XMAT Oxidation Modeling Report

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Abstract

placeholder

Keywords: oxidation, spallation, XFEM, moving interface

1. Model

Consider a sector of a centered circular domain with radius c. The oxide-metal interface is initially located at $\|\boldsymbol{x}\| = b$, and the steam-oxide interface is initially located at $\|\boldsymbol{x}\| = a$.

Two levelset functions are used to define the interfaces:

$$\phi_{\text{so}}(\boldsymbol{x}) = \|\boldsymbol{x}\| - a, \tag{1}$$
$$\phi_{\text{om}}(\boldsymbol{x}) = \|\boldsymbol{x}\| - b. \tag{2}$$

Interfaces and boundaries are defined as

$$\Gamma_{\text{so}} = \{\boldsymbol{x} \mid \phi_{\text{so}}(\boldsymbol{x}) = 0\}, \tag{3}$$
$$\Gamma_{\text{om}} = \{\boldsymbol{x} \mid \phi_{\text{om}}(\boldsymbol{x}) = 0\}, \tag{4}$$
$$\Gamma_{\text{mg}} = \{\boldsymbol{x} \mid \|\boldsymbol{x}\| = c\}, \tag{5}$$
$$\Gamma_{\text{bottom}} = \{\boldsymbol{x} \mid x_2 = 0\}, \tag{6}$$
$$\Gamma_{\text{left}} = \{\boldsymbol{x} \mid x_1 = 0\}, \tag{7}$$

Domains are partitioned as

$$\Omega = \Omega_{\text{s}} \cup \Omega_{\text{o}} \cup \Omega_{\text{m}}, \tag{8}$$
$$\Omega_{\text{s}} = \{\boldsymbol{x} \mid \phi_{\text{so}}(\boldsymbol{x}) < 0, \phi_{\text{om}}(\boldsymbol{x}) < 0\}, \tag{9}$$
$$\Omega_{\text{o}} = \{\boldsymbol{x} \mid \phi_{\text{so}}(\boldsymbol{x}) > 0, \phi_{\text{om}}(\boldsymbol{x}) < 0\}, \tag{10}$$
$$\Omega_{\text{m}} = \{\boldsymbol{x} \mid \phi_{\text{so}}(\boldsymbol{x}) > 0, \phi_{\text{om}}(\boldsymbol{x}) > 0\}. \tag{11}$$

Deformation is described by displacements $\boldsymbol{u}$, and heat conduction is described by temperature T, governed by

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma} = \boldsymbol{0}, \quad \forall \boldsymbol{x} \in \Omega_{\text{o}} \cup \Omega_{\text{m}}, \tag{12}$$
$$\int_\Omega \boldsymbol{n} \cdot \boldsymbol{\varepsilon}\boldsymbol{n} \; \mathrm{d}V = 0, \quad \forall \boldsymbol{x} \in \Omega_{\text{o}} \cup \Omega_{\text{m}}, \tag{13}$$
$$\boldsymbol{\nabla}\cdot\kappa\boldsymbol{\nabla}T = 0, \quad \forall \boldsymbol{x} \in \Omega_{\text{o}} \cup \Omega_{\text{m}}. \tag{14}$$

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where $\boldsymbol{n}$ is the surface (boundary) normal, κ is the thermal conductivity, and $\boldsymbol{\sigma}$ is the stress with constitutive relation to be defined, subject to constraints

$$\begin{aligned}
\boldsymbol{\sigma n} &= -p\boldsymbol{n}, \quad \forall \boldsymbol{x} \in \Gamma_{\text{so}} \cup \Gamma_{\text{mg}}, && (15)\\
\kappa \boldsymbol{\nabla} T \cdot \boldsymbol{n} &= -h(T - T_\infty), \quad \forall \boldsymbol{x} \in \Gamma_{\text{so}} \cup \Gamma_{\text{mg}}, && (16)\\
\boldsymbol{u} \cdot \boldsymbol{n} &= 0, \quad \forall \boldsymbol{x} \in \Gamma_{\text{bottom}} \cup \Gamma_{\text{left}}, && (17)\\
[\![\boldsymbol{u}]\!] &= \boldsymbol{0}, \quad \forall \boldsymbol{x} \in \Gamma_{\text{om}}, && (18)\\
[\![T]\!] &= 0, \quad \forall \boldsymbol{x} \in \Gamma_{\text{om}}. && (19)
\end{aligned}$$

where h is the heat convection coefficient, p is the pressure, and T_∞ is the environment temperature.

$\boldsymbol{\sigma}$ is defined as

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}_{\text{el}}, \tag{20}$$

where $\mathbb{C}$ is the elasticity tensor. The total strain is updated based on an incremental scheme with polar decomposition [1], and is additively decomposed into

$$\boldsymbol{\varepsilon}_{\text{total}} = \boldsymbol{\varepsilon}_{\text{el}} + \boldsymbol{\varepsilon}_{\text{th}} + \boldsymbol{\varepsilon}_{\text{cr}} + \boldsymbol{\varepsilon}_{\text{ox}}, \tag{21}$$

where $\boldsymbol{\varepsilon}_{\text{th}}$ is the thermal eigenstrain, $\boldsymbol{\varepsilon}_{\text{cr}}$ is the effective creep strain, and $\boldsymbol{\varepsilon}_{\text{ox}}$ is the accumulated strain due to oxidation.

The thermal eigenstrain is defined as

$$\boldsymbol{\varepsilon}_{\text{th}} = \int_{T_1}^{T_2} \alpha \, \mathrm{d}T, \tag{22}$$

where α is the instantaneous thermal expansion coefficient.

The creep strain follows a temperature dependent power law:

$$\dot{\boldsymbol{\varepsilon}}_{\text{cr}} = A(\sigma_{\text{vm}})^n \exp\left(-\frac{Q}{RT}\right), \tag{23}$$

where A is the creep rate coefficient, σ_{vm} is the Von Mises stress, Q is the creep activation energy, R is the ideal gas constant.

Following [2], the oxide growth strain is decomposed into intrinsic growth strain and geometric growth strain:

$$\boldsymbol{\varepsilon}_{\text{ox}} = \boldsymbol{\varepsilon}_{\text{ox}}^{\text{intr}} + \boldsymbol{\varepsilon}_{\text{ox}}^{\text{geo}}. \tag{24}$$

The intrinsic growth strain is given as $\boldsymbol{\varepsilon}_{\text{ox},\theta}^{\text{intr}} = \boldsymbol{\varepsilon}_{\text{ox},z}^{\text{intr}} = \tau/B$, $\boldsymbol{\varepsilon}_{\text{ox},r}^{\text{intr}} = 0$, where $\tau = \sqrt{2A_{\text{ox}} \exp(-\frac{Q_{\text{ox}}}{RT})t}$ is the oxide thickness. The geometric growth strain is given as $\boldsymbol{\varepsilon}_{\text{ox},r}^{\text{geo}} = \boldsymbol{\varepsilon}_{\text{ox},z}^{\text{geo}} = 0$, $\boldsymbol{\varepsilon}_{\text{ox},\theta}^{\text{geo}} = -\ln(r_c/r_0)$, where r_c is the current radial coordinate and r_0 is the initial radial coordinate where the oxide is formed.

All model parameters and material properties are summarized in the appendix.

2. Benchmark

3. Creep strain

4. LAROMANCE

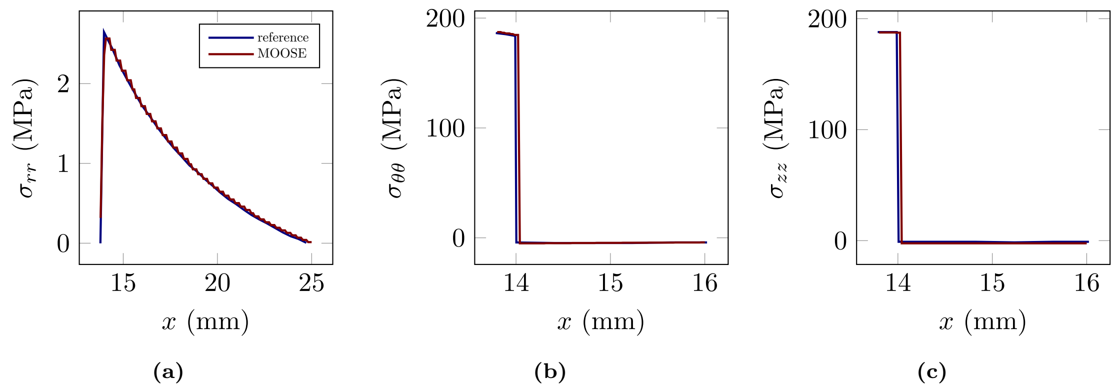


Figure 1. Comparison among the analytical solution, the numerical solution from [2], and the numerical solution obtained using MOOSE for (a) radial stress, (b) hoop stress and (c) axial stress.

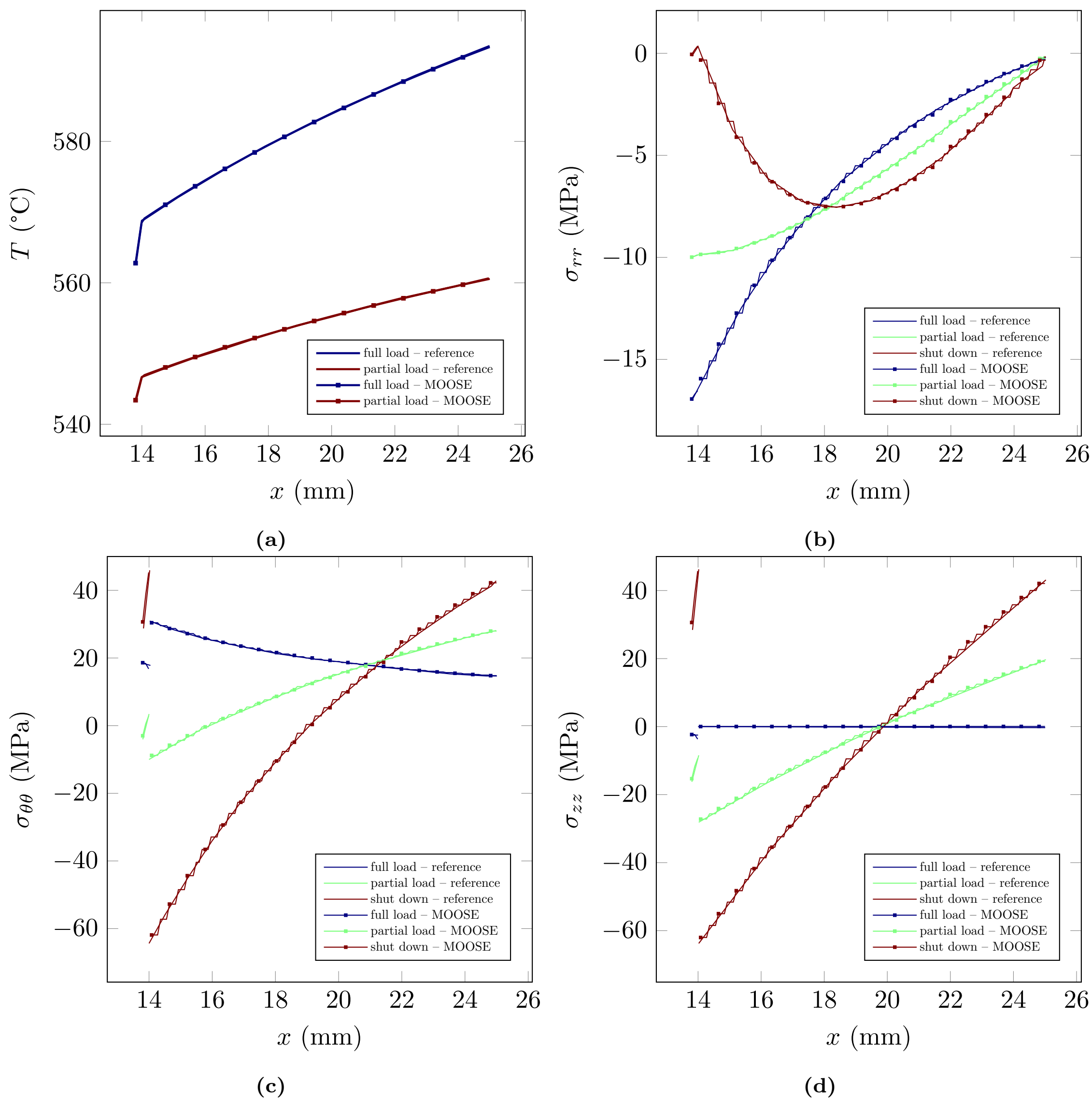
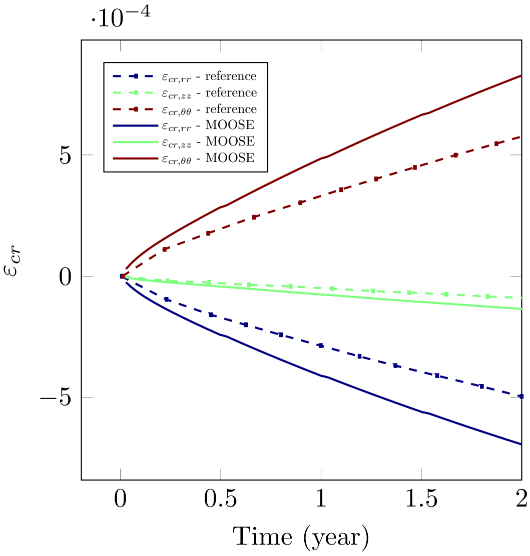
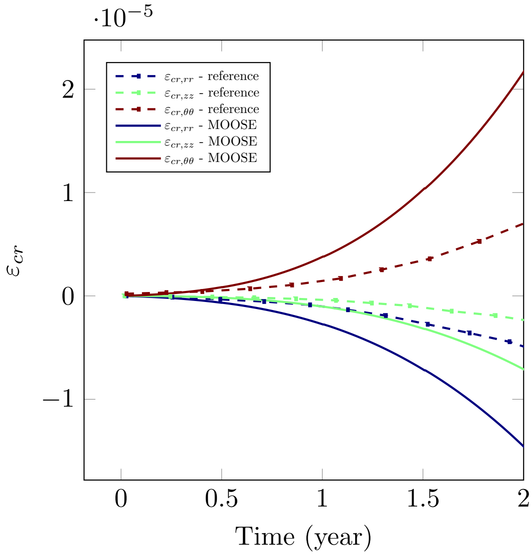


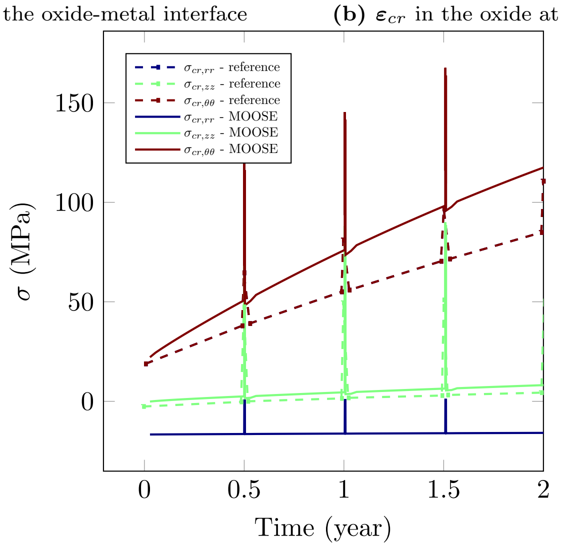
Figure 2. Comparison between the numerical solution from [2] and the numerical solution obtained using MOOSE for (a) temperature, (b) radial stress, (c) hoop stress and (d) axial stress at different load profiles.



(a) $\boldsymbol{\varepsilon}_{cr}$ in the metal near the oxide-metal interface

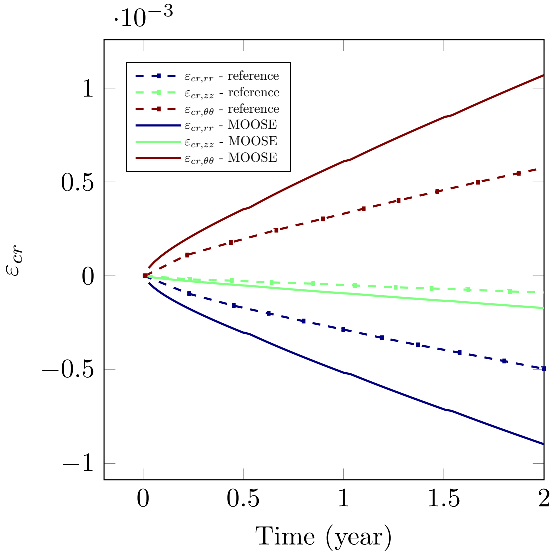


(b) $\boldsymbol{\varepsilon}_{cr}$ in the oxide at the middle of the oxide

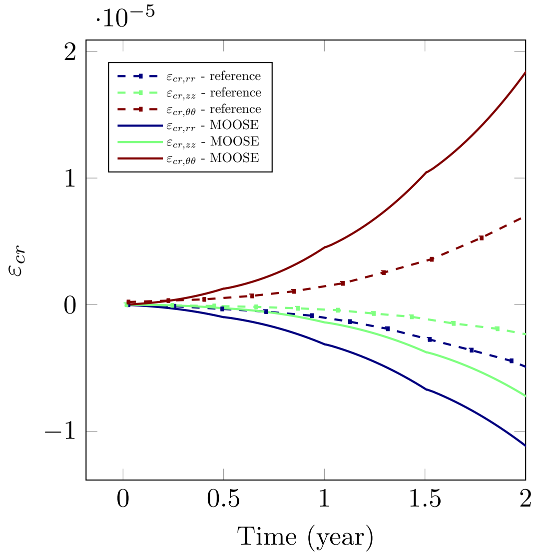


(c) $\boldsymbol{\sigma}$ at the middle of the oxide

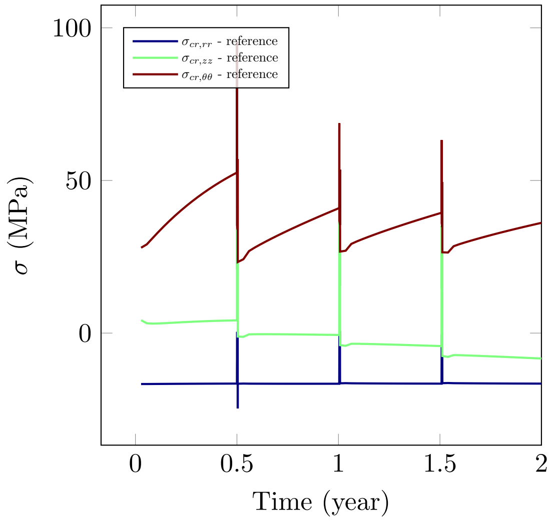
Figure 3



(a) $\boldsymbol{\varepsilon}_{cr}$ in the metal near the oxide-metal interface

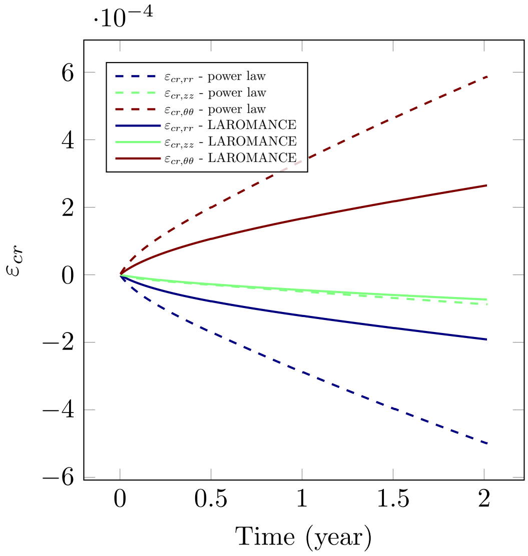


(b) $\boldsymbol{\varepsilon}_{cr}$ in the oxide at the middle of the oxide

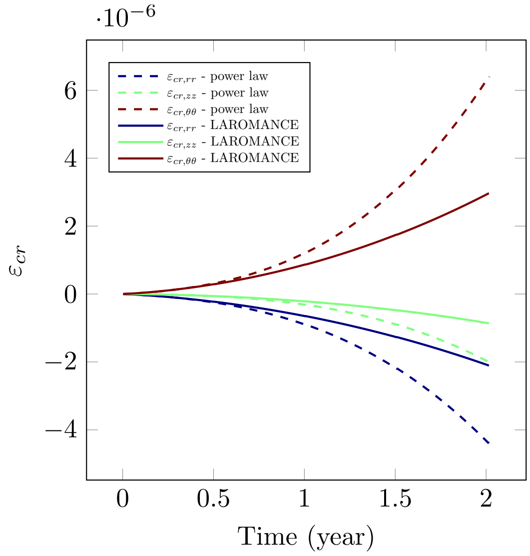


(c) $\boldsymbol{\sigma}$ at the middle of the oxide

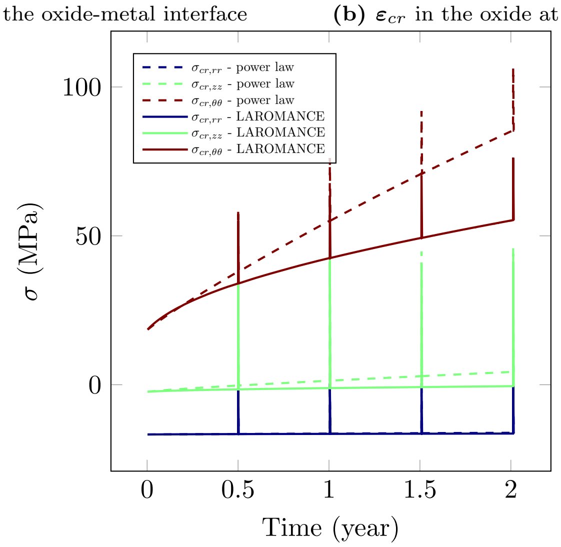
Figure 4



(a) $\boldsymbol{\varepsilon}_{cr}$ in the metal near the oxide-metal interface



(b) $\boldsymbol{\varepsilon}_{cr}$ in the oxide at the middle of the oxide



(c) $\boldsymbol{\sigma}$ at the middle of the oxide

Figure 5

Appendix A Model parameters and material properties

Table A.1. Summary of material properties and model parameters for metal

Property/Parameter	Symbol	Value	Unit
Outer radius	c	25	mm
Thickness	τ	11	mm
Young's modulus	E	190	GPa
Poisson's ratio	ν	0.3	nondim.
Thermal conductivity	κ	30	$\mathrm{W\,m^{-1}\,K^{-1}}$
Convection coefficient (metal-gas)	h	100	$\mathrm{W\,m^{-2}\,K^{-1}}$
Creep coefficient	A	2.3×10^6	$\mathrm{s^{-1}}$
Creep exponent	n	5.06	nondim.
Creep activation energy	Q	400	$\mathrm{kJ\,mol^{-1}}$

Table A.2. Summary of material properties and model parameters for oxide

Property/Parameter	Symbol	Value	Unit
Young's modulus	E	120	GPa
Poisson's ratio	ν	0.24	nondim.
Thermal conductivity	κ	3	$\mathrm{W\,m^{-1}\,K^{-1}}$
Convection coefficient (steam-oxide)	h	2800	$\mathrm{W\,m^{-2}\,K^{-1}}$
Creep coefficient	A	8.5875×10^7	$\mathrm{s^{-1}}$
Creep exponent	n	3	nondim.
Creep activation energy	Q	421.62	$\mathrm{kJ\,mol^{-1}}$
Growth strain scale factor	B	0.3	m
Oxidation coefficient	A_{ox}	6.22×10^8	$\mathrm{m^2\,h^{-1}}$
Oxidation activation energy	Q_{ox}	326	$\mathrm{kJ\,mol^{-1}}$

Table A.3. Summary of operation schedule

Load	Duration (h)	T_s (°C)	T_g (°C)	p_s (MPa)	p_g (MPa)	Transition (h)
Full	14	530	1100	17	0.2	Full to Partial: 1
Partial	8	525	845	10	0.1	Partial to Full: 1
Shutdown	25	25	25	0.1	0.1	Full to Shutdown: 6
						Shutdown to Full: 3

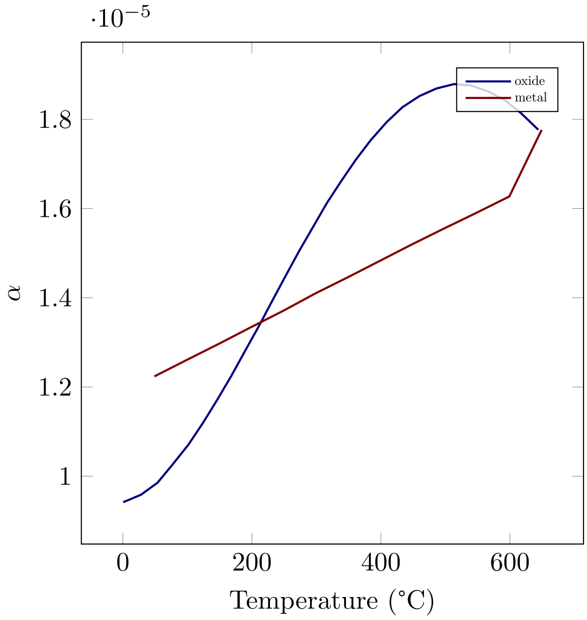
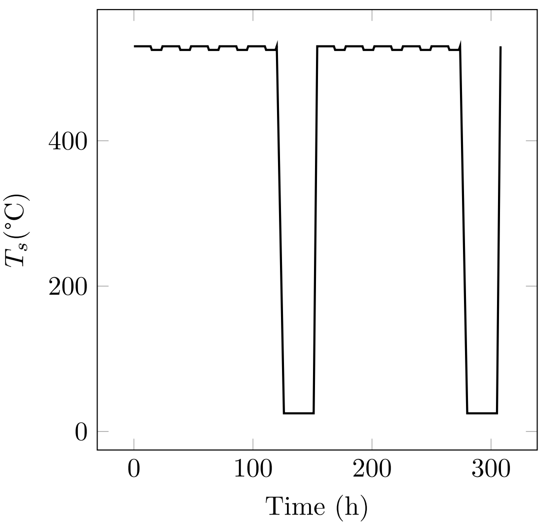
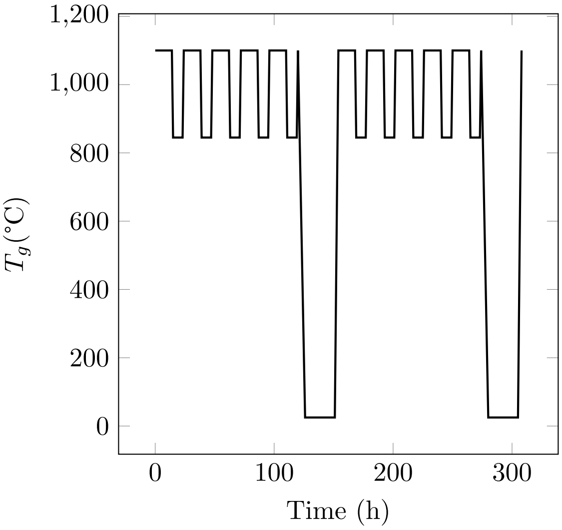


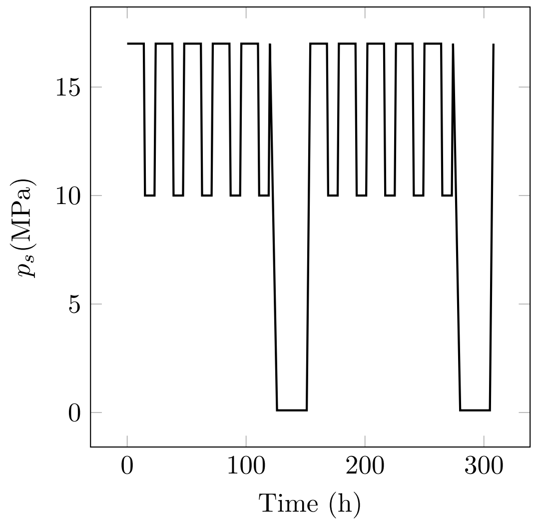
Figure A.6. instantaneous thermal expansion coefficients for oxide and metal.



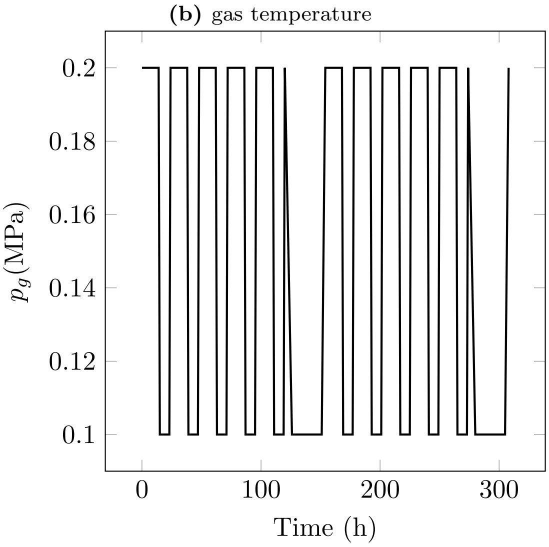
(a) steam temperature



(b) gas temperature



(c) steam pressure



(d) gas pressure

Figure A.7. Example schedule: five full – partial cycles followed by a shutdown.

References

[1] M. Rashid, Incremental kinematics for finite element applications, International journal for numerical methods in engineering 36 (1993) 3937–3956.

[2] F. Xue, T.-L. Cheng, Y.-H. Wen, Stress analysis of the steam-side oxide of boiler tubes: Contributions from thermal strain, interface roughness, creep, and oxide growth, Oxidation of Metals (2020) 1–29.