<Paper review>

Evaluating MT3DMS for heat transport simulation of closed geothermal systems

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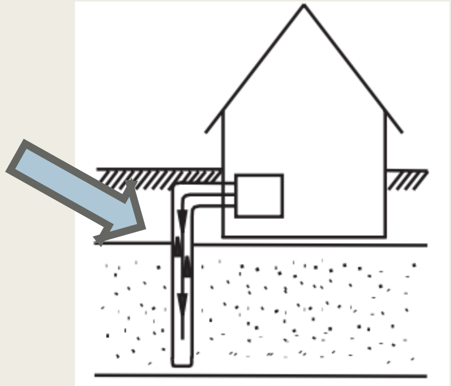
Outline

- Introduction
- Method
- Model setting
- Results and discussion
- Conclusions
- Future work

Introduction

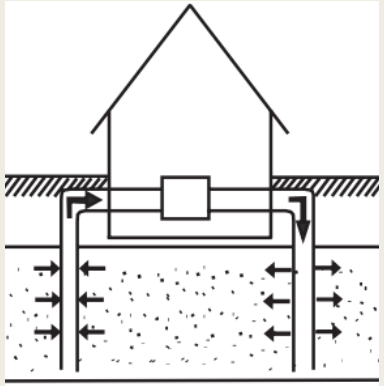
- MT3DMS (Modular Transport, 3-Dimensional, Multi-Species model) is a widely used program for simulation of solute transport in porous media. (Zheng and Wang,1999)
- Since the governing equations for solute transport are mathematically identical to those for heat transport, this program appears also applicable to simulation of thermal transport phenomena in saturated aquifers.
- Using MT3DMS for heat transport in aquifers has limitations, because it is decoupled from the flow model.
- MT3DMS uses the flow regime predicted by flow simulators such as MODFLOW (Harbaugh et al. 2000)
- So, evaluating the utility of MT3DMS for shallow geothermal systems would be discuss in this research.

Introduction



Ground source heat pump (GSHP) system

- a pair of heat exchangers
- the fluid never mixing with the groundwater



Ground water heat pump (GWHP) system

- production and injection wells
- groundwater is directly brought to the surface

Method (governing equations)

Solute transport in transient groundwater flow systems solved by MT3DMS (Zheng and Wang 1999)

$$\left(1+\frac{\rho_b K_d}{n}\right)\frac{\partial C^k}{\partial t} = \nabla \cdot [(D_m + \alpha v_a)\nabla C^k] - \nabla \cdot \left(v_a C^k\right) + \frac{q_{ss} C_{ss}}{n}$$

Retardation factor * transient term   Dispersion & advection   Source & sink

symbol	unit	variable
ρ_b	kg/m^3	Dry bulk density ρb = (1 − n)ρs
K_d	m^3/kg	Distribution coefficient
C^k	kg/m^3	Dissolved mass concentration
D_m	m^2/s	thermal diffusivity
α	m	Dispersivity
v_a	m/s	Seepage velocity
q_{ss}	$m^3/s/m^3$	Volumetric flow rate per unit volume of aquifer
C_{ss}	kg/m^3	Concentration of the sources or sinks

Method (comparison Metric)

Comparison of the simulations is based on residual errors and follows the method of efficiencies (EF)

$$EF = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2 - \sum_{i=1}^{n}(x_i' - x_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

(Loague and Green, 1991)

x_i	Observed values (analytical solution)
$\bar{x}$	The mean of the observed values
x_i'	The values simulated by MT3DMS

- $0 \leqq \text{EF} \leqq 1$
- EF = 1, representing no difference between analytical and simulated results.
- EF = 0, representing high residual error.

Method (comparison Metric)

Comparison of the simulations is based on residual errors and follows the method of efficiencies (EF)

$$EF = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2 - \sum_{i=1}^{n}(x_i' - x_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

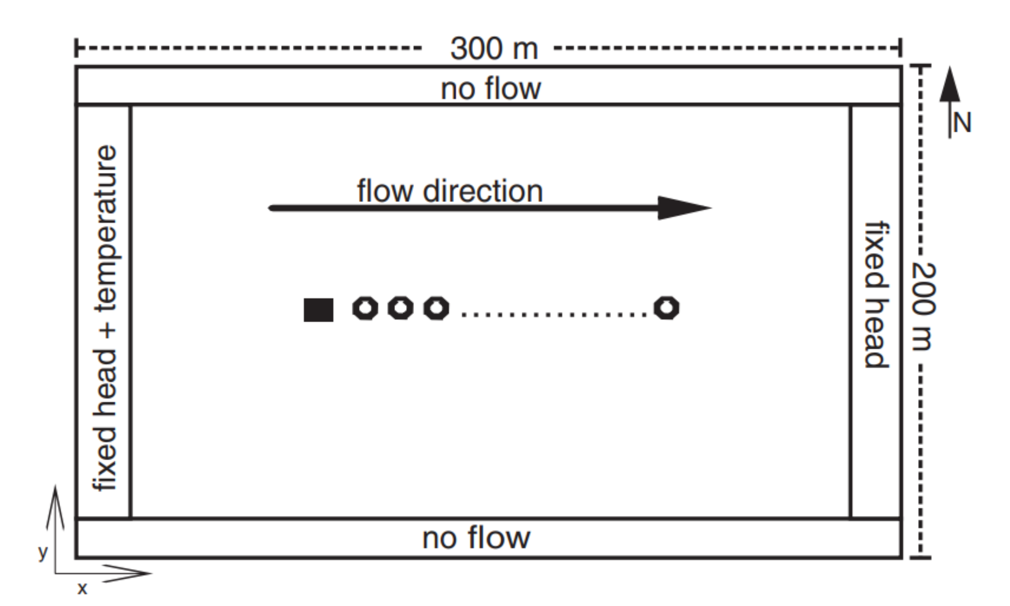
(Loague and Green, 1991)

x_i	Observed values (analytical solution)
$\bar{x}$	The mean of the observed values
x_i'	The values simulated by MT3DMS

Very good	$0.98 \leqq \text{EF} \leqq 1$
Good	$0.8 \leqq \text{EF} \leqq 0.97$
Moderate	$0.5 \leqq \text{EF} \leqq 0.79$
Bad	$\text{EF} < 0.5$

Model setting

- 300 m × 200 m with regular grid spacing (Δx = Δy =0.5m)
- Source cell (heat changer) is at x = 50 m, y = 100 m, and size is 0.1 × 0.1 m
- Fixed head boundary conditions at west and east.
- Fixed temperature at west border (285.15 K or 12°C).
- For 2D cases, vertical heat transfer is ignored.
- For 3D cases
  - 13 identical uniform 1-m layers
  - Source is at 6,7,8 layers with the same coordinates as 2D.



Model setting

Table 2
Scenarios Classified According to the Underlying Thermal Péclet Numbers (Pe)

Scenario	Pe	Gradient	Seepage Velocity (v_a) (m/s)
1	0	0	0
2	1	1.2×10^{-4}	3.7×10^{-6}
3	10	1.2×10^{-3}	3.7×10^{-5}

symbol	variable
q	Darcy's velocity
l	Characteristic length (grid spacing)
ρ_w	Density of water
C_w	Specific heat capacity of the water
λ_m	Effective thermal conductivity of porous media

- Péclet number $(P_e) = \frac{ql\rho_w C_w}{\lambda_m} = \frac{heat\ convection}{heat\ conduction}$
- Scenario 1 (S1) : conduction-dominant, no groundwater flow
- Scenario 2 (S2) : convection and conduction processes have a similar influence
- Scenario 3 (S3) : convection-dominant, high flow velocity

Results and discussion

MT3DMS vs. analytical solutions

	2D	3D
Scenario 1		
Scenario 2		
Scenario 3		

MT3DMS vs. numerical solutions
(FEFLOW, SEAWAT)

	2D	3D
Scenario 1		
Scenario 2		
Scenario 3		

Results and discussion

MT3DMS compares with analytical solutions

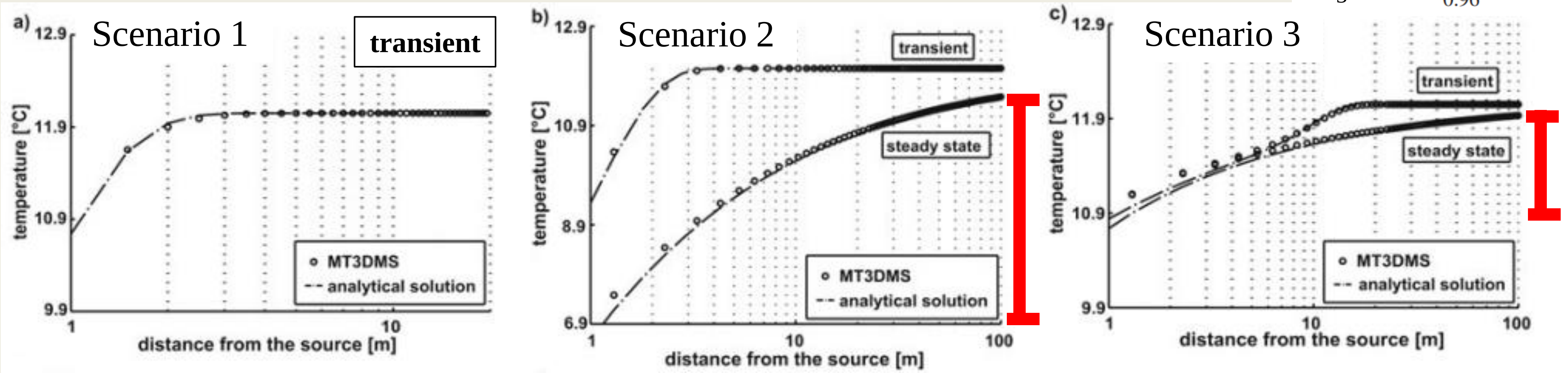
Table 5
Efficiencies of the Comparison Between MT3DMS and Analytical Results, Steady-State and Transient Conditions

	2D				3D			
	<10 m		>10 m		<10 m		>10 m	
Scenario	Steady State	Transient	Steady State	Transient	Steady State	Transient	Steady State	Transient
1 (no flow)	—	0.98	—	1.00	—	—	—	—
2 (Pe = 1)	0.99	1.00	0.99	1.00	0.93	0.96	1.00	1.00
3 (Pe = 10)	0.96	0.96	0.96	1.00	0.92	0.84	0.94	1.00

- Two sectors (from the source)：**proximate sector**, 1-10m；**distant sector**, 10-100m
- Transient results are shown for 10 days

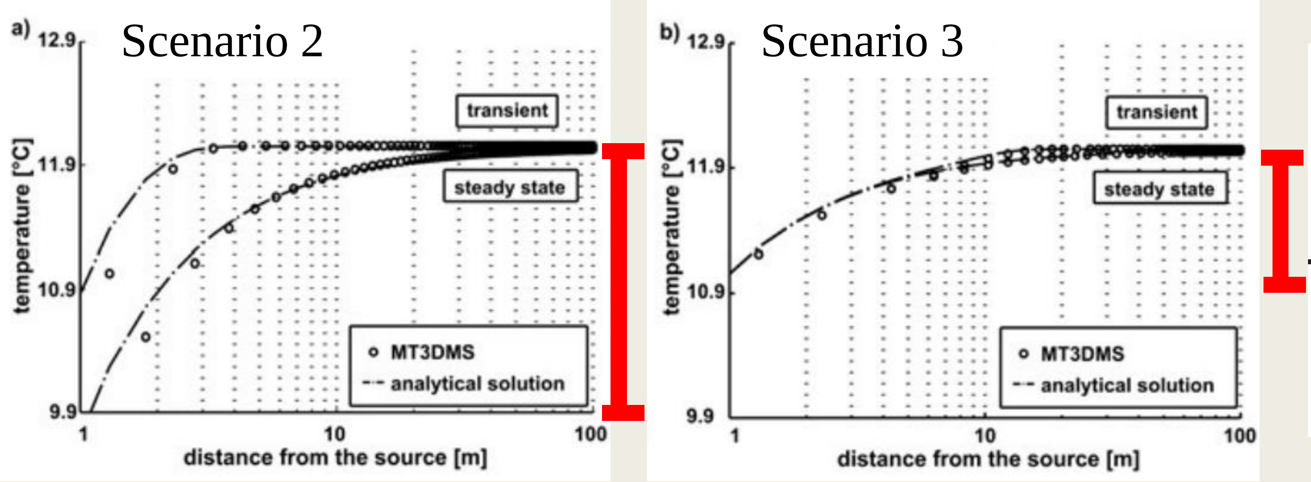
Results and discussion (2D cases)

Scenario	2D			
	<10 m		>10 m	
	Steady State	Transient	Steady State	Transient
1	—	0.98	—	1.00
2	0.99	1.00	0.99	1.00
3	0.96	0.96	0.96	1.00



- The calculated efficiency for the proximate and distant sector have a very good agreement between both curves.
- To compare the temperature differences of S2 and S3 under steady state conditions, the convection-dominated (S3) case brings out a lower absolute temperature change near the source.
- This reflects the important role of groundwater flow for the energy supply at the borehole.

Results and discussion (3D cases)



	3D			
	<10 m		>10 m	
Scenario	Steady State	Transient	Steady State	Transient
1 (no flow)	—	—	—	—
2 (Pe = 1)	0.93	0.96	1.00	1.00
3 (Pe = 2)	0.92	0.84	0.94	1.00

- S1 is not considered due to the lack of a 3D analytical solution for pure conduction.
- Shows good to very good agreement between steady state and transient numerical and analytical results at the proximate and distant sector.
- The temperature differences are similar with 2D cases.

Results and discussion MT3DMS compare with numerical solutions

Table 6
Model Efficiencies of the Comparison Between MT3DMS-SEAWAT and MT3DMS-FEFLOW Results

	2D				3D			
	<10 m		>10 m		<10 m		>10 m	
Scenario	Steady State	Transient	Steady State	Transient	Steady State	Transient	Steady State	Transient
FEFLOW								
1 (no flow)	—	—	—	—	—	—	—	—
2 (Pe = 1)	0.99	0.99	1.00	1.00	0.64	0.64	0.93	1.00
3 (Pe = 10)	0.93	0.91	0.95	0.97	0.64	0.64	0.87	1.00
SEAWAT								
1 (no flow)	—	—	—	—	—	—	—	—
2 (Pe = 1)	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
3 (Pe = 10)	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Note: Two sectors are distinguished: proximate, from 1 to 10 m distance (downgradient) from the source; and distant, from 10 to 100 m.

- These differences are likely to be dominated by differences in how the source is represented in MT3DMS(like a planar source) and FEFLOW (like a line source).
- The close match between MT3DMS and SEAWAT is consistent with the overall efficiency of 1.0 for all cases.
- Because the results of SEAWAT and MT3DMS have a high degree of agreement, the calculation time of the two is further discussed.

Results and discussion MT3DMS compare with numerical solutions

Table 7
Execution Time for the Different Scenarios

Code	Execution Time (s)			
	2D		3D	
	Scenario 2 (Pe = 1)	Scenario 3 (Pe = 10)	Scenario 2 (Pe = 1)	Scenario 3 (Pe = 10)
MT3DMS	238	1,070	5,484	20,051
SEAWAT	507	1,595	11,114	31,737

Hardware specifications: Pentium IV, CPU 3 GHz, and 1 GB RAM.

- Execution times for S1 are not shown since no significant differences are noticeable.
- SEAWAT requires longer running times for the same simulated scenarios than MT3DMS.

Conclusions

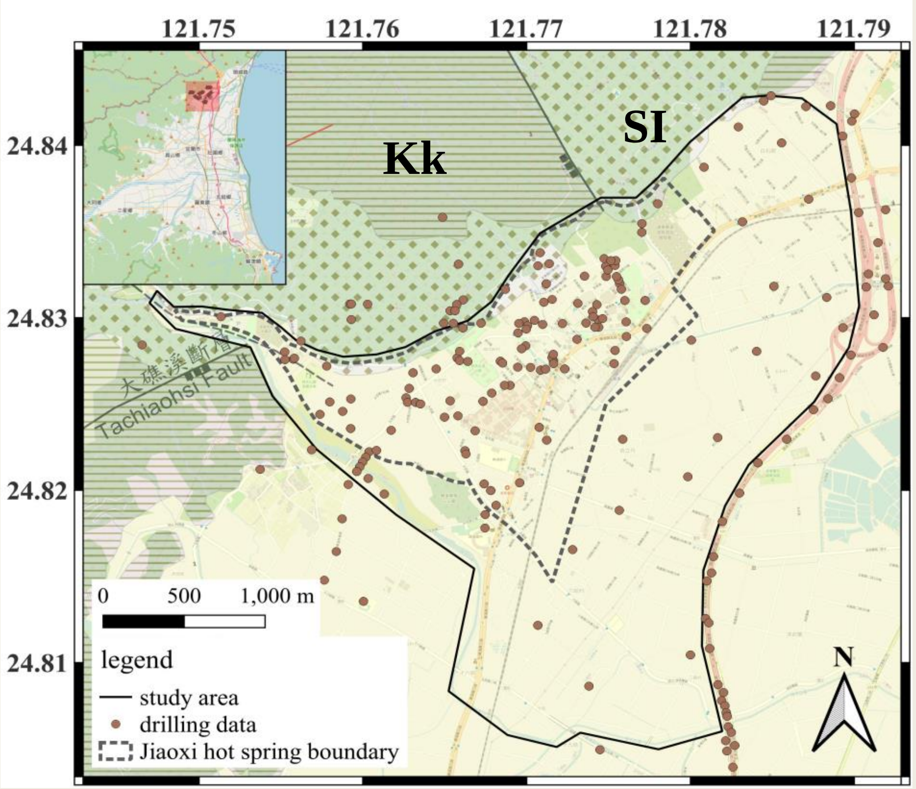
- They used three different scenarios for comparison, which differ with respect to the assumed groundwater flow velocities.
- The overall agreement of MT3DMS with analytical solutions, SEAWAT and FEFLOW is good to very good. ($0.8 \leqq EF \leqq 1$)
- Highest absolute temperature differences reach 5℃ if heat is transported by conduction and convection, and 1℃ if convection dominates.

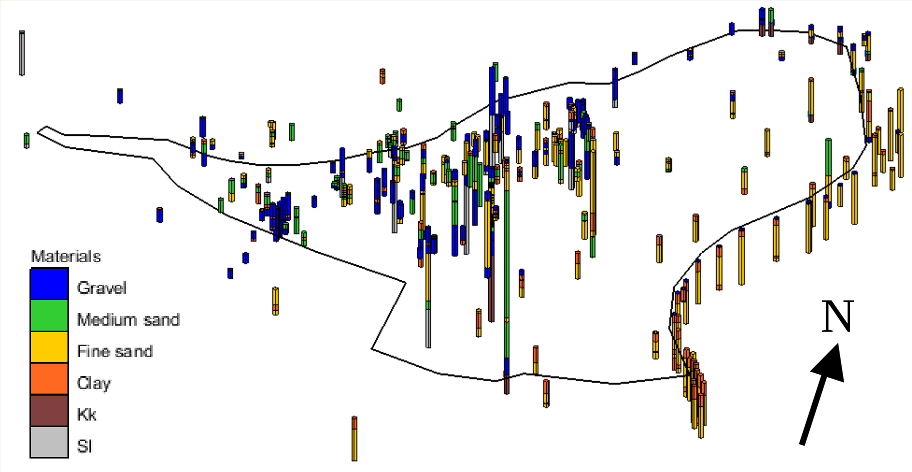
Future work

- Study area : Yilan, Jiaoxi
- Software : GMS(Groundwater Modeling System)
- Motivation : Doing the hot spring management so that the hot spring can be used longer.

<u>Step 1</u>

- Build the 3D model with sediment and bedrock
- Kankou formation (Kk) , Szuling sandstone (SI)

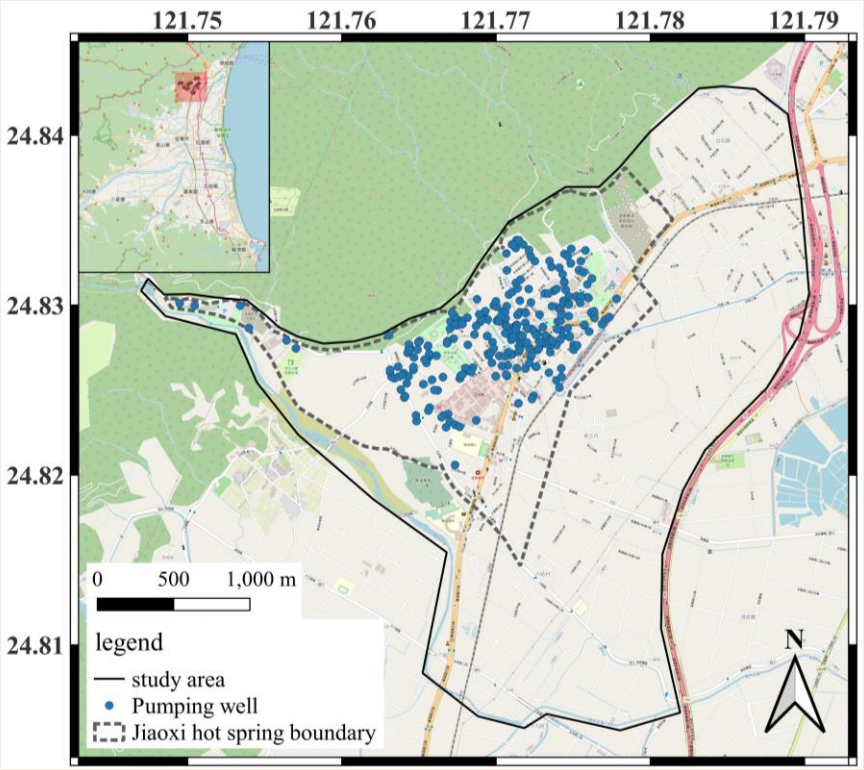




Future work

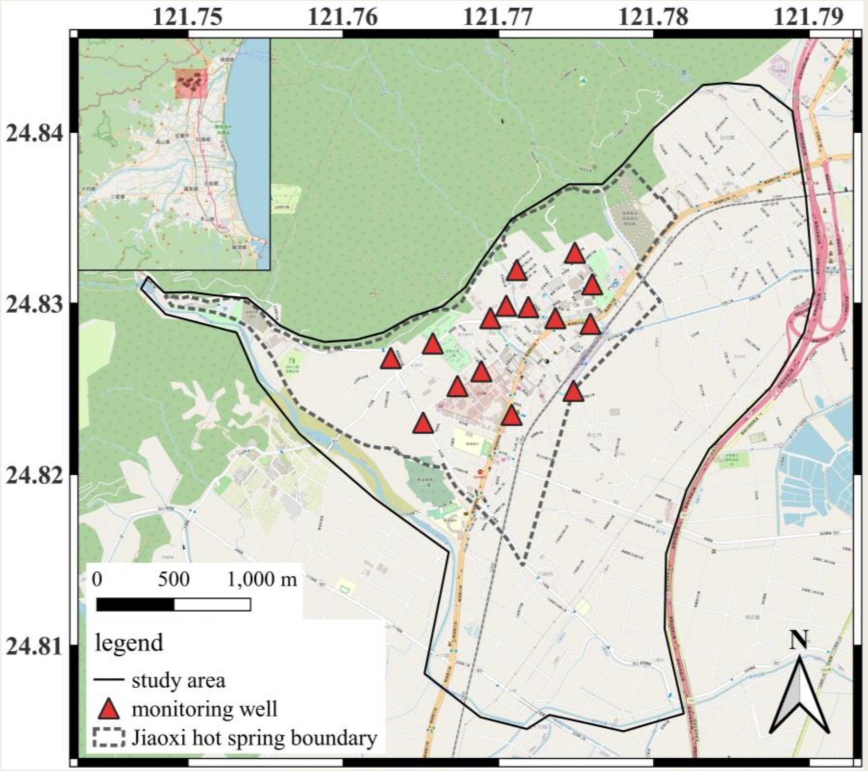
<u>Step 2</u>

- Collect pumping well, river recharge, rain data.
- Use MODFLOW to simulate the flow field.



<u>Step 3</u>

- Input MODFLOW solution to MT3DMS
- Use MT3DMS to simulate the heat transport.



Thanks for your listening

Governing equations

Symbol	Variable	Unit
K_d	Distribution coefficient	(m^3/kg)
C^k	Dissolved mass concentration	(kg/m^3)
q_{ss}	Volumetric flow rate per unit volume of aquifer representing sources and sinks	(m^3/s/m^3)
q_h	Heat injection/extraction	(W/m^3)
C_{ss}	Concentration of the sources or sinks	(kg/m^3)
F_o	Energy extraction (point source)	(W)
F_L	Energy extraction per unit length of the borehole (line source)	(W/m)
F_A	Energy extraction per area of the source (planar source)	(W/m^2)
L	Characteristic length (grid spacing)	(m)
λ_m	Effective thermal conductivity of the porous media	(W/m/K)
λ_w	Water thermal conductivity	(W/m/K)
λ_s	Solid thermal conductivity	(W/m/K)
n	Porosity	(–)
ρ_w	Density of water	(kg/m^3)
c_w	Specific heat capacity of the water	(J/kg/K^1)
$\rho_w c_w$	Volumetric heat capacity of the water	(J/m^3/K^1)
ρ_s	Density of the solid material (=minerals)	(kg/m^3)
c_s	Specific heat capacity of the solid	(J/kg/K)
$\rho_s c_s$	Volumetric heat capacity of the solid	(J/m^3/K)
ρ_b	Dry bulk density $\rho_b = (1 - n)\rho_s$	(kg/m^3)
α, α_l	Dispersivity, longitudinal dispersivity	(m)
α_{th}	Transverse horizontal dispersivity	(m)
α_{tv}	Transverse vertical dispersivity	(m)
$q = v_f$	Darcy velocity	(m/s)
v_a	Seepage velocity	(m/s)
D_m, D_h	Molecular diffusion, thermal diffusivity	(m^2/s)
D_l	Longitudinal heat dispersion coefficient	(m^2/s)
D_{th}	Transverse horizontal heat dispersion coefficient	(m^2/s)
D_{tv}	Transverse vertical heat dispersion coefficient	(m^2/s)
x, y, z	Cartesian coordinates	(m)
R	Radial coordinate	(m)
Y	Dimension (length) of the source in y direction	(m)
Z	Dimension (length) of the source in z direction	(m)
ΔT	Temperature difference	(K)
ΔT_o	Temperature difference at the source	(K)
t	Time	(s)

Symbol	Variable	Unit
T, T_s	Temperature, temperature of the solid	(K)
T_u	Undisturbed temperature of the underground	(K)
R	Retardation factor	(–)
E_i	Exponential integral function	(–)
η	Integration parameter	(–)
K_o	Modified Bessel function of second kind and order zero	(–)

$$R = \frac{\rho_m c_m}{n\rho_w C_w} \qquad D_m = \frac{\lambda_m}{n\rho_w c_w}$$

$$k_d = \frac{c_s}{\rho_w c_w} \qquad q_{ss} = \frac{q_h}{\rho_w c_w}$$

$$n\rho_w c_w \frac{\partial T}{\partial t} + (1-n)\rho_s c_s \frac{\partial T_s}{\partial t} = \nabla \cdot [(\lambda_m + n\rho_w c_w \alpha v_a)\nabla T] - \nabla \cdot (n\rho_w c_w v_a T) + q_h$$

$$n\rho_w c_w \frac{\partial T}{\partial t} + (1-n)\rho_s c_s \frac{\partial T_s}{\partial t} = \rho_m c_m \frac{\partial T}{\partial t}$$

$$\rho_m c_m = n\rho_w c_w + (1-n)\rho_s c_s = np_w c_w + \rho_b c_s$$

$$\Rightarrow \quad \frac{\rho_m c_m}{n\rho_w C_w}\frac{\partial T}{\partial t} = \nabla \cdot [(\frac{\lambda_m}{n\rho_w c_w} + \alpha v_a)\nabla T] - \nabla \cdot (v_a T) + \frac{q_h}{n\rho_w c_w}$$

$$\left(1 + \frac{\rho_b K_d}{n}\right)\frac{\partial C^k}{\partial t} = \nabla \cdot [(D_m + \alpha v_a)\nabla C^k] - \nabla \cdot \left(v_a C^k\right) + \frac{q_{ss} C_{ss}}{n}$$

Model setting

https://www.energy.gov/energysaver/geothermal-heat-pumps

Table 3
MT3DMS Specification for All Scenarios

Symbol	Variable	Value	Unit	MT3DMS Package
n	Porosity	0.26	(–)	BTN
λ_m	Effective thermal conductivity of the porous media	2.0	(W/m/K)	—
$\rho_w c_w$	Volumetric heat capacity of the water	$4.18 \times 10^{+6}$	($J/m^3/K$)	—
ρ_s	Density of the solid material (= minerals)	2650	(kg/m^3)	—
c_s	Specific heat capacity of the solid	880	(J/kg/K)	—
ρ_b	Dry bulk density	1961	(kg/m^3)	RCT
K_d	Partition coefficient	2.10×10^{-4}	(m^3/kg)	RCT
α_l	Longitudinal dispersivity	0.5	(m)	DSP
α_{th}	Transverse horizontal dispersivity	0.05	(m)	DSP
α_{tv}	Transverse vertical dispersivity	0.05	(m)	DSP
D_h	Thermal diffusivity	1.86×10^{-6}	(m^2/s)	DSP
Tu	Undisturbed temperature of the ground	285.15	(K)	BTN
R	Retardation factor	2.59	(–)	RCT

Note: Last column indicates the name of the corresponding package within MT3DMS.

- Hydraulic conductivity = $8 \times 10^{-3}\ m/s$ (typical sand aquifers)
- Density = $999.49\ kg/m^3$

Analytical solutions (2D)

- Transient conditions, closed system, and no groundwater flow velocity.

$$\Delta T(r,t) = \frac{F_L}{4\pi\lambda_m} E_i \left[- \frac{r^2}{4\left({}^{\lambda_m}/_{P_m C_m}\right) t} \right]$$

(Carslaw and Jager 1959)

- Transient conditions, closed system, and groundwater flow velocity considering heat dispersivity.

$$\Delta T(x,t) = \frac{F_L}{4\pi n \rho_w C_w \sqrt{D_1 D_{th}}} \exp\left[\frac{v_a x}{2D_1}\right] \int \frac{1}{n} \times \exp\left[-\eta - \frac{V_a^2 x^2}{16 D_{th}^2 \eta}\right] \mathrm{d}\eta$$

(Metzger et al. 2004)

- Steady-state conditions, closed system, and groundwater flow velocity.

$$\Delta T(x) = \frac{F_L}{2\pi n \rho_w c_w D_{\mathrm{th}}} \exp\left[\frac{v_a x}{2D_{th}}\right] K_0 \left[\frac{v_a x}{2D_{th}}\right]$$

(Diao et al. 2004)

Analytical solutions (3D)

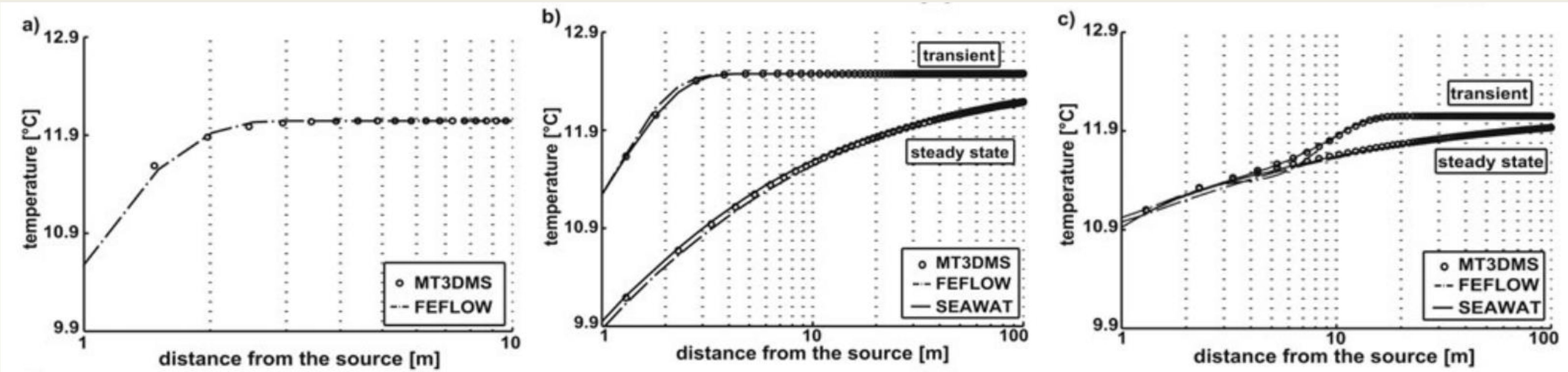
- Transient and steady-state conditions, closed system, and groundwater flow velocity.

$$\Delta T(x,y) = \frac{F_0}{v_a n \rho_w c_w \sqrt{4\pi D_{th}(x/v_a)}} \times \exp\left(\frac{-v_a(y^2)}{4D_{th}x}\right)$$

$$\Delta T(x,y) = \left(\frac{\Delta T_0}{2}\right) \operatorname{erfc}\left[\frac{(Rx - v_a t)}{2\sqrt{D_1 R_t}}\right] \times \operatorname{erf}\left[\frac{Y}{4\left(D_{th}(x/v_a)\right)^{0.5}}\right] \times \operatorname{erf}\left[\frac{Z}{4\left(D_{tv}(x/v_a)\right)^{0.5}}\right]$$

(Fried et al. 1979; Domenico and Robbins 1985)

Results and discussion (numerical_2D cases)



Results and discussion (numerical_3D cases)