

Supplementary material 1 for "A numerical model for precursory time sequences of the phreatic eruptions of Mt. Ontake, central Japan" by Yuta Maeda

Numerical procedures and parameters

This supplementary material provides the exact steps and parameters used in the simulations. COMSOL Multiphysics 6.1 was used with licenses for Chemical Reaction Engineering, Porous Media Flow, and Structural Mechanics modules. Notations and abbreviations not explained in the supplementary material are based on the main text.

A: Simulation for a cylindrical model

This section explains the numerical steps and parameters of the cylindrical model (Fig. 1a and 3).

A1. Model selection

- The simulation used "Darcy's Law" and "Heat Transfer in Porous Media" physics.
- (a) Start COMSOL Multiphysics, click "Model Wizard" and then "2D Axisymmetric".
 - (b) Choose "Fluid Flow" -> "Porous Media and Subsurface Flow" -> "Darcy's Law (dl)" and click "Add".
 - (c) Choose "Heat Transfer" -> "Porous Media" -> "Heat Transfer in Porous Media (ht)" and click "Add".
 - (d) Click "Study".
 - (e) Choose "Time Dependent" and click "Done".

A2. Definition of constants

- (a) Click "Global Definitions" -> "Parameter 1" in the left menu.
- (b) Define the parameters summarized in Table S1.

Table S1. Constants for the cylindrical model.

Name	Expression (fully liquid scenario)	Expression (supercritical scenario)	Description
L	1.2 [km]	1.2 [km]	Channel length
Rc	0.2 [km]	0.2 [km]	Channel radius
porosity	0.05	0.05	Porosity of the medium
k	3e-11 [m ²]	2e-12 [m ²]	Permeability of the medium
rho_s	2500 [kg/m ³]	2500 [kg/m ³]	Density of solid
C_ps	800 [J/kg/K]	800 [J/kg/K]	Isobaric heat capacity of solid
K_s	1 [W/m/K]	1 [W/m/K]	Thermal conductivity of solid
Tout	300 [K]	500 [K]	Outlet temperature
Pout	0.1 [MPa]	30 [MPa]	Outlet pressure
Tin	350 [K]	1000 [K]	Inlet temperature
Vin	2.5e-4 [m/s]	1e-3 [m/s]	Inlet flow velocity

A3. Definition of water properties

The properties of water were given as functions of temperature and pressure based on the IF-97 of IAPWS. They were implemented in COMSOL Multiphysics using the following steps. Despite the choice of the liquid phase in (f), it well approximated the fluid properties of the liquid, gas, and supercritical phases (see Section A3-1).

- Right click "Global Definitions" in the left menu and select "Thermodynamics" -> "Thermodynamic System".
- Choose "Vapor-liquid" in the middle window and click "Next".
- Double click "water (7732-18-5, H₂O)" in the "Species" field of the middle window to add it to "Selected species" list, and click "Next".
- By default, "Water (IAPWS)" are chosen for liquid and gas phase models. Confirm it in the middle window and click "Finish".
- Right click "Global Definitions" -> "Thermodynamics" -> "Vapor-Liquid System 1 (pp1)" in the left menu and select "Generate Material".
- Choose "Liquid" in the middle window and click "Next".

- (g) Choose "Mass fraction" for "Species composition" selection in the middle window and click "Next".
- (h) Confirm that "kg" is selected for "Amount base unit" in the middle window and click "Next".
- (i) Click "Finish".

These steps create functions "Densitypp1", "Viscositypp1", "ThermalConductivitypp1", "HeatCapacityCp1", and "HeatCapacityRatioCpCvpp1", which give the density, viscosity, thermal conductivity, isobaric heat capacity, and heat capacity ratio of water, respectively, for a given temperature and pressure on the basis of the IF-97 of IAPWS.

A3-1. Checking the function (optional)

Despite the selection of "Liquid" phase in the step (f) above, the functions seem to well approximate the water properties over the liquid, gas, and supercritical phases, as is confirmed by the following steps.

- (a) Click "Global Definitions" -> "Thermodynamics" -> "Vapor-Liquid System 1 (pp1)" -> "water" -> "Liquid" -> "Density 1" in the left menu.
- (b) Change "Plot Parameters" in the middle window to 300–1000 K and 10^5 – 10^8 Pa, and click "Plot".

Subsequently, an abrupt change in the water density between the liquid and gas phases and a gradual change in the supercritical region were observed, consistent with the actual density of water over the three phases.

A4. Creating a cylinder geometry object

- (a) Right click "Component 1 (comp1)" -> "Geometry 1" in the left menu and select "Rectangle".
- (b) Modify the width to "Rc", height to "L", base z to "-L", and click "Build Selected".

A5. Setting Darcy's law physics

A5-1. Incorporating the gravity

By default, the Darcy's Law physics does not incorporate gravity. This was

incorporated into the model using the following steps.

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" in the left menu.
- (b) Check ``Gravity Effects" -> ``Include gravity" in the middle window.

A5-2. Fluid properties

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" -> ``Porous Medium 1" -> ``Fluid 1" in the left menu.
- (b) Change ``Model Input" -> ``Temperature" in the middle window from ``Common model input" to ``Temperature (ht)". By this, the temperature field computed by Heat Transfer in Porous Media physics is coupled with Darcy's Law physics.
- (c) Change ``Fluid properties" -> ``Density" in the middle window from ``From material" to ``User defined" and set the value as ``Densitypp1(T,p)".
- (d) Change ``Fluid properties" -> ``Dynamic viscosity" in the middle window from ``From material" to ``User defined" and set the value as ``Viscositypp1(T,p)".

A5-3. Porous matrix properties

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" -> ``Porous Medium 1" -> ``Porous Matrix 1" in the left menu.
- (b) Change ``Matrix Properties" -> ``Porosity" in the middle window from ``From material" to ``User defined" and set the value as ``porosity".
- (c) Change ``Matrix Properties" -> ``Permeability model" -> `` $\kappa$ " from ``From material" to ``User defined" and set the value as ``k".

A5-4. Initial condition

The initial condition should be a zero Darcy velocity ($V = 0$). However, the Darcy velocity cannot be directly specified in the Darcy's Law physics of COMSOL Multiphysics. Therefore, hydrostatic pressure $P = P_{out} - \rho_f g z$ was used instead, which was equivalent to zero Darcy velocity (Eq. 2). Exactly, ρ_f depends on the pressure, and thus on the location. For simplicity, this study assumed a constant ρ_f corresponding to a temperature T_{out} and a pressure P_{out} in the calculation of hydrostatic pressure.

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" -> ``Initial values 1" in the left menu.
- (b) Set the initial value in the middle window as ``Pout-Densitypp1(Tout,Pout)\*g\_const\*z". Here, ``g_const" is a built-in constant that represents the gravitational acceleration.

A5-5. Boundary condition at the inlet

- (a) Right click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" and select ``Inlet".
- (b) Click the bottom of the computational domain from the geometry in the right window to select it as the inlet.
- (c) In the ``Velocity" -> ``Normal inflow velocity" field in the middle window, set the value as ``Vin".

A5-6. Boundary condition at the outlet

- (a) Right click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" and select ``Outlet".
- (b) Click the top of the computational domain from the geometry in the right window to select it as the outlet.
- (c) Change ``Boundary Condition" -> ``Boundary condition" in the middle window from ``Velocity" to ``Pressure".
- (d) In the ``Pressure" -> ``Pressure" field in the middle window, set the value as ``Pout".

A6. Setting heat transfer physics

A6-1. Fluid properties

- (a) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``Porous medium 1" -> ``Fluid 1" in the left menu.
- (b) Change ``Model Input" -> ``Absolute pressure" in the middle window from ``Common model input" to ``Absolute pressure (dl)". By this, the pressure field computed by Darcy's Law physics is coupled with Heat Transfer in Porous Media physics.
- (c) Change ``Heat Convection" -> ``Velocity field" in the middle window from ``User defined" to ``Darcy's velocity field (fl/porous1)". By this, the velocity field computed by Darcy's Law physics is coupled with Heat Transfer in Porous Media physics.

- (d) Change "Heat Conduction, Fluid" -> "Thermal conductivity" in the middle window from "From material" to "User defined" and set the value as $\text{ThermalConductivitypp1}(T,p)$.
- (e) Change "Thermodynamics, Fluid" -> "Density" in the middle window from "From material" to "User defined" and set the value as $\text{Densitypp1}(T,p)$.
- (f) Change "Thermodynamics, Fluid" -> "Heat capacity at constant pressure" in the middle window from "From material" to "User defined" and set the value as $\text{HeatCapacityCp1}(T,p)$.
- (g) Change "Thermodynamics, Fluid" -> "Ratio of specific heats" in the middle window from "Automatic" to "User defined" and set the value as $\text{HeatCapacityRatioCpCv1}(T,p)$.

A6-2. Porous matrix properties

- (a) Click "Component 1 (comp1)" -> "Heat Transfer in Porous Media (ht)" -> "Porous medium 1" -> "Porous matrix 1" in the left menu.
- (b) Change "Model Input" -> "Absolute pressure" in the middle window from "Common model input" to "Absolute pressure (dl)".
- (c) Change "Matrix Properties" -> "Porosity" in the middle window from "From material" to "User defined" and set the value as porosity .
- (d) Change "Matrix Properties" -> "Define" in the middle window from "Dry bulk properties" to "Solid phase properties".
- (e) Change "Heat Conduction, Porous Matrix" -> "Solid phase thermal conductivity" in the middle window from "From material" to "User defined" and set the value as K_s .
- (f) Change "Thermodynamics, Porous Matrix" -> "Solid phase density" in the middle window from "From material" to "User defined" and set the value as ρ_s .
- (g) Change "Thermodynamics, Porous Matrix" -> "Solid phase heat capacity at constant pressure" in the middle window from "From material" to "User defined" and set the value as C_{ps} .

A6-3. Initial condition

- (a) Click "Component 1 (comp1)" -> "Heat Transfer in Porous Media (ht)" -> "Initial

Values 1" in the left menu.

- (b) Set the value of the initial temperature as ``Tout``.

A6-4. Boundary condition at the inlet

- (a) Right click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" in the left menu and select ``Temperature".
- (b) Change the label in the middle window from ``Temperature 1" to ``Temperature (inlet)".
- (c) Click the bottom of the computational domain from the geometry in the right window to select it as the inlet.
- (d) In the ``Temperature" -> ``Temperature" field in the middle window, set the value as ``Tin".

A6-5. Boundary condition at the outlet

- (a) Right click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" in the left menu and select ``Temperature".
- (b) Change the label in the middle window from ``Temperature 2" to ``Temperature (outlet)".
- (c) Click the top of the computational domain from the geometry in the right window to select it as the outlet.
- (d) In the ``Temperature" -> ``Temperature" field in the middle window, set the value as ``Tout".

A7. Study

- (a) Click ``Study 1" -> ``Step 1: Time Dependent" in the left menu.
- (b) Change ``Study Settings" -> ``Time unit" in the middle window from ``s" to ``d".
- (c) Change ``Study Settings" -> ``Output times" in the middle window to ``range(0,1,30)".
- (d) Click ``Compute".

A8. Evaluating the results

A8-1. Pressure

- (a) Click ``Results" -> ``Pressure (dl)" in the left menu.
- (b) Select a time step concerned from ``Data" -> ``Time (d)" field in the middle window and click ``Plot".
- (c) Right click ``Results" -> ``Pressure (dl)" -> ``Surface" in the left menu and select ``Add Plot Data to Export".
- (d) Define the output file name in ``Output" -> ``Filename" field in the middle window and Click ``Export". This step creates a text file that consists of the pressures on all mesh nodes at the selected time step.

A8-2. Temperature

- (a) Click ``Results" -> ``Pressure (dl)" -> ``Surface" in the left menu.
- (b) From the inverse triangle at the right of ``Expression" section in the middle window, select ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media" -> ``Temperature" -> ``T - Temperature - K".
- (c) Repeat the steps of Section A8-1.

B: Simulation for a 2-D model

This section explains the numerical steps and parameters of the 2-D model (Fig. 1b and 5).

B1. Model selection

The simulation used ``Darcy's Law", ``Heat Transfer in Porous Media", and ``Solid Mechanics" physics.

- (a) Start COMSOL Multiphysics, click ``Model Wizard" and then ``2D Axisymmetric".
- (b) Choose ``Fluid Flow" -> Porous Media and Subsurface Flow" -> ``Darcy's Law (dl)" and click ``Add".
- (c) Choose ``Heat Transfer" -> ``Porous Media" -> ``Heat Transfer in Porous Media (ht)" and click ``Add".
- (d) Choose ``Structural Mechanics" -> ``Solid Mechanics (solid)" and click ``Add".

- (e) Click ``Study".
- (f) Choose ``Time Dependent" and click ``Done".

B2. Definition of constants

- (a) Click ``Global Definitions" -> ``Parameter 1" in the left menu.
- (b) Define the parameters summarized in Tables S2–S6.

Table S2. Constants for geometrical parameters in the 2-D model from the surface topography of Mt. Ontake and the subsurface structure model proposed by Maeda and Watanabe (2023).

Name	Expression	Description
Rc	0.2 [km]	Channel radius
Ry	4 [km]	YED radius
Ro	15 [km]	OED radius
Zs	3 [km]	Altitude of summit
Zyo	1.9 [km]	Altitude of YED–OED boundary
Zob	0.9 [km]	Altitude of OED–basement boundary
Zin	-0.3 [km]	Altitude of fluid inlet
Hi	5 [km]	Thickness of infinite element

Table S3. Constants for porous medium properties. The parameter study in Fig. 4 used various sets of different values, and the final values adopted in Fig. 5 are shown here.

Name	Expression	Description
phi_o	0.05	Porosity (OED)
phi_c	0.2	Porosity (channel)
k_o	4e-12 [m ²]	Permeability (OED)
k_c	100*k_o	Permeability (channel)
alpha_B	0.4	Biot-Willis coefficient

Table S4. Constants for solid material properties; these values were based on Maeda and Watanabe (2023) and Gardner (1974).

Name	Expression	Description
Vpy	2.4 [km/s]	P-wave velocity (YED)
Vpo	3.6 [km/s]	P-wave velocity (OED)
Vpb	5.6 [km/s]	P-wave velocity (basement)
Vsy	$V_{py}/\sqrt{3}$	S-wave velocity (YED)
Vso	$V_{po}/\sqrt{3}$	S-wave velocity (OED)
Vsb	$V_{pb}/\sqrt{3}$	S-wave velocity (basement)
rho_sy	$1700[\text{kg/m}^3]+0.2[\text{kg/m}^3/(\text{m/s})]*V_{py}$	Solid density (YED)
rho_so	$1700[\text{kg/m}^3]+0.2[\text{kg/m}^3/(\text{m/s})]*V_{po}$	Solid density (OED)
rho_sb	$1700[\text{kg/m}^3]+0.2[\text{kg/m}^3/(\text{m/s})]*V_{pb}$	Solid density (basement)

Table S5. Constants for solid material properties; these values were based on Heap et al. (2020).

Name	Expression	Description
C_ps	800 [J/kg/K]	Isobaric heat capacity of solid
K_s	1 [W/m/K]	Thermal conductivity of solid

Table S6. Constants for inlet and outlet conditions. The parameter study in Fig. 4 used various sets of different values, and the final values adopted in Fig. 5 are shown here.

Name	Expression (2014 scenario)	Expression (2007 scenario)	Description
Tout	300 [K]	300 [K]	Outlet temperature
Pout	0.1 [MPa]	0.1 [MPa]	Outlet pressure
Tin	600 [K]	800 [K]	Inlet temperature
Vin	6e-4 [m/s]	1.2e-3 [m/s]	Inlet flow velocity

B3. Definition of water properties

Repeat Section A3.

B4. Creating geometry objects

B4-1. YED

- (a) Right-click "Component 1 (comp1)" -> "Geometry 1" in the left menu and select "More Primitives" -> "Polygon".
- (b) Change the label in the middle window as "YED".
- (c) Define the coordinates in the middle window as shown in Table S7 and click "Build Selected".

Table S7. Coordinates of the polygon that represents the YED.

r (m)	z (m)
0	Zs
Ry	Zyo
0	Zyo

B4-2. OED

Repeat the steps of Section B4-1 with a label "OED" and the coordinates given in Table S8.

Table S8. Coordinates of the polygon that represents the OED.

r (m)	z (m)
0	Zyo
Ry	Zyo
Ro	Zob
0	Zob

B4-3. Channel

Repeat the steps of Section B4-1 with a label "Channel" and the coordinates given in Table S9.

Table S9. Coordinates of the polygon that represents the channel.

r (m)	z (m)
0	Zob
Rc	Zob
Rc	Zin
0	Zin

B4-4. Basement other than the channel

Repeat the steps of Section B4-1 with a label ``Basement" and the coordinates given in Table S10.

Table S10. Coordinates of the polygon that represents the basement except for the channel part.

r (m)	z (m)
Rc	Zob
Ro	Zob
Ro	Zin
Rc	Zin

B4-5. Side infinite element

Repeat the steps of Section B4-1 with a label ``Side infinite element" and the coordinates given in Table S11.

Table S11. Coordinates of the polygon that represents the side infinite element.

r (m)	z (m)
Ro	Zob
Ro+Hi	Zob
Ro+Hi	Zin
Ro	Zin

B4-6. Bottom infinite element

Repeat the steps of Section B4-1 with a label "Bottom infinite element" and the coordinates given in Table S12. Note that the side and bottom infinite elements must be created separately; an L-shaped infinite element is not applicable.

Table S12. Coordinates of the polygon that represents the bottom infinite element.

r (m)	z (m)
0	Z_{in}
$R_o + H_i$	Z_{in}
$R_o + H_i$	$Z_{in} - H_i$
0	$Z_{in} - H_i$

B5. Definition of hydrostatic pressure

The pore-fluid pressure is the summation of the hydrostatic pressure and the deviation of the pressure from it. A hydrothermal equilibrium was assumed for the initial state. Only the deviation should act as the crustal deformation source, whereas the absolute pressure should be used to compute the fluid properties. To satisfy this requirement, a function of the location representing the hydrostatic pressure was defined. Exactly, the hydrostatic pressure depends on the spatial distribution of the fluid density. For simplicity, this study used a uniform fluid density corresponding to a temperature T_{out} and a pressure P_{out} to compute the hydrostatic pressure.

B5-1. A function for hydraulic head

A function $Z_h(r)$ was created to represent the altitude of the hydraulic head for a given horizontal location (the blue line in Fig. 1b).

- Right click "Global Definitions" in the left menu and select "Functions" -> "Interpolation".
- Change the label in the middle window from "Interpolation 1" to "Hydraulic head".
- Change "Definition" -> "Function name" in the middle window from "int1" to " Z_h ".
- Enter the values shown in Table S13 into the table in the "Definition" section of the middle window.

(e) Write ``m" in ``Units" -> ``Function" -> ``Zh" and ``Units" -> ``Argument" -> ``t" fields in the middle window.

Table S13. Definition of the hydraulic head function. In this table, t and $f(t)$ represent the horizontal location r and the vertical location z of the hydraulic head, respectively.

t	f(t)
0	Zyo
Ry	Zyo
Ro	Zob

B5-2. A function for hydrostatic pressure

A function Phs(r,z) was created to represent the hydrostatic pressure at an arbitrary location (r,z), assuming that the fluid density in the entire region was equal to that for a temperature T_{out} and a pressure P_{out} .

- Right click ``Global Definitions" in the left menu and select ``Functions" -> ``Analytic".
- Change the label in the middle window from ``Analytic 1" to ``Hydrostatic pressure".
- Change the function name in the middle window from ``an1" to ``Phs".
- Change ``Definition" -> ``Expression" in the middle window as

$$P_{out} + \text{Densitypp1}(T_{out}, P_{out}) * g_const * (Zh(r) - z).$$
- Change ``Arguments" as ``r,z".
- Write ``Pa" in ``Units" -> ``Function" field in the middle window.
- Write ``m" in ``Units" -> ``Argument" -> ``r" and ``Units" -> ``Argument" -> ``z" fields in the middle window.

B6. Setting Darcy's law physics

Throughout Darcy's Law physics, the fluid pressure p was used to express the deviation of the pressure from its initial value (hydrostatic pressure). The absolute pressure was expressed as $p + \text{Phs}(r,z)$. The purpose of this treatment was to prevent the hydrostatic pressure from acting as a source of crustal deformation.

For certain parameters, the simulation indicated a localized high-temperature region

with $T > T_{in}$. This is physically unreasonable and suggests numerical instability. The growth of the localized high-temperature region was significantly suppressed by using a temperature T_{in} instead of T for the calculation of fluid properties when $T > T_{in}$. Therefore, all fluid properties were calculated for a temperature $\min(T, T_{in})$.

B6-1. Domain selection

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" in the left menu.
- (b) Deselect the YED, basement (except for the channel), and infinite elements from the domain selection; remain only the OED and channel be selected.

B6-2. Storage model

A variant of Darcy's law, known as a storage model, needs to be selected for applying the pore-fluid pressure computed by Darcy's Law physics as the source of crustal deformation in Solid Mechanics physics.

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" -> ``Porous Medium 1" and change the label as ``OED"; simply rename the label without modifying the domain selection now.
- (b) Change ``Porous Medium" -> ``Storage model" in the middle window from ``From density and porosity" to ``Poroelastic storage".

B6-3. Fluid properties (OED)

- (a) Click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" -> ``OED" -> ``Fluid 1" in the left menu.
- (b) Change ``Model Input" -> ``Temperature" in the middle window from ``Common model input" to ``Temperature (ht)".
- (c) Change ``Fluid properties" -> ``Density"" in the middle window from ``From material" to ``User defined" and set the value as ``Densitypp1(min(T,Tin),p+Phs(r,z))".
- (d) Change ``Fluid properties" -> ``Dynamic viscosity" ' in the middle window from ``From material" to ``User defined" and set the value as ``Viscositypp1(min(T,Tin),p+Phs(r,z))".
- (e) Change ``Fluid properties" -> ``Compressibility" in the middle window from ``From material" to ``User defined" and set the value as

$\frac{\rho_f(T, P)}{\rho_f(T_{in}, P_{in})}$, which represents a compressibility $\chi_f = (1/\rho_f)(\partial\rho_f/\partial P)$.

B6-4. Porous matrix properties (OED)

- (a) Click "Component 1 (comp1)" -> "Darcy's Law (dl)" -> "OED" -> "Porous Matrix 1" in the left menu.
- (b) Change "Matrix Properties" -> "Porosity" in the middle window from "From material" to "User defined" and set the value as ϕ_o .
- (c) Change "Matrix Properties" -> "Permeability model" -> " κ " from "From material" to "User defined" and set the value as k_o .

B6-5. Fluid and porous matrix properties (channel)

The easiest way to define the material properties in the channel is to copy the settings of the OED and modify the values of the matrix properties; no modification is required for the fluid properties.

- (a) Right click "Component 1 (comp1)" -> "Darcy's Law (dl)" -> "OED" and click "Duplicate".
- (b) Click "Component 1 (comp1)" -> "Darcy's Law (dl)" -> "OED1" and rename the label as "Channel".
- (c) Deselect the OED from the domain selection. After this step, the domain selections for the OED and the channel are both correct.
- (d) Click "Component 1 (comp1)" -> "Darcy's Law (dl)" -> "Channel" -> "Porous Matrix 1" in the left menu.
- (e) Modify the value of "Matrix Properties" -> "Porosity" as ϕ_c .
- (f) Modify the value of "Matrix Properties" -> "Permeability model" -> " κ " as k_c .

B6-6. Initial condition

Nothing needs to be done for the initial value because the pressure is defined as its deviation from the initial (hydrostatic) pressure in the present treatment, and zero pressure is the default for Darcy's Law physics.

B6-7. Boundary condition at the inlet

- (a) Right click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" and select ``Inlet".
- (b) Click the bottom of the channel from the geometry in the right window to select it as the inlet.
- (c) In the ``Velocity" -> ``Normal inflow velocity" field in the middle window, set the value as ``Vin".

B6-8. Boundary condition at the outlet

- (a) Right click ``Component 1 (comp1)" -> ``Darcy's Law (dl)" and select ``Outlet".
- (b) Click the top of the OED (both the YED–OED boundary and the ground surface above the OED; blue in Fig. 1b) from the geometry in the right window to select it as the outlet.
- (c) Change ``Boundary Condition" -> ``Boundary condition" in the middle window from ``Velocity" to ``Pressure". The default value (0) for the outlet pressure needs not be modified because the pressure in this simulation is defined as its deviation from the hydrostatic pressure.

B7. Setting heat transfer physics

As in Darcy's Law physics (Section B6), pressure $p + P_{hs}(r, z)$ and temperature $\min(T, T_{in})$ were used to compute the flow properties in the heat transfer physics. The domain applied to this physics was the same as that used in Darcy's law (OED and the channel).

B7-1. Domain selection

- (a) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" in the left menu.
- (b) Deselect the YED, basement (except for the channel), and infinite elements from the domain selection; remain only the OED and channel be selected.

B7-2. Fluid properties (OED)

- (a) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``Porous

Medium 1" and change the label as ``OED"; simply rename the label without modifying the domain selection now.

- (b) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``OED" -> ``Fluid 1" in the left menu.
- (c) Change ``Model Input" -> ``Absolute pressure" in the middle window from ``Common model input" to ``User defined" and set the value as `` $p + P_{hs}(r,z)$ ".
- (d) Change ``Heat Convection" -> ``Velocity field" in the middle window from ``User defined" to ``Darcy's velocity field (dl)".
- (e) Change ``Heat Conduction, Fluid" -> ``Thermal conductivity" in the middle window from ``From material" to ``User defined" and set the value as `` $\text{ThermalConductivity}_{pp1}(\min(T, T_{in}), p + P_{hs}(r,z))$ ".
- (e) Change ``Thermodynamics, Fluid" -> ``Density" in the middle window from ``From material" to ``User defined" and set the value as `` $\text{Density}_{pp1}(\min(T, T_{in}), p + P_{hs}(r,z))$ ".
- (f) Change ``Thermodynamics, Fluid" -> ``Heat capacity at constant pressure" in the middle window from ``From material" to ``User defined" and set the value as `` $\text{HeatCapacity}_{C_{ppp1}}(\min(T, T_{in}), p + P_{hs}(r,z))$ ".
- (g) Change ``Thermodynamics, Fluid" -> ``Ratio of specific heats" in the middle window from ``Automatic" to ``User defined" and set the value as `` $\text{HeatCapacityRatio}_{C_p C_{vpp1}}(\min(T, T_{in}), p + P_{hs}(r,z))$ ".

B7-3. Porous matrix properties (OED)

- (a) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``OED" -> ``Porous matrix 1" in the left menu.
- (b) Change ``Model Input" -> ``Absolute pressure" in the middle window from ``Common model input" to ``User defined" and set the value as `` $p + P_{hs}(r,z)$ ".
- (c) Change ``Matrix Properties" -> ``Porosity" in the middle window from ``From material" to ``User defined" and set the value as `` ϕ_o ".
- (d) Change ``Matrix Properties" -> ``Define" in the middle window from ``Dry bulk properties" to ``Solid phase properties".
- (e) Change ``Heat Conduction, Porous Matrix" -> ``Solid phase thermal conductivity" in the middle window from ``From material" to ``User defined" and set the value as `` K_s ".

- (f) Change ``Thermodynamics, Porous Matrix" -> ``Solid phase density" in the middle window from ``From material" to ``User defined" and set the value as ``rho_so".
- (g) Change ``Thermodynamics, Porous Matrix" -> ``Solid phase heat capacity at constant pressure" in the middle window from ``From material" to ``User defined" and set the value as ``C_ps".

B7-4. Fluid and porous matrix properties (channel)

The easiest way to define the material properties in the channel is to copy the settings of the OED and modify the values of the matrix properties; no modification is required for the fluid properties.

- (a) Right click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> "OED" and click ``Duplicate".
- (b) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> "OED1" and rename the label as ``Channel".
- (c) Deselect the OED from the domain selection. After this step, the domain selections for the OED and the channel are both correct.
- (d) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``Channel" -> ``Porous Matrix 1" in the left menu.
- (e) Modify the value of ``Matrix Properties" -> ``Porosity" as ``phi_c".
- (f) Modify the value of ``Heat Conduction, Porous Matrix" -> ``Solid phase density" as ``rho_sb".

B7-5. Initial condition

- (a) Click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" -> ``Initial Values 1" in the left menu.
- (b) Set the value of the initial temperature as ``Tout".

B7-6. Boundary condition at the inlet

- (a) Right click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" in the left menu and select ``Temperature".
- (b) Change the label in the middle window from ``Temperature 1" to ``Temperature (inlet)".

- (c) Click the bottom of the channel from the geometry in the right window to select it as the inlet.
- (d) In the ``Temperature" -> ``Temperature" field in the middle window, set the value as ``Tin".

B7-7. Boundary condition at the outlet

- (a) Right click ``Component 1 (comp1)" -> ``Heat Transfer in Porous Media (ht)" in the left menu and select ``Temperature".
- (b) Change the label in the middle window from ``Temperature 2" to ``Temperature (outlet)".
- (c) Click the top of the OED (both the YED–OED boundary and the ground surface above the OED; blue in Fig. 1b) from the geometry in the right window to select it as the outlet.
- (d) In the ``Temperature" -> ``Temperature" field in the middle window, set the value as ``Tout".

B8. Setting solid mechanics physics

B8-1. Matrix properties for YED

- (a) Click ``Solid Mechanics (solid)" -> ``Linear Elastic Material 1" and change the label as ``YED"; simply rename the label without modifying the domain selection now.
- (b) Change ``Linear Elastic Material" -> ``Specify" in the middle window from ``Young's modulus and Poisson's ratio" to ``Pressure-wave and shear-wave speeds".
- (c) Change ``Linear Elastic Material" -> ``Pressure-wave speed" in the middle window from ``From material" to ``User defined" and set the value as ``Vpy".
- (d) Change ``Linear Elastic Material" -> ``Shear-wave speed" in the middle window from ``From material" to ``User defined" and set the value as ``Vsy".
- (e) Change ``Linear Elastic Material" -> ``Density" in the middle window from ``From material" to ``User defined" and set the value as ``rho_sy".

B8-2. Matrix properties for OED

The easiest way to define the material properties in the OED is to copy the settings of

the YED and modify the values of the matrix properties.

- (a) Right click ``Component 1 (comp1)" -> ``Solid Mechanics (solid)" -> "YED" and click ``Duplicate".
- (b) Click ``Component 1 (comp1)" -> ``Solid Mechanics (solid)" -> "YED1" and rename the label as ``OED".
- (c) Deselect all geometric elements other than the OED in the right window.
- (d) Modify the value of ``Linear Elastic Material" -> ``Pressure-wave speed" in the middle window as ``V_{po}".
- (e) Modify the value of ``Linear Elastic Material" -> ``Shear-wave speed" in the middle window as ``V_{so}".
- (f) Modify the value of ``Linear Elastic Material" -> ``Density" in the middle window as ``ρ_{so}".

B8-3. Matrix properties for the basement

The material properties of the basement were set in the same manner as those of the OED. In the solid mechanics, the material properties of the basement were applied to the channel and the infinite elements.

- (a) Right click ``Component 1 (comp1)" -> ``Solid Mechanics (solid)" -> "YED" and click ``Duplicate".
- (b) Click ``Component 1 (comp1)" -> ``Solid Mechanics (solid)" -> "YED1" and rename the label as ``Basement".
- (c) Deselect YED and OED geometry elements in the right window; remain the channel, basement, and the two infinite elements be selected.
- (d) Modify the value of ``Linear Elastic Material" -> ``Pressure-wave speed" in the middle window as ``V_{pb}".
- (e) Modify the value of ``Linear Elastic Material" -> ``Shear-wave speed" in the middle window as ``V_{sb}".
- (f) Modify the value of ``Linear Elastic Material" -> ``Density" in the middle window as ``ρ_{sb}".

B8-4. Boundary conditions

By default, a free surface boundary condition is applied to the Solid Mechanics physics.

The outer sides of infinite elements must be changed to fixed boundaries.

- (a) Right click ``Component 1 (comp1)" -> ``Solid Mechanics (solid)" and select ``Fixed Constraint".
- (b) Select the right and bottom boundaries of the entire domain from the geometry in the right window.

B8-5. Infinite elements

- (a) Right click ``Component 1 (comp1)" -> ``Definitions" and select ``Infinite Element Domain".
- (b) Select right and bottom infinite elements from the geometry in the right window.
- (c) Change ``Geometry" -> ``Type" in the middle window from ``Spherical" to ``Cylindrical".

B9. Poroelasticity multiphysics

The crustal deformation caused by the pore-fluid pressure change was computed using ``Poroelasticity" multiphysics, which was introduced and configured as follows.

- (a) Right click ``Component 1 (comp1)" -> ``Multiphysics" and select ``Poroelasticity".
- (b) Select the OED and channel from the geometry in the right window for the domain selection.
- (c) Change ``Poroelastic Coupling Properties" -> ``Biot-Willis coefficient" in the middle window from ``From material' to ``User defined" and set the value as ``alpha_B".

B10. Identification of phase

Functions to identify the phase type (liquid, gas, or supercritical) were prepared before computation.

B10-1. Existence or absence of liquid and vapor phases

A built-in function `Flash1_1_PhaseExist_Vapor` is available in COMSOL Multiphysics, which gives 1 if the vapor phase is present at a given temperature and pressure, and 0 otherwise. This function was activated through the following steps.

- (a) Right click ``Global Definitions" -> ``Thermodynamics" -> ``Vapor-Liquid System 1

- (pp1)" and select "Equilibrium Calculation".
- (b) Double click "water" in the middle window to add it into "Selected species" and click "Next".
- (c) Check that the amount base unit is "kg" and the first and second equilibrium conditions are "Temperature" and "Pressure". Click "Next".
- (d) Click "Finish".

B10-2. Critical temperature and pressure.

- (a) Right click "Global Definitions" -> "Thermodynamics" -> "Vapor-Liquid System 1 (pp1)" -> "water" and select "Species Property".
- (b) Change "Amount base unit" in the middle window from "mol" to "kg".
- (c) Double click "Critical temperature (K)" and "Critical pressure (Pa)" in the middle window to add them into "Selected properties", and click "Next".
- (d) Click "Finish".
- (e) Click "Global Definitions" -> "Parameters 1" and add the constants listed in Table S14.

Table 14. Constants representing the critical point of water.

Name	Expression	Description
Tc	CriticalTemperature_water11	Critical temperature of water
Pc	CriticalPressure_water12	Critical pressure of water

B10-3. A function to identify the phase type

The function `Flash1_1_PhaseExist_Vapor` (Section B10-1) did not behave correctly in the supercritical region. Therefore, a function "Phase" was created, which returns 2 if the phase of water at a given temperature and pressure is vapor, 1 if supercritical, and 0 if liquid. This function used the following branches. First, the phase was identified as supercritical if both temperature and pressure exceeded the critical point. Next, the phase was identified as vapor if the temperature exceeded the critical point but the pressure did not, and identified as liquid if via versa. Finally, if both the temperature and pressure were below the critical point, the function `Flash1_1_PhaseExist_Vapor` was used to identify whether a gas or liquid phase was present. These branches were realized as follows.

- (a) Right click ``Global Definitions" and select ``Functions" -> ``Analytic".
- (b) Change the label and function name in the middle window as ``Phase"
- (c) Modify ``Definition" -> ``Expression" in the middle window as

$$\text{``}(T \geq T_c) * (P \geq P_c) + 2 * (T \geq T_c) * (P < P_c) + 2 * (T < T_c) * (P < P_c) * \text{Flash1_1_PhaseExist_Vapor}(T, P, 1)\text{'}$$
- (d) Modify ``Definition" -> ``Arguments" in the middle window as ``T,P".
- (e) Write ``1" in ``Units" -> ``Function" field in the middle window.
- (f) Write ``K" in ``Units" -> ``Argument" -> ``T" field in the middle window.
- (g) Write ``Pa" in ``Units" -> ``Argument" -> ``P" field in the middle window.

B11. Refining the mesh size

The default mesh size was not fine enough to obtain stable simulation results. Therefore, a finer mesh size was used.

- (a) Click ``Component 1 (comp1)" -> ``Mesh 1".
- (b) Change ``Physics-Controlled Mesh" -> ``Element size" in the middle window from
 ``Normal" to ``Extremely fine".
- (c) Click ``Build All".

B12. Study

Solving all physics simultaneously resulted in numerical instabilities in many choices of parameters. Therefore, Darcy's Law and Heat Transfer in Porous Media physics were solved first, and then the results were used to compute the crustal deformation (one-way coupling).

B12-1. Solving Darcy's law and heat transfer physics

- (a) Click ``Study 1" -> ``Step 1: Time Dependent" in the left menu.
- (b) Change ``Study Settings" -> ``Time unit" in the middle window from ``s" to ``d".
- (c) Change ``Study Settings" -> ``Output times" in the middle window as

$$\text{``range}(0, 1, 1000)\text{'}$$
 This means that the results were evaluated every 1 day for up to 1000 days. For some parameters, the computation did not progress for this length of time. In this case, a shorter length of 600 days was used.

- (d) In "Physics and Variables Selection" section in the middle window, deselect "Solid Mechanics (solid)" and "Poroelectricity 1 (poro1)".
- (e) Click "Compute".

B12-2. Solving the solid mechanics physics

- (a) Right click "File name (root)" at the top of the left menu and select "Add Study".
- (b) Select "General Studies" -> "Time Dependent" in the right window and click "Add Study".
- (c) Click "Study 2" -> "Step 1: Time Dependent" in the left menu.
- (d) Change "Study Settings" -> "Time unit" in the middle window from "s" to "d".
- (e) Change "Study Settings" -> "Output times" in the middle window as "range(0,1,1000)".
- (f) In "Physics and Variables Selection" section in the middle window, deselect "Darcy's Law (dl)" and "Heat Transfer in Porous Media (ht)".
- (g) Change "Values of Dependent Variables" -> "Values of variables not solved for" -> "Settings" in the middle window from "Physics controlled" to "User controlled".
- (h) Change "Values of Dependent Variables" -> "Values of variables not solved for" -> "Method" in the middle window from "Initial expression" to "Solution".
- (i) Change "Values of Dependent Variables" -> "Values of variables not solved for" -> "Study" in the middle window from "Zero solution" to "Study 1, Time Dependent".
- (j) Change "Values of Dependent Variables" -> "Values of variables not solved for" -> "Time (d)" from "Automatic (single solution)" to "Automatic (all solutions)".
- (k) Click "Compute".

B13. Evaluating the results

The computational results were evaluated from two perspectives: when and where the vapor phase was first observed and how much displacement occurred on the ground surface.

B13-1. Time and location of vaporization

- (a) Right click "Results" -> "Derived Values" and select "Maximum" -> "Surface Maximum".

- (b) Select the OED and channel from the geometries in the right window.
- (c) In the ``Expression" field in the middle window, remove ``p" and ``T" in the table and write ``Phase(min(T,Tin),p+Phs(r,z))".
- (d) Check ``Configuration" -> ``Include position" in the middle window.
- (e) Click ``Evaluate".

Then, the maximum values of the phase function (2: vapor, 1: supercritical, and 0: liquid) for each time step are summarized in the bottom-right window.

B13-2. Ground surface deformation

- (a) Right click ``Results" -> ``Derived Values" and select ``Maximum" -> ``Line Maximum".
- (b) Select ``Study 2/Solution 2 (sol2)" from ``Data" -> ``Dataset" in the middle window.
- (c) Select the ground surface (other than infinite elements) from the geometries in the right window.
- (d) In the ``Expression" field in the middle window, remove ``p" and ``T" in the table. Then, click the inverse triangle at the right of the ``Expression" section in the middle window and select ``Component 1 (comp1)" -> ``Solid Mechanics" -> ``Displacement" -> ``solid.disp - Displacement magnitude - m".
- (e) Click ``Evaluate".

B13-3. Pressure distribution for a given time step

- (a) Click ``Results" -> ``Pressure (dl)" -> ``Surface" in the left menu.
- (b) Modify ``Expression" -> ``Expression" field as ``p+Phs(r,z)".
- (c) Click ``Results" -> ``Pressure (dl)" in the left menu.
- (d) Select a time step concerned from ``Data" -> ``Time (d)" field in the middle window and click ``Plot".
- (e) Right click ``Results" -> ``Pressure (dl)" -> ``Surface" in the left menu and select ``Add Plot Data to Export".
- (f) Define the output file name in ``Output" -> ``Filename" field in the middle window and Click ``Export". This step creates a text file that consists of the pressures on all mesh nodes at the selected time step.

B13-4. Temperature distribution for a given time step

Same as Section A8-2.

B13-5. Density and specific volume distributions for a given time step

Although the `Densitypp1` function (Section A3) yielded a good approximation for the water density, there were some differences in the temperature–pressure conditions between the jump in the density from liquid to vapor and the phase boundary based on the function `Flash1_1_PhaseExist_Vapor` (Section B10). Consequently, a low-density region corresponding to the vapor phase was absent in some cases if the density was evaluated based on `Densitypp1` at the time step when Section B13-1 indicated that the vapor phase was present. Careful examination suggested that the function `Flash1_1_PhaseExist_Vapor` was more accurate for the phase boundary. Therefore, this study used the results of Section B13-1 to determine the time step of the phase transition and then re-computed the densities from the temperature and pressure distribution exported in Section B13-3 using IAPWS-95 (Wagner and Pruss 2002) that was implemented in `ymaeda_opentools` (Maeda 2022).

References not in the main text

- Gardner GHF, Gardner LW, Gregory AR (1974) Formation velocity and density – The diagnostic basics for stratigraphic traps. *Geophysics* 39(6):770–780. <https://doi.org/10.1190/1.1440465>
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