

1 Cylindrical Void Thermomigration Benchmark

1.1 Introduction

This benchmark considers the thermomigration of a cylindrical void in a solid subjected to an imposed temperature gradient. The objective is to develop a simple analytic or semi-analytic reference solution that can be compared with finite element calculations in which surface diffusion transports material around the void surface. The benchmark is intended to test the thermal solution, the thermomigration contribution to the surface flux, and the conversion of the resulting deposition/removal rates into a void migration velocity.

The two-dimensional cylindrical void problem is also a useful stepping stone toward later three-dimensional calculations. In three dimensions, a void in a box can be interpreted as a representative cell for a periodic array of voids in metallic nuclear fuel. The resulting cell calculations can then be used to construct homogenized descriptions of macroscopic mass transport under a macroscopic temperature gradient. The present two-dimensional benchmark provides a simpler setting in which the same basic ideas can be tested.

Two analytic comparisons are considered. The first is an isolated cylindrical void in an infinite medium subjected to a uniform temperature gradient. This problem has a closed-form solution and provides a transparent derivation of the surface temperature, deposition/removal rate, and void velocity. The second is a cylindrical void in a finite box with specified temperatures on the left and right boundaries and insulated top and bottom boundaries. This finite box problem is the problem solved in the finite element benchmark. It can also be interpreted as a representative cell for a periodic array of cylindrical voids, where the insulated top and bottom boundaries correspond to symmetry planes between neighboring voids transverse to the imposed temperature gradient.

1.2 Objective

The objective of this benchmark is to determine whether the finite element implementation reproduces the thermomigration-driven translation velocity of a cylindrical void. The calculation assumes that the void remains circular during translation. This assumption is appropriate when the void is small enough, and the surface energy is large enough, that capillarity suppresses shape changes while allowing the void to translate.

The benchmark does not impose the void velocity directly. Instead, the thermal elements compute the temperature field in the solid. The surface diffusion elements use the tangential temperature gradient on the void surface to compute a thermomigration-driven surface flux. The divergence of this flux gives the normal deposition/removal rate on the void surface. The void velocity is then extracted from the deposition/removal rates at the left and right sides of the void.

1.3 Analytic Solutions

1.3.1 Void in an Infinite Medium

Consider a cylindrical void of radius a in an infinite solid. The void center is located at $x = X$, and the far-field temperature is assumed to be linear in x :

$$T_b(x) = T_h + Gx, \quad (1.1)$$

where

$$G = \frac{T_c - T_h}{L}. \quad (1.2)$$

For a problem in which the left side is hot and the right side is cold, $T_h > T_c$, and therefore

$$G < 0. \quad (1.3)$$

Local polar coordinates are introduced around the void center:

$$x = X + r \cos \theta, \quad (1.4)$$

$$y = r \sin \theta. \quad (1.5)$$

The angle $\theta = 0$ corresponds to the right side of the void, and $\theta = \pi$ corresponds to the left side of the void.

For an insulating cylindrical void in an infinite medium, the temperature field is

$$T(r, \theta) = T_b(X) + G \left(r + \frac{a^2}{r} \right) \cos \theta. \quad (1.6)$$

This solution satisfies Laplace's equation in the solid, approaches the imposed linear temperature field far from the void, and gives zero normal heat flux on the void surface. The temperature on the void surface is obtained by setting $r = a$:

$$T_s(\theta) = T_b(X) + 2aG \cos \theta. \quad (1.7)$$

The surface temperature is therefore a first harmonic in θ , with amplitude $2aG$.

Let s denote arclength along the void surface. Since

$$s = a\theta, \quad (1.8)$$

the first and second derivatives of the surface temperature are

$$\frac{\partial T_s}{\partial s} = -2G \sin \theta, \quad (1.9)$$

$$\frac{\partial^2 T_s}{\partial s^2} = -\frac{2G}{a} \cos \theta. \quad (1.10)$$

For this benchmark, the thermomigration surface flux is written in the form

$$J_T = -M_T \frac{\partial T_s}{\partial s}, \quad (1.11)$$

where M_T is the thermomigration mobility. The corresponding normal material deposition/removal rate is

$$v_n = -\Omega \frac{\partial J_T}{\partial s}, \quad (1.12)$$

where Ω is the atomic volume. Combining Equations (1.11) and (1.12) gives

$$v_n = K_T \frac{\partial^2 T_s}{\partial s^2}, \quad (1.13)$$

where

$$K_T = \Omega M_T. \quad (1.14)$$

The coefficient K_T is treated as constant in the analytic benchmark.

Using Equation (1.10), the thermomigration-driven normal deposition/removal rate is

$$v_n(\theta) = -\frac{2K_T G}{a} \cos \theta. \quad (1.15)$$

Since $G < 0$ for a hot-left, cold-right problem, Equation (1.15) predicts positive deposition on the right side of the void and negative deposition on the left side of the void.

It remains to relate the normal deposition/removal rate to the void translation velocity. The unit normal used by HeavyMetal points outward from the solid surface. On an internal void surface, this normal points into the void. Thus, on the left side of the void,

$$\mathbf{n}_L = \mathbf{e}_x, \quad (1.16)$$

and on the right side of the void,

$$\mathbf{n}_R = -\mathbf{e}_x. \quad (1.17)$$

If the void translates with velocity

$$\mathbf{V}_{\text{void}} = V_{\text{void}} \mathbf{e}_x, \quad (1.18)$$

then the scalar normal velocity on a circular void is

$$v_n(\theta) = -V_{\text{void}} \cos \theta. \quad (1.19)$$

Comparison of Equations (1.15) and (1.19) gives the analytic void velocity

$$V_{\text{void}} = \frac{2K_T G}{a}. \quad (1.20)$$

For a hot-left, cold-right problem, $G < 0$, so the predicted velocity is negative. The void therefore migrates toward the hot side.

The same result can be obtained directly from the deposition/removal rates at the left and right sides of the void. Let

$$v_{n,L} = v_n(\pi), \quad (1.21)$$

$$v_{n,R} = v_n(0). \quad (1.22)$$

For rigid translation of a circular void,

$$v_{n,L} = V_{\text{void}}, \quad (1.23)$$

$$v_{n,R} = -V_{\text{void}}. \quad (1.24)$$

Therefore the void velocity can be computed from the two endpoint values as

$$V_{\text{void}} = \frac{v_{n,L} - v_{n,R}}{2}. \quad (1.25)$$

This is the primary scalar quantity used for comparison with the finite element solution.

1.3.2 Void in a Finite Box

The finite element benchmark uses a cylindrical void in a rectangular box. The box has length L in the direction of the imposed temperature gradient and height H transverse to the gradient. The left boundary is held at temperature T_h , and the right boundary is held at temperature T_c . The top and bottom boundaries are insulated. The cylindrical void is also thermally insulating.

The finite box problem can also be interpreted as a representative cell for a periodic array of cylindrical voids. The insulated top and bottom boundaries correspond to symmetry planes between neighboring voids in the direction transverse to the imposed temperature gradient. The specified temperatures on the left and right boundaries impose the macroscopic thermal gradient across the representative cell. In this sense, the finite box model provides a simple way to include void-to-void thermal interactions while retaining a well-defined, easily reproducible benchmark problem.

The thermal problem is

$$\nabla^2 T = 0 \quad (1.26)$$

in the solid, with boundary conditions

$$T = T_h \quad \text{on} \quad x = 0, \quad (1.27)$$

$$T = T_c \quad \text{on} \quad x = L, \quad (1.28)$$

$$\frac{\partial T}{\partial y} = 0 \quad \text{on} \quad y = \pm H/2, \quad (1.29)$$

and

$$\frac{\partial T}{\partial n} = 0 \quad \text{on} \quad \Gamma_v, \quad (1.30)$$

where Γ_v is the void surface and $\mathbf{n}$ is the outward normal from the solid.

It is useful to decompose the temperature field into the background linear solution and a disturbance caused by the void:

$$T(x, y) = T_b(x) + u(x, y), \quad (1.31)$$

where

$$T_b(x) = T_h + Gx. \quad (1.32)$$

The disturbance u satisfies

$$\nabla^2 u = 0 \quad (1.33)$$

with homogeneous boundary conditions on the external box boundaries:

$$u = 0 \quad \text{on} \quad x = 0 \quad \text{and} \quad x = L, \quad (1.34)$$

$$\frac{\partial u}{\partial y} = 0 \quad \text{on} \quad y = \pm H/2. \quad (1.35)$$

On the void surface,

$$\frac{\partial u}{\partial n} = -Gn_x. \quad (1.36)$$

This equation states that the disturbance cancels the normal heat flux that the background linear temperature field would otherwise produce on the insulating void surface.

The finite box solution does not reduce to a simple elementary expression like Equation (1.6). However, the boundary value problem is linear and can be solved independently of the finite element surface evolution calculation. One convenient semi-analytic representation uses a Green's function that satisfies the homogeneous boundary conditions on the outer rectangular boundary. The disturbance may be written formally as

$$u(\mathbf{x}) = \int_{\Gamma_v} \rho(\boldsymbol{\xi}) G_R(\mathbf{x}, \boldsymbol{\xi}) d\Gamma_{\boldsymbol{\xi}}, \quad (1.37)$$

where G_R is the rectangular Green's function and ρ is an unknown source strength distributed around the void surface. The source strength is chosen so that Equation (1.36) is satisfied on Γ_v . The resulting surface temperature is then

$$T_s(\theta) = T_b(X + a \cos \theta) + u(X + a \cos \theta, a \sin \theta). \quad (1.38)$$

For a void centered vertically in the box, symmetry about the horizontal mid-plane eliminates sine terms in the surface temperature expansion. The surface temperature may therefore be written as

$$T_s(\theta) = T_0 + \sum_{m=1}^{\infty} A_m \cos(m\theta), \quad (1.39)$$

where the coefficients A_m depend on the void radius, the box dimensions, and the void position. In the isolated-void limit, the leading coefficient approaches

$$A_1 \rightarrow 2aG, \quad (1.40)$$

and the higher-order coefficients approach zero.

Using Equation (1.13), the corresponding normal deposition/removal rate is

$$v_n(\theta) = -\frac{K_T}{a^2} \sum_{m=1}^{\infty} m^2 A_m \cos(m\theta). \quad (1.41)$$

The first harmonic represents the rigid-translation component of the normal velocity field. The corresponding first-harmonic void velocity is

$$V_1 = \frac{K_T A_1}{a^2}. \quad (1.42)$$

For the isolated-void solution, $A_1 = 2aG$, and Equation (1.42) reduces to Equation (1.20).

The endpoint velocity measure used in the finite element comparison is

$$V_{\text{end}} = \frac{v_{n,L} - v_{n,R}}{2}. \quad (1.43)$$

Using Equation (1.41), this may be written as

$$V_{\text{end}} = \frac{K_T}{a^2} (A_1 + 9A_3 + 25A_5 + \dots). \quad (1.44)$$

Thus, the endpoint measure equals the first-harmonic migration velocity when the deposition/removal field is dominated by the first harmonic. Higher odd harmonics contribute to the endpoint value and provide a useful diagnostic of finite-box effects and shape-change tendencies. For a small void in a large box, these higher harmonics are expected to be small, and V_{end} approaches V_1 .

1.4 Benchmark Setup

The benchmark uses a rectangular cell containing a circular cylindrical void. The finite element calculations were performed using half-symmetry about the horizontal mid-plane, $y = 0$. The lower half of the void was not included in the computational mesh. Where full-pore images are shown below, the computed field has been reflected across the symmetry plane for visualization only.

The cell dimensions were scaled with the pore radius. For each radius a , the left and right thermal boundaries were placed at

$$x = -2a \quad \text{and} \quad x = 2a, \quad (1.45)$$

and the upper boundary of the half-symmetry model was placed at $y = 2a$. The reflected visualization therefore corresponds to a full cell with dimensions $4a \times 4a$. The resulting two-dimensional pore area fraction is

$$f_A = \frac{\pi a^2}{(4a)(4a)} = \frac{\pi}{16} \approx 0.196. \quad (1.46)$$

Thus, the radius series isolates the effect of pore size at fixed normalized geometry. Finite-volume-fraction effects can be assessed in later calculations by varying the cell size at fixed pore radius.

The imposed macroscopic temperature gradient was

$$G = \frac{dT}{dx} = -100 \text{ }^\circ\text{C/mm}, \quad (1.47)$$

with the left boundary hotter than the right boundary. The boundary temperature was centered about $900 \text{ }^\circ\text{C}$, so that

$$T(-2a) = 900 - 2aG, \quad T(2a) = 900 + 2aG, \quad (1.48)$$

where a is expressed in mm. The pore surface was treated as thermally insulating. Surface diffusion was active on the pore surface, with the thermomigration coefficient evaluated from the material parameters in the surface-diffusion material file.

For the analytic comparison, the thermomigration coefficient was written as

$$K_T = \Omega M_s \frac{Q^*}{T_{\text{ref}}}, \quad (1.49)$$

where T_{ref} is the absolute reference temperature. The material parameters used in the calculations are summarized in Table 1.1.

Table 1.1: Primary input parameters for the cylindrical void thermomigration benchmark. The cell size and boundary temperatures were scaled with pore radius so that all cases used the same normalized geometry and the same imposed macroscopic temperature gradient.

Parameter	Symbol	Value	Units
Pore radii	a	0.1, 1, 10, 100	μm
Horizontal cell extent	–	$-2a \leq x \leq 2a$	mm
Half-symmetry vertical extent	–	$0 \leq y \leq 2a$	mm
Macroscopic temperature gradient	G	-100	$^\circ\text{C/mm}$
Reference temperature	T_{ref}	≈ 1173.15	K
Atomic volume	Ω	2.07×10^{-20}	mm^3/atom
Heat of transport	Q^*	3.2654×10^{-17}	N mm/atom
Surface mobility	M_s	3.37166×10^{27}	$\text{atoms}^2/(\text{N mm s})$
Transport prefactor	K_T	$\approx 1.94266 \times 10^{-12}$	$\text{mm}^3/(\text{K s})$

The analytic velocity used for comparison was evaluated from the temperature variation computed on the pore surface. If T_L and T_R denote the reference surface temperatures at the left and right sides of the pore, respectively, then

$$A_1 = \frac{T_R - T_L}{2} \quad (1.50)$$

is the first-harmonic surface-temperature coefficient. The corresponding analytic migration velocity is

$$V_{\text{analytic}} = K_T \frac{A_1}{a^2} = K_T \frac{T_R - T_L}{2a^2}. \quad (1.51)$$

This surface-temperature comparison was used as the primary analytic reference. The velocity obtained from the imposed boundary gradient was also computed as a diagnostic, but the surface-temperature value is the more direct comparison because the thermomigration surface flux is driven by the temperature variation on the pore surface.

The finite element void velocity was extracted from the displacement histories of the left and right pore nodes. Equivalently, it may be interpreted as the endpoint velocity measure

$$V_{\text{void}} = \frac{v_{n,L} - v_{n,R}}{2}, \quad (1.52)$$

where $v_{n,L}$ and $v_{n,R}$ are the deposition/removal rates at the left and right void-surface symmetry nodes. For the hot-left, cold-right orientation, the expected signs are

$$v_{n,L} < 0, \quad (1.53)$$

$$v_{n,R} > 0, \quad (1.54)$$

and therefore

$$V_{\text{void}} < 0. \quad (1.55)$$

The negative sign indicates motion toward the hot side of the cell.

1.5 Results

Figure 1.1 shows the temperature field for the $a = 10 \mu\text{m}$ case at the beginning of the analysis, at an intermediate time, and at the end of the analysis. The results have been reflected across the $y = 0$ symmetry plane for visualization. The pore migrates toward the hot side of the domain while remaining nearly circular. The temperature field moves with the pore, and the first-harmonic variation of temperature on the pore surface remains the dominant thermomigration driving term.

The primary velocity comparison is given in Table 1.2. The finite element velocity agrees closely with the analytic velocity evaluated from the pore-surface temperature variation for all four pore radii. The largest relative error is 5.90×10^{-4} for the $100 \mu\text{m}$ case, and the relative error is less than 3×10^{-5} for the three smaller radii.

Figure 1.2 compares the finite element velocities with the analytic prediction over three orders of magnitude in pore radius. The analytic solution predicts

$$|V_{\text{void}}| \propto \frac{1}{a} \quad (1.56)$$

for a fixed macroscopic thermal gradient and fixed material properties. The finite element results reproduce this scaling over the full radius range.

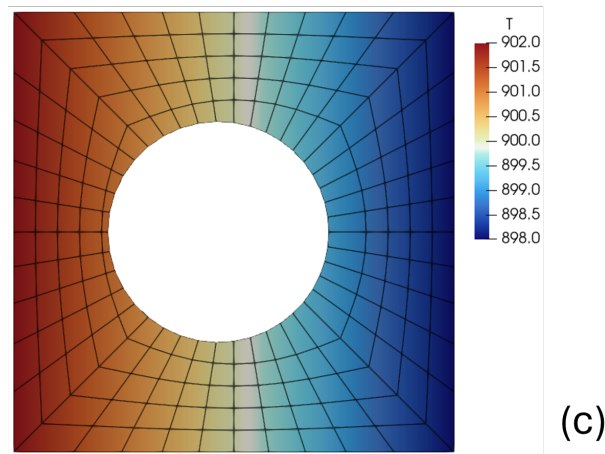
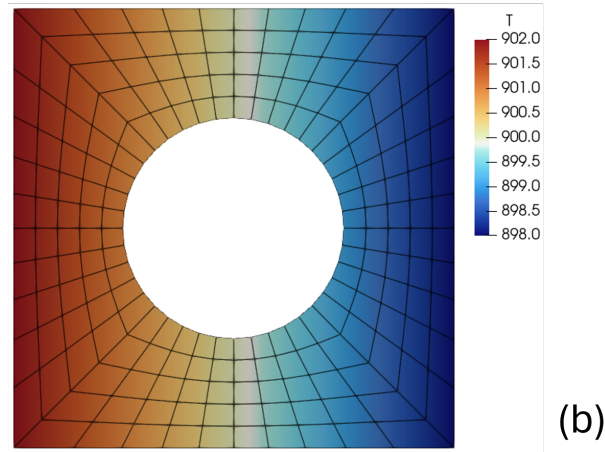
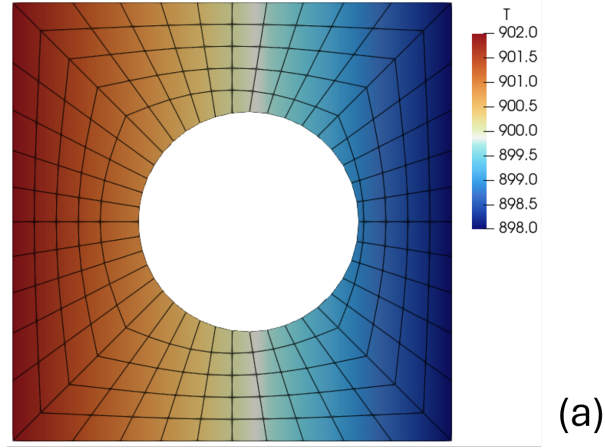


Figure 1.1: Temperature field for the $a = 10 \mu\text{m}$ 2D single-pore thermomigration benchmark at (a) the beginning of the analysis, (b) an intermediate time, and (c) the end of the analysis. The finite element model used half-symmetry about the $y = 0$ axis; the results shown here have been reflected across the symmetry plane for visualization. The pore migrates toward the hot side of the domain while remaining nearly circular.

Table 1.2: Finite element and analytic pore velocities for the 2D single-pore thermomigration benchmark. The analytic velocity is evaluated from the first-harmonic temperature variation on the pore surface.

a (μm)	V_{FE} (mm/s)	V_{analytic} (mm/s)	Absolute error (mm/s)	Relative error —
0.1	$-1.9428690 \times 10^{-6}$	$-1.9429174 \times 10^{-6}$	4.8390×10^{-11}	2.4906×10^{-5}
1	$-1.9427063 \times 10^{-7}$	$-1.9426867 \times 10^{-7}$	1.9587×10^{-12}	1.0083×10^{-5}
10	$-1.9426466 \times 10^{-8}$	$-1.9426638 \times 10^{-8}$	1.7144×10^{-13}	8.8251×10^{-6}
100	$-1.9415143 \times 10^{-9}$	$-1.9426603 \times 10^{-9}$	1.1460×10^{-12}	5.8991×10^{-4}

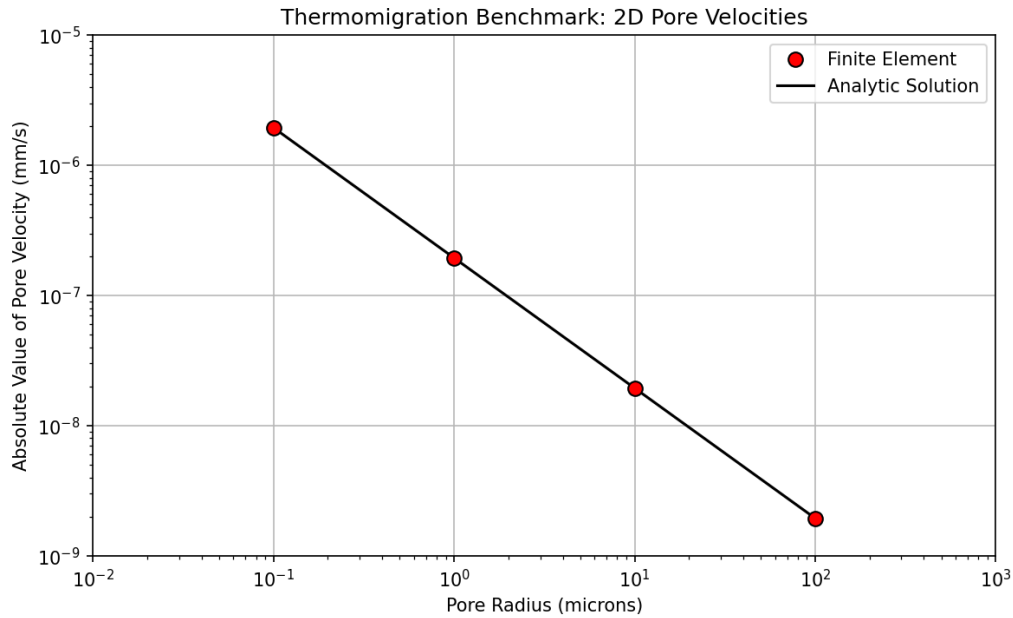


Figure 1.2: Comparison of finite element and analytic pore thermomigration velocities for circular 2D pores with radii from 0.1 to 100 μm . The imposed macroscopic temperature gradient is 100 $^{\circ}\text{C}/\text{mm}$. The analytic solution predicts $|V_{\text{void}}| \propto a^{-1}$, and the finite element velocities agree closely with the analytic prediction over three orders of magnitude in pore radius.

1.6 Discussion

The cylindrical void thermomigration benchmark provides an end-to-end test of the surface thermomigration machinery. The thermal elements compute the insulated-pore temperature field, the surface diffusion elements use the tangential temperature gradient to compute a thermomigration surface flux, and the divergence of that flux produces material removal and deposition around the void surface. With the normal convention used by HeavyMetal, the hot-left, cold-right temperature gradient gives a negative void velocity, meaning that the void migrates toward the hot side of the cell.

The finite element results reproduce the analytic velocity over pore radii from 0.1 to 100 μm . This verifies the expected scaling

$$V_{\text{void}} \propto \frac{G}{a}. \quad (1.57)$$

The scaling is important for later homogenized models of porosity redistribution. At fixed porosity, smaller pores provide more pore surface area per unit bulk volume. Because pore migration is mediated by surface diffusion, this implies that the macroscopic thermomigration transport coefficient depends not only on pore volume fraction, but also on a characteristic pore size or surface area density.

For a distribution of nearly circular or spherical pores, the void-volume flux can be written schematically as

$$\mathbf{J}_v = \int V_p(a) v_p(a) n(a) da, \quad (1.58)$$

where $V_p(a)$ is the volume of one pore, $v_p(a)$ is the pore velocity, and $n(a)$ is the pore number density. Since the present benchmark gives $v_p(a) \propto 1/a$, the resulting macroscopic transport law is controlled by pore surface area per unit bulk volume. Thus, a fine distribution of pores can transport porosity more rapidly than a coarse distribution at the same total porosity.

The present calculations were not intended to follow long-time pore coalescence, shape instability, or topology change. Those problems require improved time integration and remeshing methods. However, the short-time velocity extraction used here is sufficient for estimating the leading-order pore migration coefficient. The benchmark therefore provides the pore-scale validation needed to construct homogenized models of thermomigration-driven porosity redistribution and associated mass transport in metallic nuclear fuel.