

1 Gas Gap and Thermomigration-Induced Surface Instability Benchmark

1.1 Introduction

This benchmark case is intended to show that the combination of heat generation within a solid, heat transfer from the solid to a temperature reservoir through a poorly conducting gas, and a perturbation in the surface profile of the solid can lead to a surface instability by temperature-gradient-driven surface diffusion. The configuration is shown schematically in Figure 1.1. A simple analytic solution for the surface temperature is presented by assuming that heat transfer occurs only in the primary heat-conduction direction. This reduces the thermal problem to a local one-dimensional heat-transfer expression. In order for the finite element solution to match this analytic solution, highly anisotropic thermal conductivities are used in the finite element model, with the conductivities in directions orthogonal to the primary heat-conduction direction taken to be negligible.

A subtle but important feature of this benchmark is that the finite element model uses volumetric heat generation in the perturbed solid. Therefore, the local heat flux through the gas is proportional to the local solid thickness, not to the nominal solid thickness alone. The analytic solution used for this benchmark includes this effect. This distinction is important because using a constant heat flux based only on the nominal solid thickness gives a slightly larger surface-temperature perturbation than the finite element problem actually solves.

Given the temperature distribution on the surface of the solid, the surface transport equation is solved to determine the deposition or removal of material along the surface. By comparing the evolution of the surface temperature and surface profile with the analytic solution, the finite element implementation of thermomigration-driven surface diffusion can be assessed.

1.2 Objective

The objective of this benchmark is to determine whether the finite element implementation reproduces the analytic temperature perturbation and the corresponding thermomigration-driven surface evolution rate for a sinusoidally perturbed surface. The benchmark is useful because the finite element calculation does not impose the analytic growth or decay rate directly. Instead, the thermal solution produces a surface temperature variation. The surface diffusion elements then compute the thermomigration flux from the tangential temperature gradient, and the divergence of that flux determines the normal deposition/removal rate.

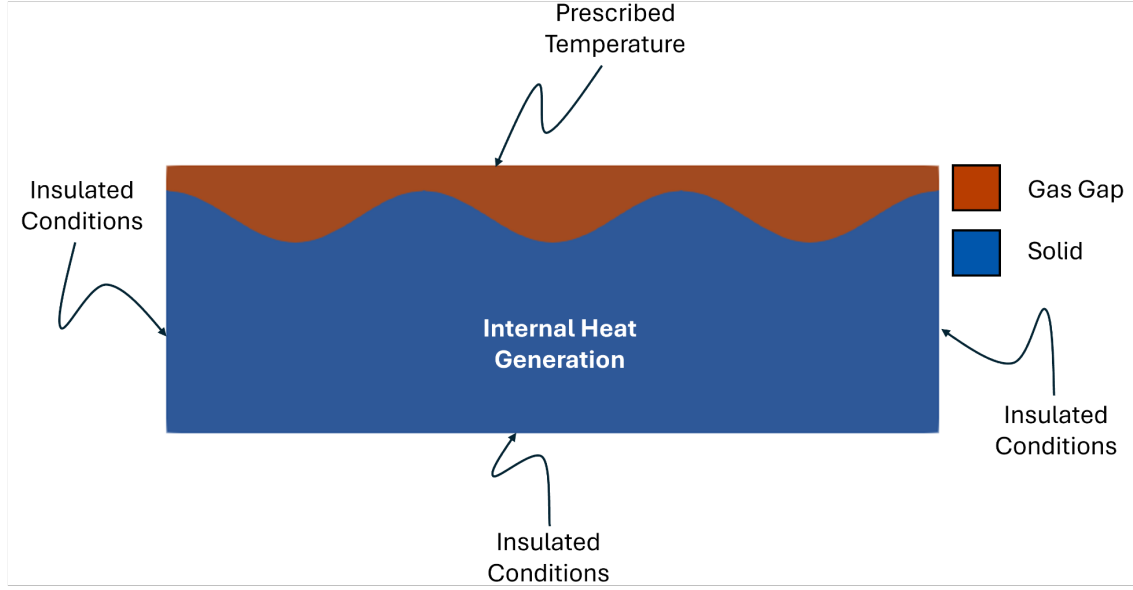


Figure 1.1: Schematic representation of the gas-gap thermomigration benchmark. Heat generated in the solid is conducted through a poorly conducting gas gap to a prescribed-temperature reservoir. A perturbation in the solid surface changes both the local solid thickness and the local gas-gap thickness, which produces a temperature perturbation along the solid surface.

1.3 Analytic Solution

1.3.1 Geometry and Assumptions

The mean solid-gas interface is taken to be at $y = 0$, and the positive y -direction is the primary heat-conduction direction. The nominal solid thickness is H_s and the solid has uniform volumetric heat generation q''' . The lower surface of the solid is insulated. The solid is separated from a temperature reservoir by a gas gap with nominal thickness H_g and gas conductivity k_g . The reservoir temperature is prescribed as T_R .

The solid surface is perturbed sinusoidally:

$$h(x, t) = A(t) \cos(kx), \quad (1.1)$$

where

$$k = \frac{2\pi}{\lambda}. \quad (1.2)$$

The small-slope and small-amplitude assumptions are

$$kA \ll 1, \quad (1.3)$$

and

$$A \ll H_g. \quad (1.4)$$

A positive value of h corresponds to upward motion of the solid surface, which reduces the local gas-gap thickness and increases the local solid thickness. Therefore,

$$g(x, t) = H_g - h(x, t), \quad (1.5)$$

and the local solid thickness is

$$s(x, t) = H_s + h(x, t). \quad (1.6)$$

The analytic solution assumes that heat transfer is locally one-dimensional in the y -direction. Lateral heat conduction is neglected. In the finite element model this condition is approximated by using a highly anisotropic conductivity tensor. The conductivity in the primary heat-conduction direction is retained, while the conductivities in the orthogonal directions are made negligible.

Because the heat generation is volumetric, the heat flux passing upward through the gas gap is proportional to the local solid thickness:

$$q_y(x, t) = q''' [H_s + h(x, t)]. \quad (1.7)$$

This is the key correction relative to a simpler constant-flux approximation. If the heat flux were prescribed as $q''' H_s$ independent of the surface perturbation, the surface-temperature perturbation would be slightly different. The finite element benchmark, however, solves the volumetric heat-generation problem, and Equation (1.7) is the appropriate local-column heat flux.

1.3.2 Surface Temperature

The temperature drop across the gas gap is

$$\Delta T_g(x, t) = \frac{q_y(x, t)g(x, t)}{k_g}. \quad (1.8)$$

Therefore, the temperature at the solid surface is

$$T_s(x, t) = T_R + \frac{q'''}{k_g} [H_s + h(x, t)] [H_g - h(x, t)]. \quad (1.9)$$

For the flat surface, the nominal interface temperature is

$$T_0 = T_R + \frac{q''' H_s H_g}{k_g}. \quad (1.10)$$

Expanding Equation (1.9) gives

$$T_s(x, t) = T_0 - \frac{q'''}{k_g} [(H_s - H_g)h(x, t) + h^2(x, t)]. \quad (1.11)$$

In the linear small-amplitude limit, the h^2 term is neglected, giving

$$T_s(x, t) \simeq T_0 - \frac{q'''(H_s - H_g)}{k_g} h(x, t). \quad (1.12)$$

Substituting the sinusoidal surface perturbation gives

$$T_s(x, t) = T_0 + \theta(t) \cos(kx), \quad (1.13)$$

where the linear first-harmonic temperature amplitude is

$$\theta(t) = -\frac{q'''(H_s - H_g)}{k_g} A(t). \quad (1.14)$$

Equation (1.14) gives the key thermal result for the linearized benchmark. If the surface moves upward at a peak of the sinusoid, the local gas gap becomes thinner and the local solid thickness becomes larger. For the present geometry, the reduction in gas-gap resistance dominates the first-order variation, so the solid surface is cooler at the peak. Conversely, the gas gap is larger at a valley, and the solid surface is hotter there.

For comparison, a constant-flux approximation would give

$$\theta_{\text{cf}}(t) = -\frac{q''' H_s}{k_g} A(t). \quad (1.15)$$

The ratio between the corrected local-column temperature amplitude and the constant-flux temperature amplitude is

$$\frac{\theta(t)}{\theta_{\text{cf}}(t)} = \frac{H_s - H_g}{H_s} = 1 - \frac{H_g}{H_s}. \quad (1.16)$$

This factor explains the difference between the original constant-flux analytic comparison and the finite element solution for the volumetric heat-generation model.

1.3.3 Thermomigration Flux

The benchmark uses a constant effective thermomigration coefficient evaluated at a reference temperature. The surface flux is written directly in terms of surface temperature as

$$J_s = -B_T \frac{\partial T_s}{\partial s}, \quad (1.17)$$

where s is distance along the surface and

$$B_T = M_s \frac{Q^*}{T_{\text{ref}}}. \quad (1.18)$$

Here M_s is the prescribed constant surface mobility for this benchmark, Q^* is the heat of transport, and T_{ref} is the reference absolute temperature. With the sign convention used here,

$B_T > 0$ corresponds to hot-to-cold material transport along the surface. The opposite sign of B_T would give the stable branch of the same linear problem.

For small slopes, $s \simeq x$. Therefore,

$$\frac{\partial T_s}{\partial s} \simeq \frac{\partial T_s}{\partial x}. \quad (1.19)$$

Using Equation (1.13),

$$\frac{\partial T_s}{\partial x} = -k\theta(t) \sin(kx). \quad (1.20)$$

The thermomigration flux is therefore

$$J_s = B_T k \theta(t) \sin(kx). \quad (1.21)$$

1.3.4 Surface Evolution

Conservation of mass along the surface gives the normal deposition/removal rate as

$$v_n = -\Omega \frac{\partial J_s}{\partial s}, \quad (1.22)$$

where Ω is the atomic volume. Under the small-slope approximation,

$$v_n \simeq -\Omega \frac{\partial J_s}{\partial x}. \quad (1.23)$$

Using Equation (1.21),

$$v_n = -\Omega B_T k^2 \theta(t) \cos(kx). \quad (1.24)$$

Since the surface profile is $h(x, t) = A(t) \cos(kx)$, the normal velocity is also

$$v_n \simeq \frac{\partial h}{\partial t} = \frac{dA}{dt} \cos(kx). \quad (1.25)$$

Equating Equations (1.24) and (1.25), and using Equation (1.14), gives

$$\frac{dA}{dt} = \Omega B_T \frac{q'''(H_s - H_g)}{k_g} k^2 A. \quad (1.26)$$

It is convenient to write this as

$$\frac{dA}{dt} = \omega A, \quad (1.27)$$

where, for the instability-producing sign convention $B_T > 0$,

$$\omega = \Omega B_T \frac{q'''(H_s - H_g)}{k_g} k^2. \quad (1.28)$$

The analytic solution for the amplitude is therefore

$$A(t) = A_0 \exp(\omega t). \quad (1.29)$$

The corresponding linearized surface temperature is

$$T_s(x, t) = T_0 - \frac{q'''(H_s - H_g)}{k_g} A_0 \exp(\omega t) \cos(kx). \quad (1.30)$$

For comparison with the finite element surface temperatures, the postprocessor uses the local-column expression

$$T_s(x, t) = T_R + \frac{q'''}{k_g} [H_s + A_0 \exp(\omega t) \cos(kx)] [H_g - A_0 \exp(\omega t) \cos(kx)], \quad (1.31)$$

while the growth-rate comparison uses the linear coefficient in Equation (1.28).

If the sign of B_T is reversed, then $\omega < 0$ and the perturbation decays. With the sign convention used in this benchmark, $B_T > 0$ produces hot-to-cold material transport. Since the valleys are hotter and the peaks are cooler, this transport moves material toward the peaks and amplifies the perturbation.

1.3.5 Explicit Time-Step Estimate

For a single Fourier mode, the amplitude equation is

$$\frac{dA}{dt} = \omega A. \quad (1.32)$$

If this equation is advanced by forward Euler, then

$$A^{n+1} = (1 + \omega \Delta t) A^n. \quad (1.33)$$

For a decaying mode, $\omega < 0$, stability requires

$$|1 + \omega \Delta t| \leq 1. \quad (1.34)$$

The corresponding maximum stable time increment is

$$\Delta t_{\max} = \frac{2}{|\omega|}. \quad (1.35)$$

Using Equation (1.28), this can be written as

$$\Delta t_{\max} = \frac{2k_g}{\Omega |B_T| q'''(H_s - H_g) k^2}. \quad (1.36)$$

This estimate applies to a decaying mode. If the sign of B_T makes $\omega > 0$, the continuum problem is physically unstable for this mode, and the time increment is then controlled by accuracy and nonlinear coupling rather than by a decaying-mode forward-Euler stability limit.

1.4 Benchmark Setup

The finite element benchmark uses the same sinusoidal surface perturbation as the analytic solution. The thermal material response is made highly anisotropic so that heat transfer occurs primarily in the vertical direction. This makes the finite element thermal solution directly comparable to the local-column analytic temperature solution.

The benchmark outputs of interest are the surface temperature amplitude $\theta(t)$, the surface profile amplitude $A(t)$, and the fitted growth or decay rate ω . The analytic comparison is

$$\frac{A(t)}{A_0} = \exp(\omega t), \quad (1.37)$$

with ω given by Equation (1.28). The analytic linear first-harmonic temperature amplitude is

$$\theta(t) = -\frac{q'''(H_s - H_g)}{k_g} A(t). \quad (1.38)$$

For plotting the full surface-temperature distribution, the local-column expression in Equation (1.31) is used. This expression includes the small quadratic contribution from the product of the local solid thickness and the local gas-gap thickness.

The reference calculation uses the parameters listed in Table 1.1. The model uses millimeters for length and seconds for time. Thermal quantities are given in the consistent HeavyMetal unit system used by the input and material files. The reference temperature in the thermomigration coefficient is the flat-interface surface temperature expressed on an absolute temperature scale.

Table 1.1: Reference parameters for the gas-gap thermomigration benchmark.

Quantity	Value	Description
λ	1.000000 mm	Wavelength
H_s	0.840219 mm	Nominal solid thickness
H_g	0.050000 mm	Nominal gas-gap thickness
A_0	1.0000×10^{-3} mm	Initial surface amplitude
q'''	3.30678	Volumetric heat generation
k_g	3.2500×10^{-4}	Gas conductivity in the heat-flow direction
T_R	500.0 °C	Prescribed reservoir temperature
T_0	927.449 °C	Flat-interface surface temperature
T_{ref}	1200.599 K	Absolute reference temperature
Ω	2.0700×10^{-20} mm ³ /atom	Atomic volume
M_s	3.37166×10^{27}	Surface mobility coefficient
Q^*	3.2654×10^{-17} N-mm/atom	Heat of transport
k	6.283185 mm ⁻¹	Wavenumber

1.5 Results

The numerical results for the gas-gap thermomigration benchmark are reported by comparing the finite element surface temperature and surface profile evolution with Equations (1.31) and (1.29). The primary scalar comparison is the growth or decay rate extracted from the finite element amplitude history.

Using the local-column analytic temperature expression removes the apparent thermal-amplitude discrepancy that results from the constant-flux approximation. In the finite element model, the generated heat per unit projected area varies with the local solid thickness. The corrected analytic first-harmonic driving coefficient is therefore reduced from $q''' H_s / k_g$ to $q''' (H_s - H_g) / k_g$. Equivalently, the corrected temperature amplitude is smaller than the constant-flux amplitude by the factor

$$1 - \frac{H_g}{H_s}. \quad (1.39)$$

With this correction, the finite element surface temperature agrees with the analytic local-column solution on the initial configuration, and the finite element growth rate is compared against the corrected value in Equation (1.28).

For the reference case, the correction factor in Equation (1.39) is

$$1 - \frac{H_g}{H_s} = 0.94049. \quad (1.40)$$

Thus, the corrected local-column thermal drive is about six percent smaller than the constant-flux estimate.

Figure 1.2 compares the finite element surface temperatures with the analytic local-column temperature solution for the initial perturbed geometry. The finite element points closely follow the analytic curve. The surface is coolest where the gas gap is thinnest and hottest where the gas gap is thickest, consistent with Equation (1.9).

Figure 1.3 compares the normalized finite element amplitude history with the analytic solution $A/A_0 = \exp(\omega t)$. The finite element points are nearly indistinguishable from the analytic curve over the simulated interval.

The analytic growth rate for the reference case is

$$\omega_{\text{analytic}} = 6.02534 \times 10^{-7} \text{ s}^{-1}. \quad (1.41)$$

The growth rate fitted from the finite element amplitude history is

$$\omega_{\text{FE}} = 5.99251 \times 10^{-7} \text{ s}^{-1}. \quad (1.42)$$

The relative difference is

$$\frac{|\omega_{\text{FE}} - \omega_{\text{analytic}}|}{|\omega_{\text{analytic}}|} = 5.45 \times 10^{-3}, \quad (1.43)$$

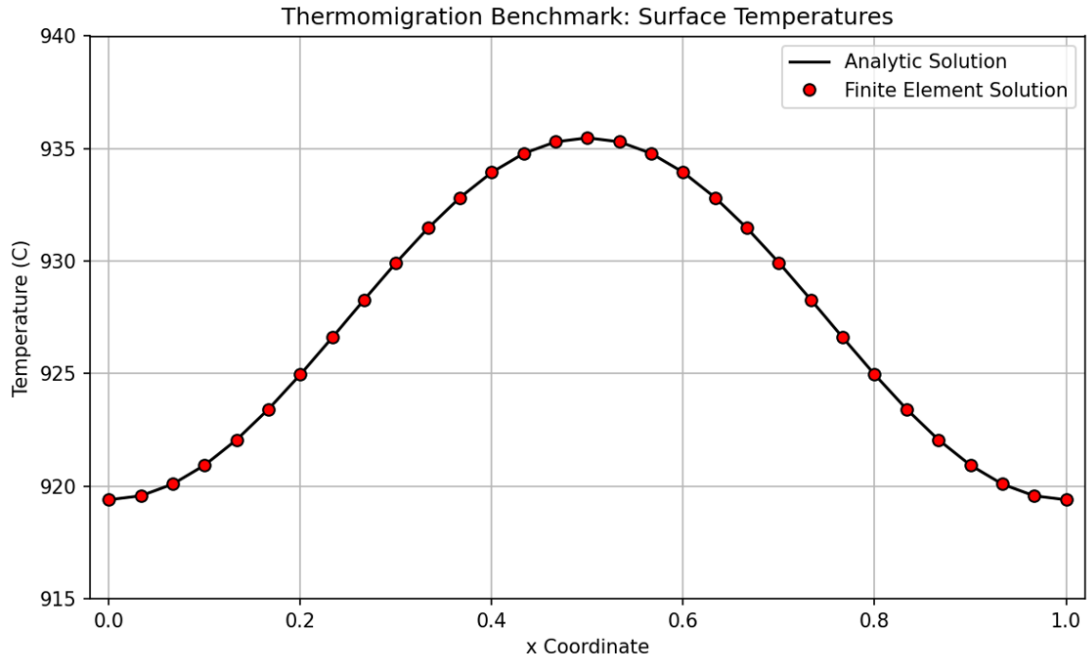


Figure 1.2: Surface temperature comparison for the gas-gap thermomigration benchmark. The analytic curve is computed from the local-column expression in Equation (1.31).

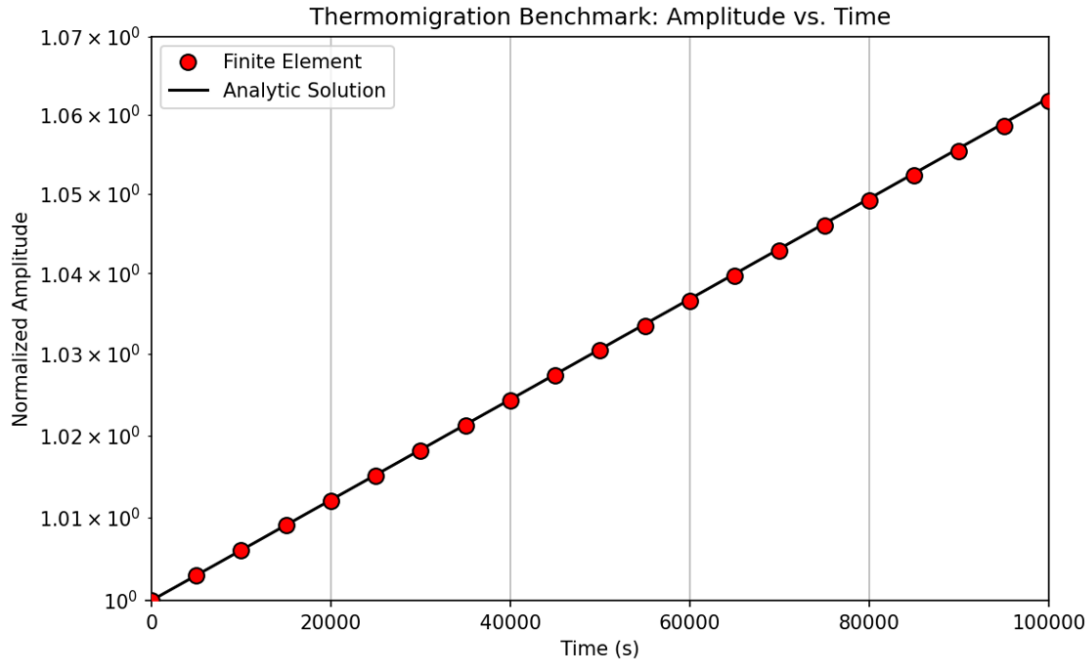


Figure 1.3: Normalized amplitude history for the gas-gap thermomigration benchmark. The finite element amplitude is compared with $A/A_0 = \exp(\omega t)$ using the corrected thermomigration growth rate in Equation (1.28).

or approximately 0.55%.

The timestep scale is also favorable for larger calculations. For the reference case, a timestep corresponding to $\omega\Delta t = 0.1$ is

$$\Delta t = 1.66 \times 10^5 \text{ s.} \quad (1.44)$$

The timestep used for the amplitude-growth calculation was $5.0 \times 10^3 \text{ s}$, giving $\omega\Delta t \simeq 3.0 \times 10^{-3}$. Thus, the benchmark does not require prohibitively small timesteps, and related two-dimensional planar thermomigration calculations should be computationally practical.

1.6 Discussion

This benchmark is a useful test of the thermomigration portion of the surface evolution formulation because the temperature perturbation has a simple analytic form and the resulting surface evolution remains dominated by a single Fourier mode in the linear regime. The thermal part of the problem tests the ability of the finite element model to reproduce the local-column gas-gap temperature perturbation for a volumetrically heated, perturbed solid. The surface evolution part tests whether the surface diffusion elements correctly convert the tangential temperature gradient into a surface flux and then into a normal deposition/removal rate.

The benchmark is intentionally limited to the small-slope, small-amplitude regime. Under these assumptions, the analytic growth rate is linear and provides a direct comparison for the finite element calculation. The full local-column surface-temperature expression is retained for plotting and for checking the thermal solution, while the linearized first-harmonic coefficient is used for the analytic growth-rate comparison.

This benchmark is a verification calculation, not a direct simulation of a specific annular metallic fuel experiment. The geometry is planar, and the purpose of the calculation is to isolate a local thermomigration mechanism for which an analytic solution is available. The close agreement between the finite element solution and the analytic solution demonstrates that the thermal coupling, thermomigration surface flux, and surface-evolution postprocessing are working consistently for this case. The resulting timestep scale also indicates that subsequent two-dimensional planar studies should be feasible. Although the present benchmark does not prove that thermomigration is responsible for experimentally observed metallic-fuel surface instabilities, it shows that the mechanism is not obviously excluded by the resulting time scale.