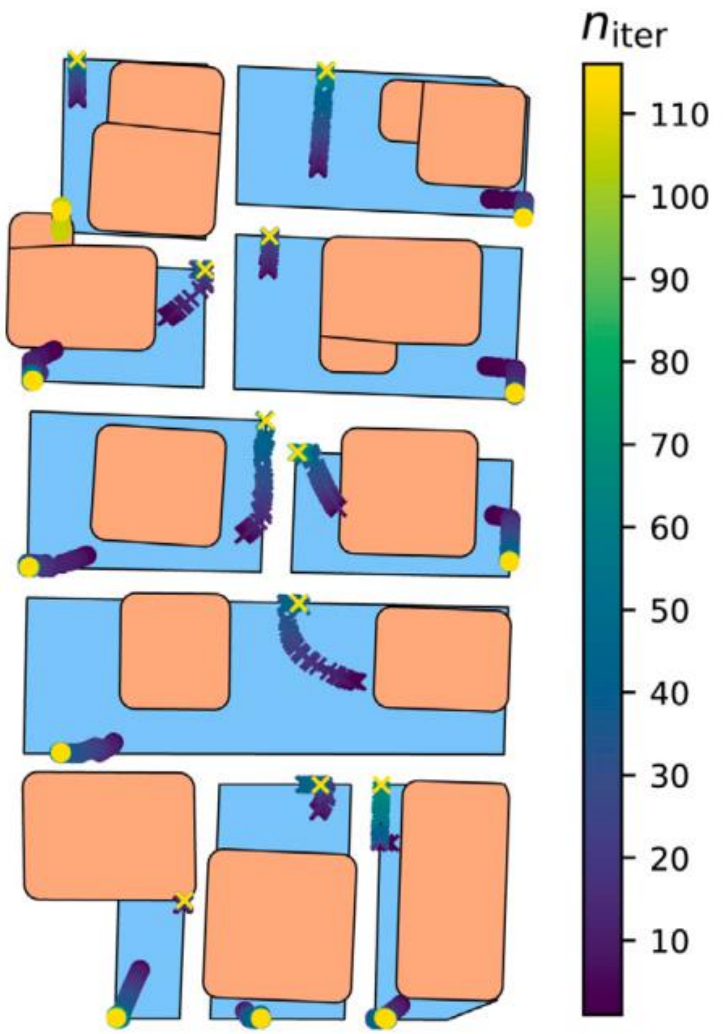
Multi-start initialization strategy [5]

PDECO – case study

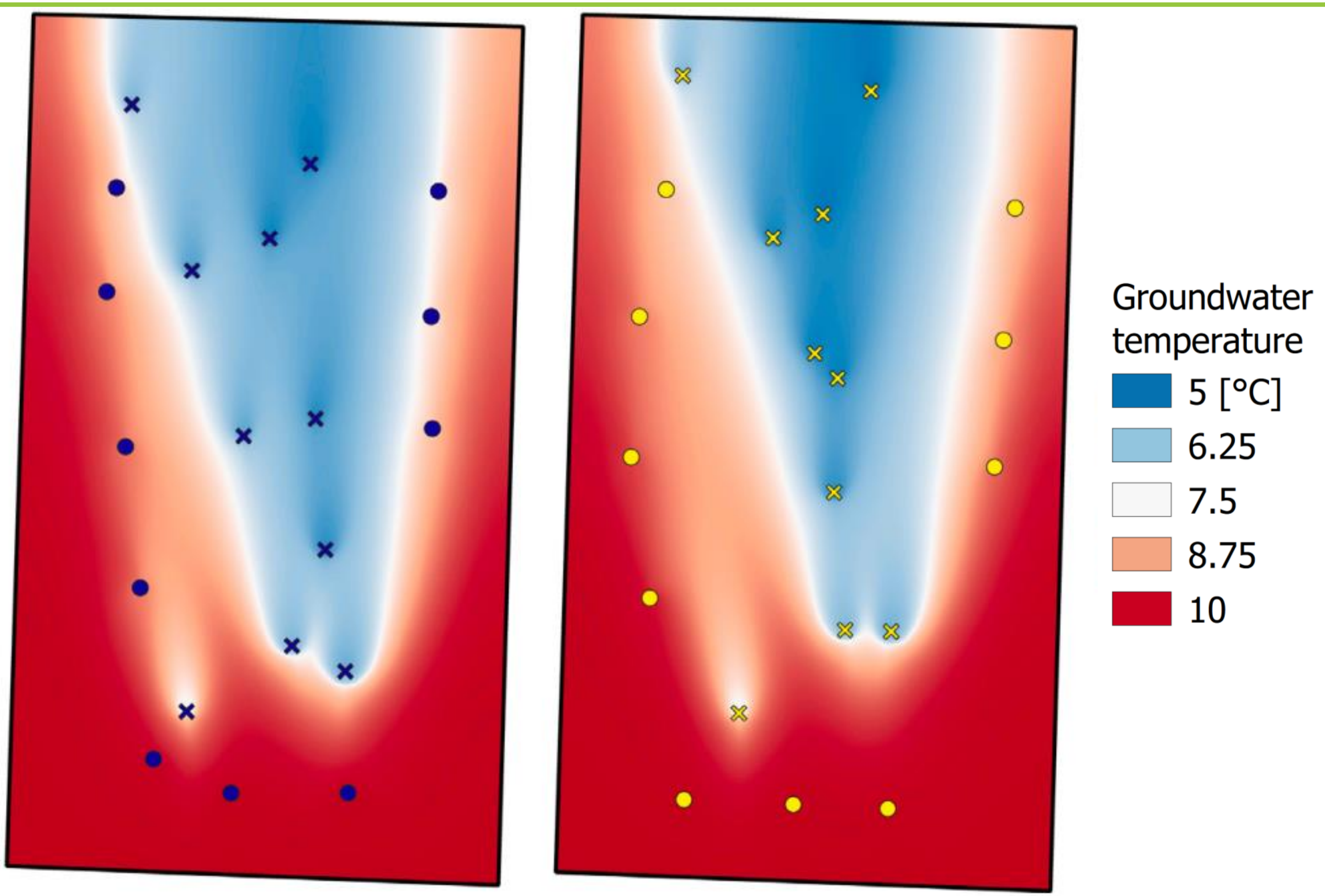


adapted from [5]

PDECO – results



Well positions during optimization [5]



Initial and final GW temperature fields and well layouts [5]

Conclusion

Main contribution

Developed and evaluated novel approaches for the optimization of GWHP systems that are efficient and tailored to specific applications

Research questions

1. What are the viable approaches for the optimization of GWHP systems, and how do they compare in terms of efficiency and applicability?
2. How to optimize the design and operation of GWHP systems?
   a) well locations?
   b) number of GWHP wells?
   c) sizing (pumping rates) of GWHP wells?
3. How to effectively integrate GWHPs into energy system optimization models?

Publications

2	
3	Analytical (thermal)
4	Analytical (hydraulic)
5	PDECO
1	

Outlook

Future work

- **Enhancement** of **analytical models** used in optimization approaches → improvement of the approaches
- **Combined** (**thermal** and **hydraulic**) analytical approach
- Extension of the **PDECO** approach to:
  - **Time-dependent** cases
  - **3D** subsurface models
- Integration of **uncertainties** (underground **parameters**) into optimization
- Integration of **economic parameters** into optimization
- Extension to **other applications**: ATES, GSHP, BTES, etc.

Potential methodological improvements

New applications

List of publications

[1] Halilovic, S., Odersky, L. and Hamacher, T., 2022. Integration of groundwater heat pumps into energy system optimization models. *Energy*, 238, p.121607. URL: https://doi.org/10.1016/j.energy.2021.121607

[2] Halilovic, S., Böttcher, F., Zosseder, K. and Hamacher, T., 2023. Optimization approaches for the design and operation of open-loop shallow geothermal systems. *Advances in Geosciences*, 62. URL: https://doi.org/10.5194/adgeo-62-57-2023

[3] Halilovic, S., Böttcher, F., Zosseder, K. and Hamacher, T., 2023. Optimizing the spatial arrangement of groundwater heat pumps and their well locations. *Renewable Energy*, 217, p.119148. URL: https://doi.org/10.1016/j.renene.2023.119148

[4] Halilovic, S., Böttcher, F., Zosseder, K. and Hamacher, T., 2023. Spatial analysis of thermal groundwater use based on optimal sizing and placement of well doublets. URL: https://doi.org/10.48550/arXiv.2311.01816

[5] Halilovic, S., Böttcher, F., Kramer, S.C., Piggott, M.D., Zosseder, K. and Hamacher, T., 2022. Well layout optimization for groundwater heat pump systems using the adjoint approach. *Energy Conversion and Management*, 268, p.116033. URL: https://doi.org/10.1016/j.enconman.2022.116033

Other literature

[6] Modified from:
D. Banks, An introduction to thermogeology: ground source heating and cooling. John Wiley & Sons, 2012.

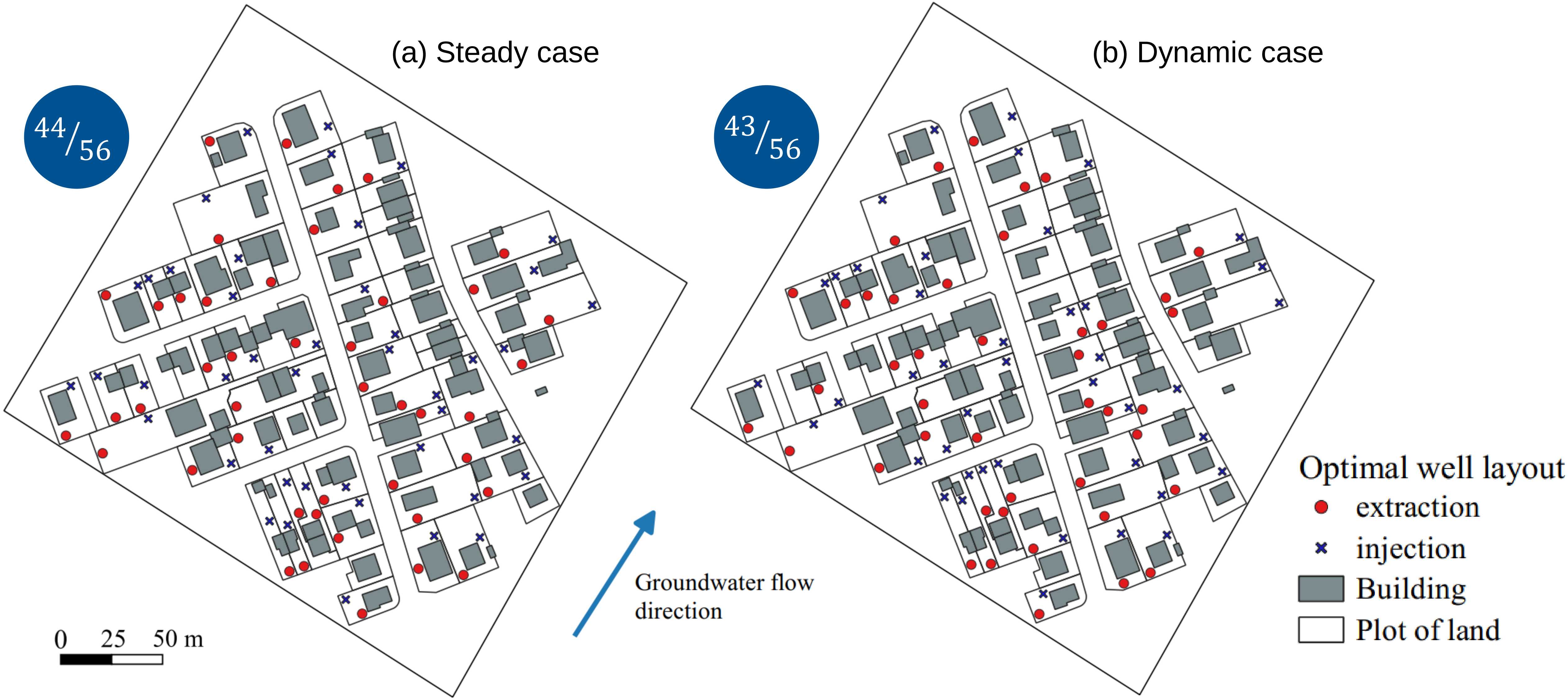
[7] W. Kinzelbach, Numerische Methoden Zur Modellierung Des Transports Von Schadstoffen Im Grundwasser, Oldenbourg, 1987.

[8] H.-J. G. Diersch, FEFLOW. Berlin, Heidelberg: Springer Berlin Heidelberg, 2014.

[9] A. Molar-Cruz, UrbanHeatPro, https://github.com/tum-ens/UrbanHeatPro, 2020.

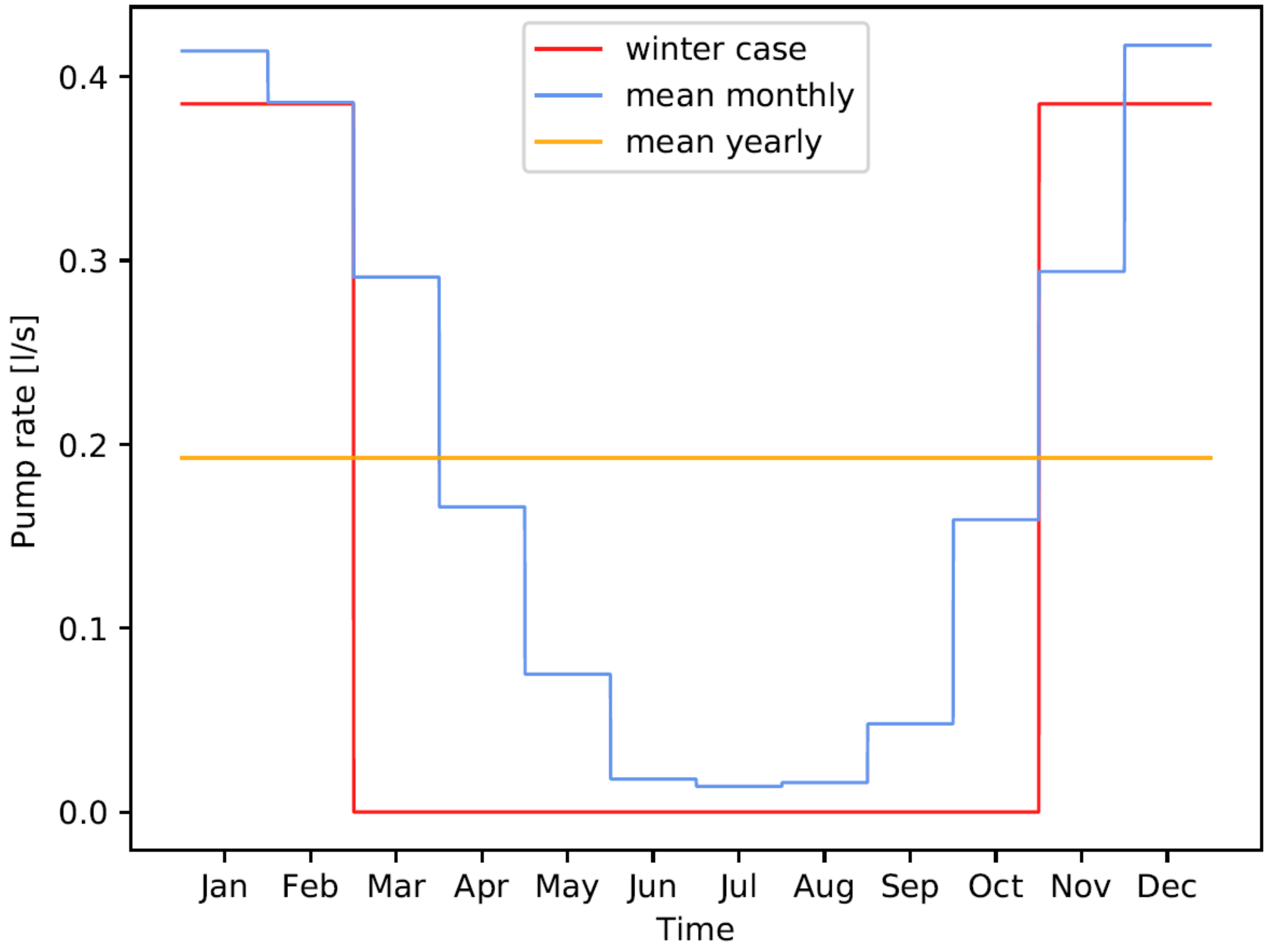
Backup

Analytical approach – Results



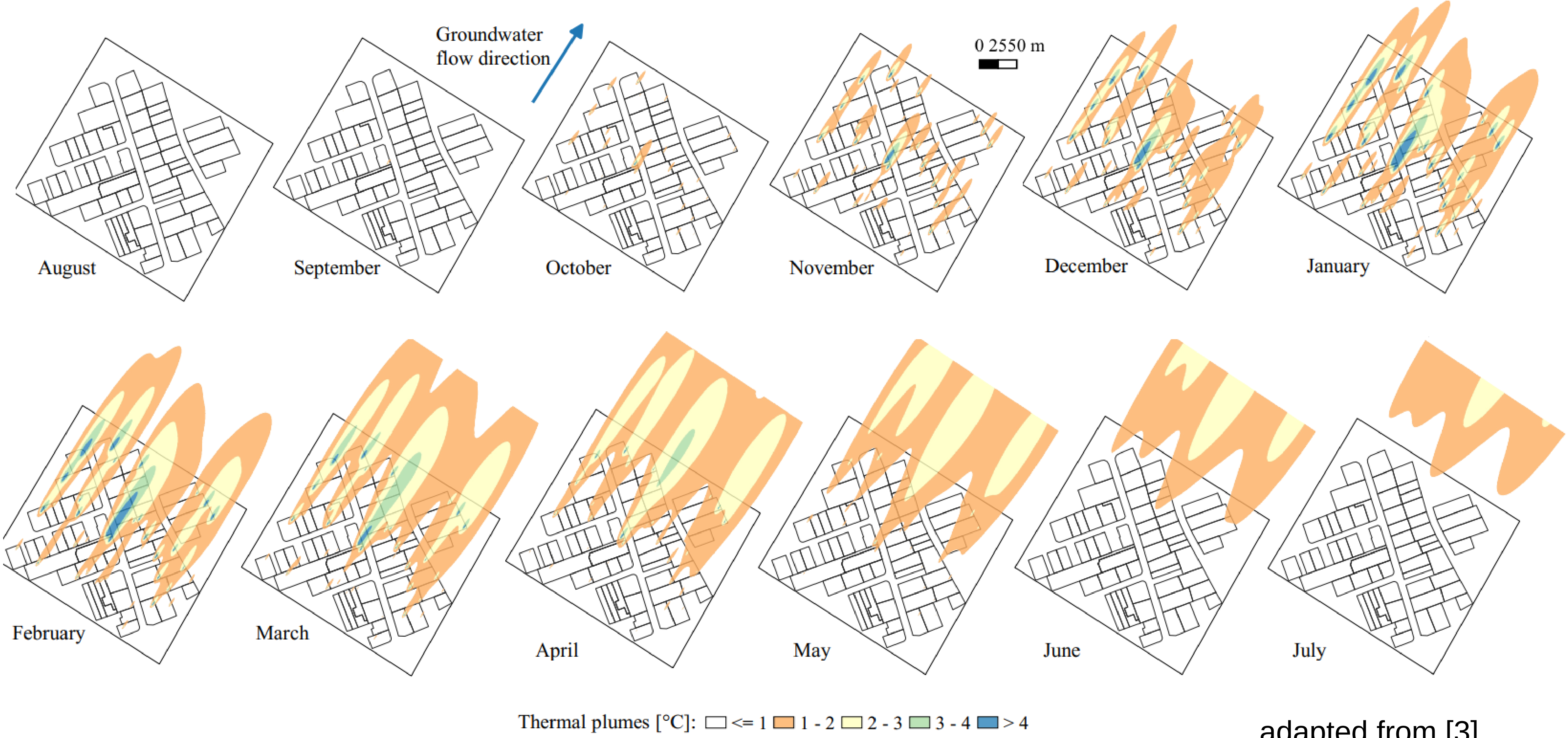
Optimal well layouts (adapted from [3])

Analytical approach



Optimization scenarios (cases) [3]

Analytical approach – Results (dynamic case)



adapted from [3]

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$$\mathbf{q} = -\mathbf{K} \cdot \nabla h$$

$$B = h - f^{\mathrm{B}}$$

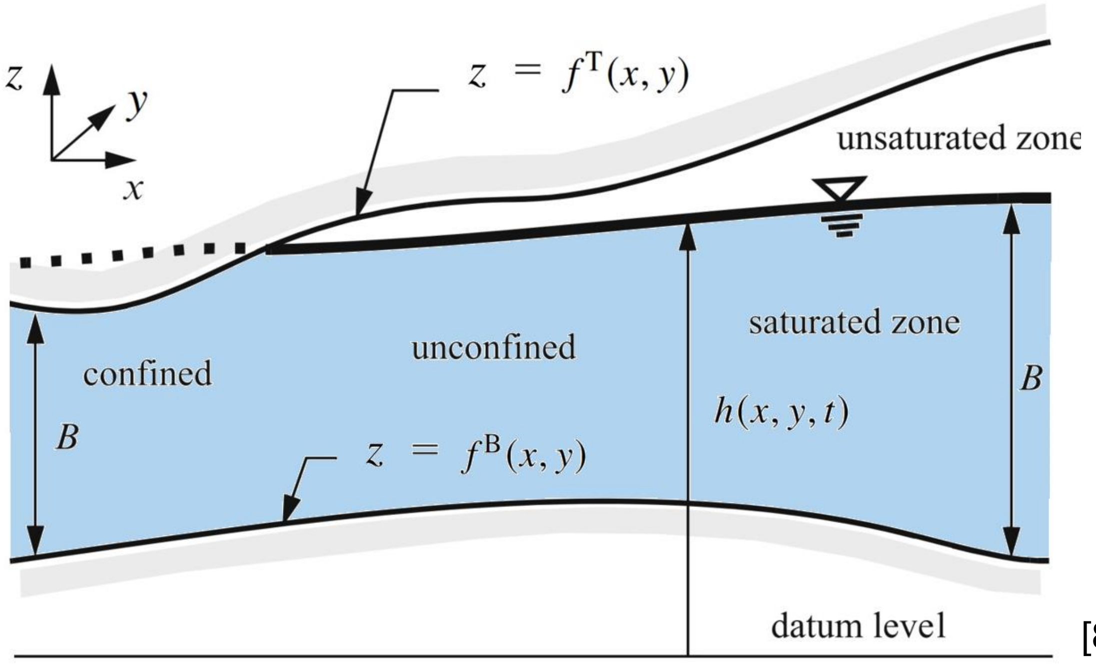
$$\overline{Q} = \sum_{i=1}^{N} q_i(t)\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{inj}}) - q_i(t)\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{ext}})$$

- 2D vertically averaged heat transport in aquifer [8]:

$$BC_{\mathrm{m}}\frac{\partial T}{\partial t} + BC_{\mathrm{w}}\mathbf{q} \cdot \nabla T - \nabla \cdot (B\boldsymbol{\Lambda} \cdot \nabla T) = \overline{P}_{\mathrm{t}}$$

$$\overline{P}_{\mathrm{t}} = \sum_{i=1}^{N} q_i(t)C_{\mathrm{w}}[T(\mathbf{x}_i^{\mathrm{inj}}, t) - T]\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{inj}})$$

h	hydraulic head [m]
$\mathbf{q}$	Darcy velocity [m/s]
T	groundwater temperature [K]
$\overline{Q}$	depth integrated liquid source term [m/s]
$\overline{P}_{\mathrm{t}}$	depth integrated heat source term [W/m^2]



[8]

- Tensor of hydrodynamic thermal dispersion:

$$\boldsymbol{\Lambda} = \boldsymbol{\Lambda}_0 + \boldsymbol{\Lambda}_0^s + \rho c\mathbf{D}_{\mathrm{mech}}$$

$$\boldsymbol{\Lambda}_0 = \varepsilon s \Lambda \mathbf{I}$$

$$\boldsymbol{\Lambda}_0^s = (1-\varepsilon)\Lambda^s\mathbf{I}$$

$$\mathbf{D}_{\mathrm{mech}} = \beta_T\|\mathbf{q}\|\mathbf{I} + (\beta_L - \beta_T)\frac{\mathbf{q}\otimes\mathbf{q}}{\|\mathbf{q}\|}$$

[8]

PDECO – forward model (simulation)

- Weak variational formulation for 2D flow [8]:

$$\int_\Omega w(BS_0 + \varepsilon_e)\frac{\partial h}{\partial t}d\Omega + \int_\Omega \nabla w \cdot (B\mathbf{K} \cdot \nabla h)d\Omega - \int_\Omega w\overline{Q}d\Omega - \int_\Gamma w(B\mathbf{K} \cdot \nabla h) \cdot \mathbf{n}d\Gamma = 0, \quad \forall w \in H_0^1(\Omega)$$

$$\int_\Omega w(BS_0 + \varepsilon_e)\frac{\partial h}{\partial t}d\Omega + \int_\Omega \nabla w \cdot (B\mathbf{K} \cdot \nabla h)d\Omega - \int_\Omega w\overline{Q}d\Omega + \int_{\Gamma_\mathrm{N}} w(Bq_h)d\Gamma = 0, \quad \forall w \in H_0^1(\Omega)$$

PDECO - problem formulation

- Reduced-space approach

$$\min_{\boldsymbol{u},\boldsymbol{m}} f(\boldsymbol{u},\boldsymbol{m})$$
$$\text{s.t. } \boldsymbol{g}(\boldsymbol{u},\boldsymbol{m}) \le \boldsymbol{0}$$
$$\boldsymbol{h}(\boldsymbol{u},\boldsymbol{m}) = \boldsymbol{0}$$

$\boldsymbol{u}$ state variables
$\boldsymbol{m}$ control variables

$$\min_{\boldsymbol{u},\boldsymbol{m}} f(\boldsymbol{u},\boldsymbol{m})$$
$$\text{s.t. } g_i(\boldsymbol{u},\boldsymbol{m}) \le 0, \quad i = 1, \dots, n_i$$
$$h_j(\boldsymbol{u},\boldsymbol{m}) = 0, \quad j = 1, \dots, n_e$$
$$R(\boldsymbol{u},\boldsymbol{m}) = 0 \quad \to \boldsymbol{u} = S(\boldsymbol{m})$$

$$\min_{\boldsymbol{m}} f(S(\boldsymbol{m}),\boldsymbol{m})$$
$$\text{s.t. } g_i(S(\boldsymbol{m}),\boldsymbol{m}) \le 0$$
$$h_j(S(\boldsymbol{m}),\boldsymbol{m}) = 0$$

- Regulation about negative interference (state constraint):

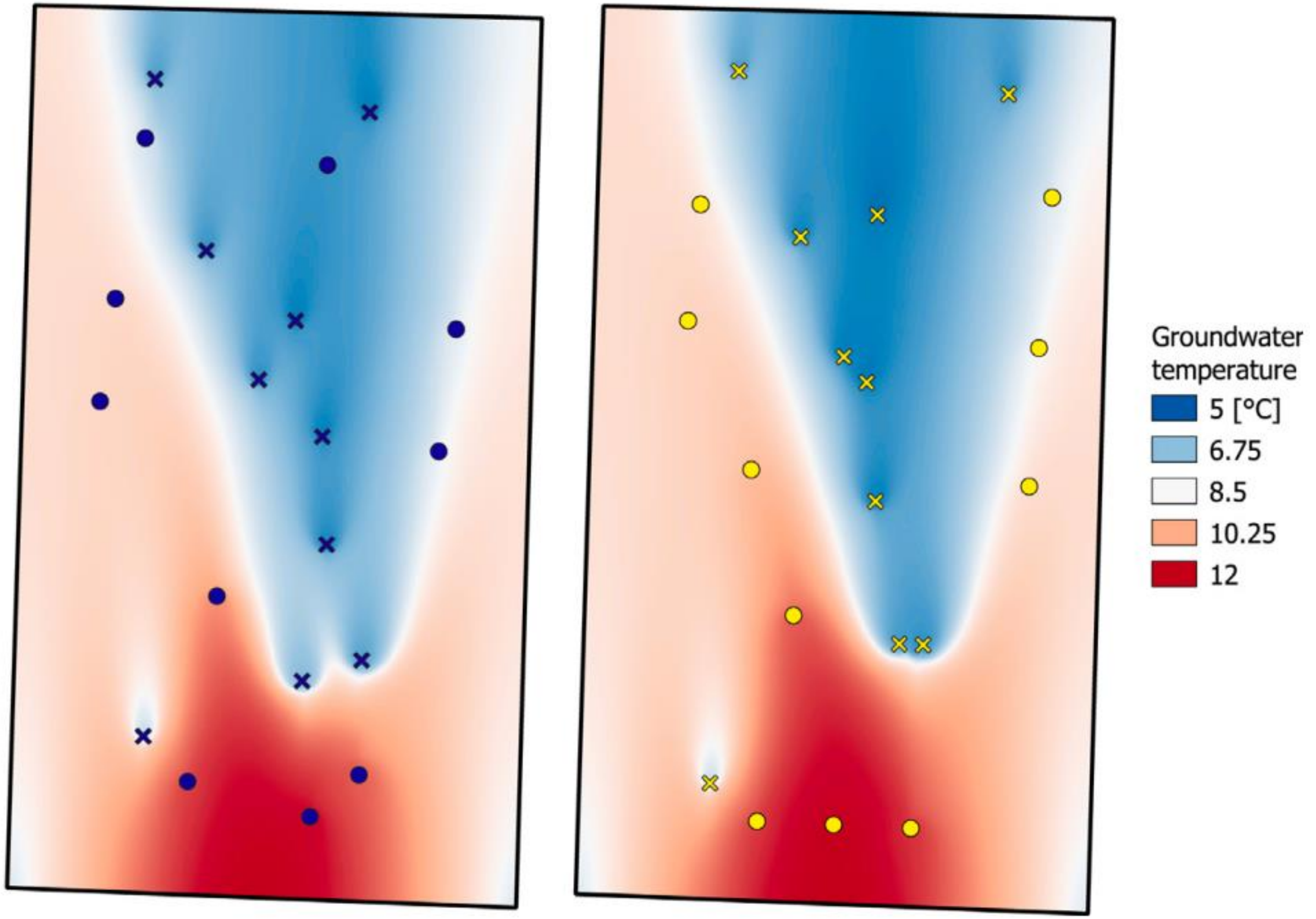
$$T_{\mathrm{n}}(\mathbf{x}_i^{\mathrm{ext}}, t) - T(\mathbf{x}_i^{\mathrm{ext}}, t) \le \mathrm{T}_1^{\mathrm{diff}} \quad \forall t \quad \forall i = 1, \dots, N$$

$$(T_{\mathrm{n}}(\mathbf{x}, t) - \mathrm{T}_1^{\mathrm{diff}})\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{ext}}) \le T(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{x}_i^{\mathrm{ext}}) \quad \forall t \quad \forall i = 1, \dots, N$$

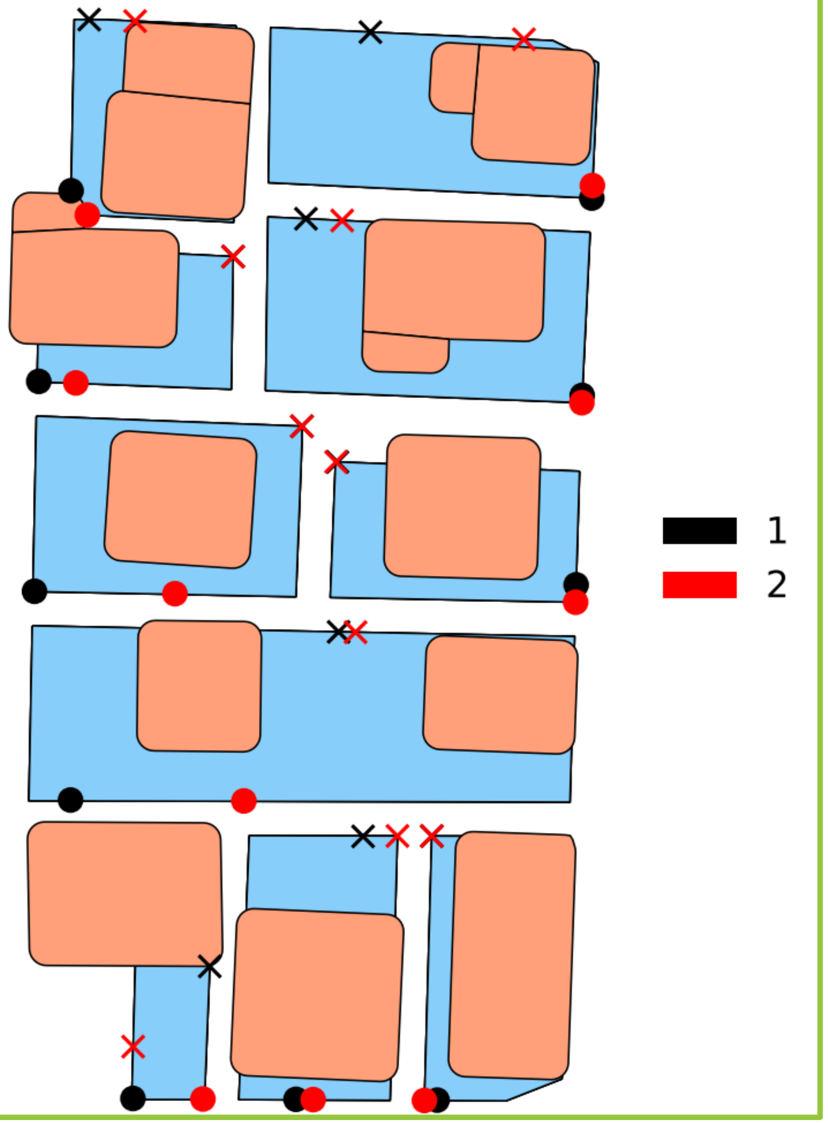
- Moreau-Yosida type of regularization:

$$y_a \le y \quad \text{in} \quad \Omega \quad \Rightarrow \quad \frac{\gamma}{2}\int_{\Omega} (\max\{0, y_a - y\})^2 \, dx$$

PDECO – results



Initial and final GW temperature fields and well layouts [3]



Optimal well layouts – Scenario 1 & 2 [3]

PDECO – optimization progress