

THERMAL STRESS ANALYSIS OF PCM CONTAINERS FOR TEMPERATURE SMOOTHING OF WASTE GAS

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Abstract

This article develops an analytical and numerical approach to evaluate thermal stress in a phase change material (PCM) system, used for temperature smoothing of waste gas of Electric Arc Furnace, in which the PCM is encapsulated in a cylindrical steel container. Thermal analysis shows that temperature distribution in the PCM system can be considered as uniform at any time instant according to the lumped capacitance method; the thermal behaviour of PCM system is thus simulated as a sequence of steady state analyses. Mechanical analysis adopts an axisymmetric plane analytical model to compare elastic thermal stress distribution for different stainless steels and to identify AISI 316 as the most suitable material for the PCM container. A simple two-bars model and a stress index are also used to allow a physical understanding and a satisfactory interpretation of the PCM system response. Mechanical analysis shows that thermal stresses exceed the yield point of both stainless steels used in the container. A finite element elastic-plastic model is then developed to estimate the extension of the plastic zone. Finally, an alternative PCM system geometry based on concentric pipes is designed to keep the maximum stresses in the PCM container below the yielding point. A sensitivity analysis shows that the most relevant design parameters of the alternative geometry are the diameter of inner pipe and thickness of the external pipe.

Keywords: Energy Recovery, Electric Arc Furnace, Phase Change Material (PCM), Thermal Stresses

Nomenclature

<i>Acronyms</i>		χ	radiation dampening factor [-]
AISI	American Iron and Steel Institute	σ	stress [MPa]
EAF	Electric Arc Furnace	τ	shear stress [MPa]
FEM	Finite element method	ψ	thermal expansion ratio [-]
PCM	Phase Change Material		
<i>Latin letters</i>		<i>Subscript</i>	
A	area [m ²]	A	aluminium bar
Bi	Biot number [-]	a	aluminium
D	outer diameter [mm]	av	average
d	inner diameter [mm]	conv	convection
e	emissivity [-]	crit	critical
E	Elastic modulus [GPa]	e	external pipe
H	latent heat [kJ/kg]	ext	external
h	heat transfer coefficient [W/m ² K]	f	fracture
i	stress index [-]	g	waste gas
k	Boltzmann Constant [W/m ² K ⁴]	i	inner side
L	characteristic length [m]	if	interface
R	thermal resistance [m ² K/W]	int	internal
r	radial coordinate [m]	m	melting
T	temperature [°C]	max	maximum
t	thickness [mm]	mec	mechanical
u	displacement [mm]	o	outer side
z	axial coordinate [m]	r	radial
		rad	radiation
		ref	reference
		rp	reduction pipe
		S	steel bar
		s	steel
		th	thermal
		tot	total
		gtr	Guest-Tresca
		vm	Von Mises
		y	yielding
		θ	tangential
		z	axial
<i>Greek letters</i>			
α	thermal expansion coefficient [K ⁻¹]		
Γ	time instant [s]		
Δ	property difference		
ε	strain [-]		
λ	thermal conductivity [W/m K]		
μ	friction coefficient [-]		
ν	Poisson ratio [-]		
ζ	Elastic modulus ratio [-]		
ρ	density [kg/m ³]		

27

28 1. INTRODUCTION

29 Heat recovery in energy intensive industries, especially in steel industry, is gaining an increasing
 30 attention due to the energy policy of the European Union and the global economic context. In particular,
 31 heat recovery in steel industry represents one of the greatest opportunity to reduce the consumption of
 32 primary energy while increasing the competitiveness of the steelmaking business [1].

33 Electric Arc Furnace (EAF), one of the most employed technology for steelmaking, generates large
 34 amounts of waste gases. The thermal energy owned by the waste gases represents about 15% to 35% of
 35 the total energy provided to the steelmaking process [2].

36 The most common heat recovery system from waste gas involves pre-heating of metal scrap; however,
 37 its diffusion is mainly limited by problems related to dioxins formation [3].

38 In the last years, new approaches of heat recovery based on steam production (e.g. in [4] and [5]) have
 39 been developed to overcome the environmental issues caused by scrap pre-heating. The efficiency of
 40 heat recovery by steam production is limited, however, by the high variability of temperature and flow
 41 rate of the waste gas. During the steelmaking process, the waste gas temperature at settling chamber
 42 inlet (see Figure 1a) generally shows a fluctuation within a wide range, e.g. from 100°C to 1000°C in
 43 tens of minutes. These operative conditions make difficult to size a direct contact heat exchanger, even
 44 by taking into account oversizing and appropriate control systems.

45 A possible solution to smooth the variability of waste gas temperature is to exploit aluminium as a phase
 46 change material (PCM) [6]. The PCM device designed in [6] is formed by a set of PCM systems, in
 47 which aluminium is encapsulated in a steel cylinder in direct contact with the surrounding waste gas.
 48 The PCM systems are vertically aligned and hung to the rooftop of the settling chamber by an
 49 appropriate hooking system (see Figure 1a). The outer surface of each PCM system is then subjected to
 50 a corrosive environment and to a thermal load, which is mainly due to convection from waste gas.

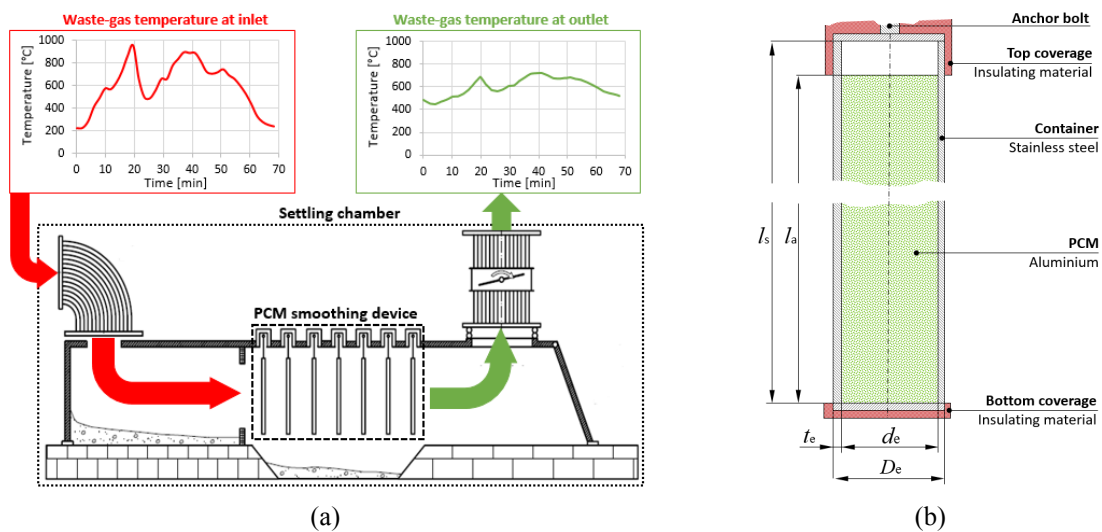


Figure 1. (a) PCM-smoothing device and (b) geometry of the PCM system

51 The PCM system is then exposed to thermal loads that vary during the steelmaking process. The thermal
 52 expansion coefficient of the contained aluminium is higher than that of the containment material; this
 53 mismatch then gives rise to thermal stresses in the PCM container, which can affect its structural
 54 integrity.

55 To the author's knowledge, design procedures and regulations specifically dedicated to high-
 56 temperature applications of this kind of components (cylindrical geometry and PCM expansion in solid

57 phase) are not available in the literature. Some examples available in literature analyse expansion of
58 PCM in liquid phase usually in spherical containers [7]-[8] and rarely in cylindrical container [9]. This
59 work then aims to propose a simplified methodology for the thermo-mechanical analysis of a PCM
60 system when in solid state, which would also allow identifying the most relevant design parameters for
61 subsequent experimental validation. The thermo-structural behaviour of the PCM container is then
62 investigated by a simple analytical thermo-elastic model, followed by an elasto-plastic finite element
63 approach. A simple two-bars model and a stress index are also derived, to allow a physical understanding
64 and a satisfactory interpretation of the PCM system response. This simplified methodology has been
65 privileged over a more complex modelling approach, as it allows the obtained results to be directly used
66 in the design.

67 After a short description of the PCM system, the article describes the analytical and numerical model
68 used to study its thermo-mechanical behaviour. Finally, an alternative design that improves the structural
69 thermo-mechanical behaviour is proposed.

70

71 **2. THE PCM SYSTEM**

72 The PCM smoothing device is based on the phase change phenomenon, which for pure materials and
73 eutectic alloys occurs with a heat exchange at constant temperature (i.e. the phase change temperature).

74 When the waste gas temperature is greater than the phase change temperature, the PCM absorbs heat
75 from waste gas, whose temperature then decreases. At the opposite, waste gas temperature increases
76 when it is lower than phase change temperature (the PCM then releases heat). The combination of these
77 two effects leads to a smoothing of waste gas temperature, which tends to stabilise at the phase change
78 temperature. The temperature-smoothing effect becomes as more effective as the average temperature
79 of the waste gas (about 600°C) is closer to the phase change temperature, which then becomes one
80 criterion to choose the PCM.

81 Other thermo-physical properties of PCM (e.g. latent heat of fusion and thermal conductivity) have also
82 to be considered as choice criteria. A high latent heat of fusion is desirable to increase the energy storage
83 capacity of the PCM system, while a high thermal conductivity assures a fast response to waste gas
84 temperature variation.

85 To summarise, the best PCM should have a high latent heat, high thermal conductivity and a melting
 86 point close to waste gas temperature. These criteria identify the aluminium as the best candidate for
 87 PCM, as it has the melting point ($T_{m,a} = 660$ °C) close to the average waste gas temperature ($T_{av,g} =$
 88 600 °C), a high latent heat of fusion ($H_a = 396$ kJ/kg) and a high thermal conductivity ($\lambda_a = 211$ W/m K).
 89 In the PCM system, the PCM material is encapsulated by a steel container, see Figure 1b. A PCM device
 90 is composed by a set of PCM systems vertically aligned and hung to the rooftop of the settling chamber
 91 by an appropriate hooking system, as shown in Figure 1a. The hooking system allows the containers to
 92 oscillate in order to prevent accumulation of dust, which could hamper the waste gas flow. Table 1
 93 reports the main characteristics of the component shown in Figure 1b.

94 Table 1. Geometric parameters of the PCM system

Outer diameter, D_e (mm)	60.3
Inner diameter, d_e (mm)	52.3
Thickness, t_e (mm)	4.0
Container length, l_s (m)	3.2
PCM length, l_a (m)	3.0

95 In the PCM device, all PCM systems are in direct contact with the surrounding waste gas; thus, they are
 96 subjected to thermal loads, corrosion (due to combination of high temperature and high concentration
 97 of chlorine compounds) and erosion (due to the high concentration of dust). In order to prevent
 98 overheating, the top and the bottom of the PCM container are protected by a coverage of insulating
 99 material, as sketched in Figure 1b. As reported in [6], the bottom coverage hampers the generation of a
 100 thermal bridge between the external wall and the bottom of the container. The presence of corrosive
 101 compounds in the settling chamber and the high temperature of the waste gas suggest the use of stainless
 102 steel as the most suitable material for the PCM container. Among available steel grades, two candidates
 103 have been identified: austenitic (AISI 316) and ferritic (AISI410S) stainless steel. Their temperature-
 104 dependent mechanical properties can be found in Eurocode 3 [10] and are listed in Table 3. Such
 105 stainless steels have differences in elastic modulus E and coefficient of thermal expansion α , which
 106 affect in a different way the thermal stresses generated in the PCM system. The stainless steel that is
 107 most suitable as PCM container will be identified by the analytical model developed in Section 4. The
 108 typical duty cycle of the PCM system is characterised by a start-up phase where the PCM temperature

109 increases, a running phase where phase change occurs, followed by a switch-off phase where the PCM
 110 system is brought back to room temperature.

111 Table 2. Thermo-physical properties of PCM system and waste gas

<i>PCM – Aluminium</i>	
Thermal conductivity (Solid State), λ_a (W/mK)	211
Melting temperature, $T_{m,a}$ (°C)	660
Latent heat of fusion, H_a (kJ/kg)	396
Density, ρ_a (kg/m ³)	2750
<i>Container – Stainless Steel</i>	
Thermal conductivity, λ_s (W/mK)	17
Density, ρ_s (kg/m ³)	7810
<i>Waste gas</i>	
Reference temperature, T_{ref} (°C)	20
Average temperature, $T_{av,g}$ (°C)	600
Convective heat transfer coefficient, h_{conv} (W/m ² K)	50÷100

112 During the start-up phase, the PCM system is heated from room temperature up to the melting point of
 113 the contained aluminium. During this phase, the aluminium always remains at solid state. Since the
 114 coefficient of thermal expansion of the steel container is lower than that of the PCM (Table 3), it is
 115 expected that the maximum stresses in the PCM container will be generated during the start-up phase,
 116 which will be then investigated in the next Sections.

117 During the running phase, instead, the PCM is subjected to phase change (melting or solidification); the
 118 coexistence of both liquid and solid states leads to a drastic reduction of PCM mechanical properties (in
 119 fact, the PCM in liquid state has almost null mechanical properties). Therefore, the mechanical stresses
 120 in the steel container are very small, as they are only due to gravity effects (i.e. the weight of PCM and
 121 steel container) and metallostatic pressure.

122 Finally, the mechanical response of the PCM system during the switch-off phase, when the PCM system
 123 comes back to solid state, is almost similar to the start-up phase.

124 The real temperature trends in Figure 1a, which lead to melting of PCM, suggest that the thermo-
 125 mechanical response of the PCM system should be studied by a transient analysis with phase change.

126 From one hand, this modelling would greatly increase the complexity of the analysis, at the expense of
 127 high computational cost, which both are not very suitable to industrial needs. Furthermore, a complex
 128 modelling approach might also hinder the understanding of the basic mechanisms that govern the system
 129 thermo-mechanical response, as well as the identification of the relevant design parameters. It is then

130 desirable to find out a simplified modelling approach, which matches high accuracy and low
131 computational cost.

132 On the other hand, the results of Appendix A, which will be discussed later in the paper, will clearly
133 show how a transient analysis with phase change is actually not necessary in the computation of thermal
134 stresses, as the highest stresses occur only at the start-up phase, when the PCM is solid, whereas much
135 lower stresses occur when the PCM is liquid. In addition, the thermal analysis presented in the next
136 Section will further confirm how a sequence of steady-state analyses with uniform temperature in the
137 PCM system is a quite good approximation of a transient thermal analysis. This conclusion thus fully
138 justifies the thermo-mechanical analysis developed in the next Sections, which considers the PCM
139 container at different temperatures limited to the range of the start-up phase, where the PCM is solid.

140

141 **3. THERMAL ANALYSIS**

142 In the start-up and switch-off phases, the thermal response of the system can be modelled as a problem
143 of transient conduction. According to [11], the simplest and most convenient method that can be used
144 to solve transient heating and cooling problems is the lumped capacitance method, which assumes that
145 the temperature of a solid body is spatially uniform at any instant during a transient process.

146 In order to check the conditions that guarantee a reasonable accuracy of this method, it is necessary to
147 estimate the Biot number Bi of the PCM system, defined as the ratio of internal thermal resistance R_{int}
148 and external thermal resistance R_{ext} (see Figure 2a):

$$149 \quad Bi = \frac{R_{int}}{R_{ext}} \quad (1)$$

150 If $Bi < 0.1$, the error associated by using the lumped capacitance method is small and the assumption of
151 uniform temperature within the PCM system can be made with a negligible error.

152 It has to be considered that the PCM system at the back receives less heat as compared to that at the
153 front area of the arrangement of Figure 1a. Therefore, each PCM system is characterized by a different
154 Biot number. According to the lumped capacitance method, the smaller the Biot number, the more
155 accurate is the assumption of uniform temperature in the body at any time instant. Therefore, only the
156 PCM system with the highest Biot number has to be checked.

157 The highest Biot number occurs when the internal thermal resistance is maximum R_{int} (i.e. thermal
 158 conductivity of the materials is minimum) and the external thermal resistance R_{ext} is minimum (i.e. heat
 159 transfer coefficients of the waste gas are maximum).

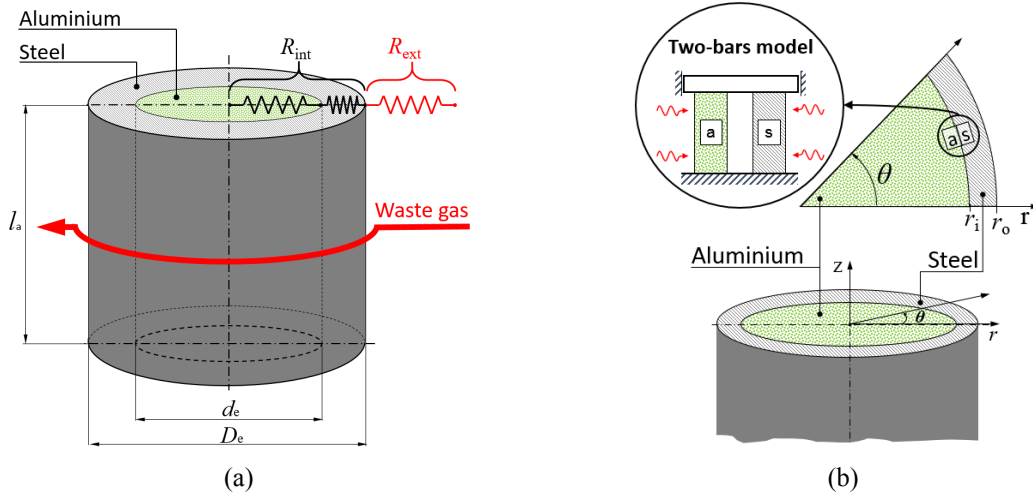


Figure 2. (a) Thermal model and (b) structural model of the PCM system

160

161 The internal thermal resistance R_{int} depends on the resistance to conduction within the materials and the
 162 contact resistance at their interface, as expressed in equation (2).

$$R_{int} = \frac{L_a}{\lambda_a} + \frac{L_s}{\lambda_s} + \frac{1}{h_{if}} \quad (2)$$

163 where L is a characteristic length associated with the length scale corresponding to the maximum spatial
 164 temperature difference, which for the aluminium part is $L_a = d_e/2$ and for the steel part is $L_s = (D_e - d_e)/2$.
 165 Symbols λ_a and λ_s represent the thermal conductivity of aluminium and steel, respectively, while h_{if}
 166 represents the interfacial heat transfer coefficient at aluminium/steel interface. In [12], interfacial heat
 167 transfer coefficients have been measured for several metal castings in cylindrical steel moulds. In [12],
 168 the interfacial heat transfer coefficients have been measured in several metal castings, where melting
 169 and solidification occurred in a cylindrical steel mould, exactly as the melting and solidification in the
 170 PCM system. Thus, a good estimation of the maximum contact resistance at the aluminium/steel
 171 interface in the PCM system can be obtained considering the minimum h_{if} measured in [12], which
 172 reports a minimum value of $h_{if} = 5000 \text{ W/m}^2\text{K}$ for an almost pure aluminium casting in a vertical
 173 cylindrical steel mould. The maximum value of $R_{int} = 5.59 \times 10^{-4} \text{ m}^2\text{K/W}$ results by using the data in Table

174 2, in which the thermal conductivity of the austenitic stainless steel AISI 316 is used because it is the
175 lowest one among selected steels.

176 According to equation (3), the external thermal resistance R_{ext} depends on heat transfer coefficients of
177 convection h_{conv} and radiation h_{rad} , which are related to the PCM system arrangement.

$$R_{\text{ext}} = (h_{\text{conv}} + h_{\text{rad}})^{-1} \quad (3)$$

178 The thermal analysis considers the PCM system where the heat transfer coefficients are maximum.

179 Estimations carried out in [6] showed that the maximum convection heat transfer coefficient h_{conv} of
180 about 100 W/m²K is achieved in the first row of the PCM system arrangement. As reported in [13],
181 radiation heat transfer coefficient h_{rad} can be estimated as:

$$h_{\text{rad}} = k e_g e_e \chi \frac{T_g^4 - T_e^4}{T_g - T_e} \quad (4)$$

182 where k is the Stefan-Boltzmann constant, e_g is the emissivity of the waste gas, e_e is the emissivity of
183 the external surface of the PCM system, T_g is the waste gas temperature and T_e is the temperature of the
184 external surface of the PCM system. The dampening factor χ takes into account the influence of dust
185 load; in order to guarantee a conservative calculation, it can be set to 1. Radiation heat transfer is strongly
186 tied to the emission coefficient of the waste gas e_g , which depends on several factors (temperature,
187 chemical composition, total pressure, partial pressure of gas species and domain geometry). In
188 particular, chemical composition is the most important factor that affects e_g . In fact, only
189 absorbing/emitting gases (e.g. water vapour and carbon dioxide) contribute significantly to the radiation
190 heat transfer, while the contribution of nonabsorbing/emitting gases (e.g. nitrogen) is negligible. Waste
191 gas at settling chamber inlet is usually composed by three components: CO₂ (30%), H₂O (20%) and N₂
192 (50%) [13]. Thus, according to [14], the emission factor of waste gas can be calculated as:

$$e_g = e_{\text{CO}_2} + e_{\text{H}_2\text{O}} - \Delta e \quad (5)$$

193 where Δe is a correction factor which takes into account the overlap of the individual emission bands
194 of the gases involved. For what concerns the emission factor e_e of the external surface of the PCM
195 system, it can be considered very close to 1. Based on the data provided in [6] the maximum heat transfer
196 coefficient of waste gas radiation h_{rad} results equal to 26 W/m²K and, according to eq. (3), the minimum
197 external resistance results $R_{\text{ext}} = 7.94\text{E-}03 \text{ m}^2\text{K/W}$.

208 The estimated maximum R_{int} and minimum R_{ext} give a maximum Biot number of the PCM system equal
 209 to 0.07, which is lower than 0.1. Thus, the internal thermal resistance R_{int} can be neglected and each
 210 PCM system can be assumed, with a negligible error, to be at uniform temperature. Since the PCM
 211 system has a very small Biot number, the system temperature can be considered almost uniform at any
 212 time instant of start-up and switch-off phases. In such phases, the thermal behaviour of PCM system can
 213 thus be simulated as a sequence of steady state analyses. The hypothesis of steady-state thermal analysis
 214 and uniform temperature distribution in the PCM system, which is used in the thermo-mechanical
 215 analysis of the following Sections, has been further justified by the transient numerical simulation
 216 presented in Appendix A.

217

218 4. ANALYTICAL MODEL

219 Before facing an elastic-plastic analysis, which will be described in Section 5, it is useful to preliminary
 220 evaluate the thermo-mechanical response of the PCM system by a simple linear elastic analysis. An
 221 analytical model is then employed to estimate the thermal stress distribution in the PCM system and to
 222 identify the most suitable stainless steel for the PCM container.

223

Table 3. Structural properties of the materials [10]-[15]

Temperature [°C]	Elastic Modulus, E [GPa]							Thermal expansion Coeff., α [$10^{-5}/K$]	Poisson ratio, ν
	20	100	200	300	400	500	550		
Aluminium	70	68	60	48	28	14	0	2.3	0.34
AISI 316 - Austenitic	200	192	184	176	168	160	154	1.7	0.3
AISI 410S - Ferritic	220	211	202	194	185	176	172	1.0	0.3

224 According to the conclusions of the thermal analysis in Section 3, the PCM system is at almost uniform
 225 temperature at any time instant. No thermal gradient then occurs along the axial direction. This allows
 226 the thermo-mechanical behaviour of the system to be studied by a plane model, as shown in Figure 2b.
 227 In addition, the axial symmetry of both geometry and thermal loads (i.e. temperature is symmetrical
 228 about the centre) allows using the “axialsymmetric plane model” of Timoshenko [16]. This plane model
 229 derives the analytical expressions for the radial σ_r and tangential (or hoop) σ_θ stresses. The axial stress
 230 σ_z , instead, can range from plane stress $\sigma_z=0$ (free axial thermal expansion) to plain strain condition $\sigma_z \neq 0$
 231 (totally constrained axial thermal expansion), depending on the axial boundary condition applied to the

222 PCM system. The plane stress and plain strain conditions are called the “plane circular disk” and “long
223 circular cylinder” in [16].

224 In the PCM system, however, the axial stress σ_z is also influenced by the mismatch in the axial thermal
225 expansion of aluminium and steel parts, which also gives rise to a shear stress τ_{rz} at the aluminium/steel
226 interface (note, instead, that $\tau_{\theta z} = \tau_{\theta r} = 0$ for symmetry). This shear stress τ_{rz} tends to prevent the free
227 sliding, and thus the free axial thermal expansion, of the aluminium part over the steel container (in fact,
228 the aluminium expands more than steel under the same temperature change). The shear stress is, then,
229 also directly influenced by the value of friction coefficient at the aluminium/steel interface.

230 This complex situation makes difficult to identify which axial boundary condition (plane stress or plane
231 strain), and thus which axial stress σ_z , can reasonably be assumed in the analytical model of the PCM
232 system. An answer is then given by a preliminary numerical study that has been performed by the plane
233 axisymmetric finite element model described in Appendix B. The obtained results, shown in Figure 11,
234 confirmed that the plane stress hypothesis, where the axial stress $\sigma_z = 0$, is a reasonable assumption for
235 the analytical model of the PCM system.

236 In the “axialsymmetric plane model”, the general expressions of radial σ_r and tangential σ_θ stresses, as
237 well as radial displacement u , are:

$$\sigma_r(r) = -\alpha E \frac{1}{r^2} \int_a^r \Delta T r dr + \frac{E}{1-\nu^2} \left[C_1(1+\nu) - C_2(1-\nu) \frac{1}{r^2} \right] \quad (6)$$

$$\sigma_\theta(r) = \alpha E \frac{1}{r^2} \int_a^r \Delta T r dr - \alpha E \Delta T + \frac{E}{1-\nu^2} \left[C_1(1+\nu) + C_2(1-\nu) \frac{1}{r^2} \right] \quad (7)$$

$$u(r) = (1+\nu)\alpha \frac{1}{r} \int_a^r \Delta T r dr + C_1 r + \frac{C_2}{r} \quad (8)$$

238 where r is the radial coordinate, a is the inner radius, E is the elastic modulus, ν the Poisson coefficient
239 and α the coefficient of thermal expansion. The temperature increment is $\Delta T = T(r) - T_{\text{ref}}$, where $T(r)$ is
240 the temperature distribution in the body and T_{ref} a reference temperature. In the above equations, symbols
241 C_1, C_2 are unknown parameters that depend on the applied boundary conditions.

242 Section 3 emphasised that, at each time instant in start-up and switch-off phases, the PCM system can
243 be considered at a uniform temperature, which means that $T(r) = T_\Gamma = \text{const.}$ is the system temperature
244 at time instant Γ . The temperature increment is also constant, $\Delta T = T_\Gamma - T_{\text{ref}}$.

245 For the system in Figure 2b, which is formed by two different materials, two sets of three equations
 246 must be defined: one set for aluminium, one set for steel. For the part of domain filled with aluminium,
 247 it is $a = 0$ (solid disk); the surrounding domain related to the container (steel), it is $a = r_i$. According to
 248 [16], for a solid disk $C_2 = 0$, in order that the displacement $u_a(r)$ is zero at the centre $r = 0$. Thus, this
 249 gives the following expressions:

$$\begin{cases} \sigma_{r_a}(r) = -\alpha_a E_a \frac{\Delta T}{2} + \frac{E_a}{1 - \nu_a^2} [C_{1,a}(1 + \nu_a)] \\ \sigma_{\theta_a}(r) = -\alpha_a E_a \frac{\Delta T}{2} + \frac{E_a}{1 - \nu_a^2} [C_{1,a}(1 + \nu_a)] \\ u_a(r) = (1 + \nu_a) \alpha_a \frac{\Delta T}{2} r + C_{1,a} r \end{cases} \quad (9)$$

$$\begin{cases} \sigma_{r_s}(r) = -\alpha_s E_s \frac{\Delta T}{2} \left(1 - \frac{r_i^2}{r^2}\right) + \frac{E_s}{1 - \nu_s^2} [C_{1,s}(1 + \nu_s) - C_{2,s}(1 - \nu_s) \frac{1}{r^2}] \\ \sigma_{\theta_s}(r) = -\alpha_s E_s \frac{\Delta T}{2} \left(1 + \frac{r_i^2}{r^2}\right) + \frac{E_s}{1 - \nu_s^2} [C_{1,s}(1 + \nu_s) - C_{2,s}(1 - \nu_s) \frac{1}{r^2}] \\ u_s(r) = (1 + \nu_s) \alpha_s \frac{\Delta T}{2} \frac{r^2 - r_i^2}{r} + C_{1,s} r + \frac{C_{2,s}}{r} \end{cases} \quad (10)$$

250 Equation (7) shows that, in the aluminium domain, the state of stress is plane hydrostatic, as the radial
 251 and hoop stresses are equal and also constant in the whole domain.

252 The remaining three unknown parameters $C_{1,a}$, $C_{1,s}$, $C_{2,s}$ can be determined by imposing the appropriate
 253 boundary conditions:

$$\sigma_{r_s}(r_o) = 0 \quad (11)$$

$$\sigma_{r_a}(r_i) = \sigma_{r_s}(r_i) \quad (12)$$

$$u_a(r_i) = u_s(r_i) \quad (13)$$

254 The above expressions represent zero radial stress (11) at outer stress-free surface of the domain, the
 255 continuity of radial stresses (12) and the continuity of radial displacement (13) at the interface $r = r_i$.

256 The conditions in equations (11)-(13), combined with the expressions in equations (9)-(10), allow one
 257 to calculate closed-form analytical equations for the parameters $C_{1,a}$, $C_{1,s}$, $C_{2,s}$:

$$C_{1,a} = \frac{\Delta T(1 - \nu_a) \alpha_a \{r_i^2(1 - \nu_s) + r_o^2(1 + \nu_s) + [2\psi\xi - \xi(1 + \nu_a)](r_o^2 - r_i^2)\}}{2[r_i^2(1 - \nu_s) + r_o^2(1 + \nu_s)] + \xi(1 - \nu_a)(r_o^2 - r_i^2)} \quad (14)$$

$$C_{1,s} = \frac{\Delta T(1 - \nu_s) \alpha_a [\psi\xi(1 - \nu_a)(r_o^2 - r_i^2) + \psi(1 + \nu_s)(r_o^2 - r_i^2) + 2r_i^2]}{2[r_i^2(1 - \nu_s) + r_o^2(1 + \nu_s)] + \xi(1 - \nu_a)(r_o^2 - r_i^2)} \quad (15)$$

$$C_{2,s} = \frac{\Delta T r_i^2 (1 + \nu_s) \alpha_a \{[\psi\xi(1 - \nu_a) - \psi(1 - \nu_s)](r_o^2 - r_i^2) + 2r_o^2\}}{2[r_i^2(1 - \nu_s) + r_o^2(1 + \nu_s)] + \xi(1 - \nu_a)(r_o^2 - r_i^2)} \quad (16)$$

258 where $\psi = \alpha_s/\alpha_a$ and $\zeta = E_s/E_a$ are dimensionless coefficients, which account for the difference in material
 259 properties between aluminium and steel. Note that in the hypothesis of same material in the whole PCM
 260 system, it is $\psi = \alpha_s/\alpha_a$ and $\zeta = E_s/E_a$. Accordingly, the expressions (9)-(10) give a stress $\sigma_{r,a} = \sigma_{\theta,a} = 0$ and
 261 $\sigma_{r,s} = \sigma_{\theta,s} = 0$ in the whole domain, which coincides with the results given in [16] for the case of solid
 262 cylinder and then confirms the correctness of the previous equations.
 263 The distribution of tangential σ_{θ} and radial σ_r stress in aluminium and steel container can be computed
 264 by expressions (9)-(10) with the coefficients in (14)-(16). The temperature increment $\Delta T = T_{\Gamma} - T_{ref}$ is
 265 calculated by considering the temperature T_{Γ} at time instant Γ in the start-up or switch-off phase; in this
 266 study, the reference temperature is $T_{ref} = 20\text{ }^{\circ}\text{C}$. The axial stress is found, instead, by a simple equilibrium
 267 condition along the axial direction. In fact, as previously said, the PCM system is free to expand along
 268 its axis, thus the axial stress σ_z in the container is only generated by the total weight of the system.
 269 Considering the parameters in Table 1, the axial stress is $\sigma_z = 0.5\text{ MPa}$ and it can be neglected for practical
 270 purposes.

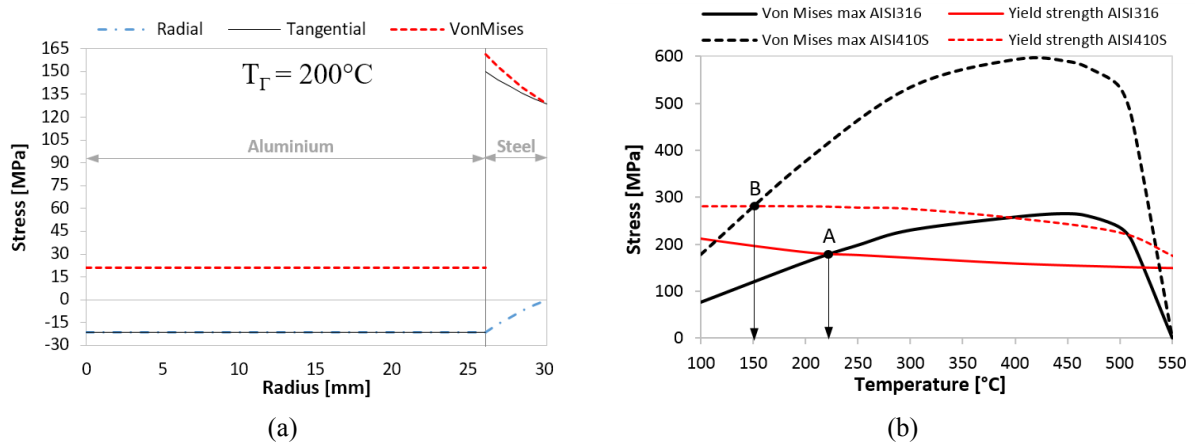


Figure 3. (a) Example of stress distribution (radial, tangential, Von Mises) in PCM system at temperature $T_{\Gamma} = 200\text{ }^{\circ}\text{C}$, steel is AISI 316; (b) yield strength (red lines) and maximum Von Mises stress (black lines) at inner radius, as a function of temperature T_{Γ} , for the two considered stainless steels

271 Figure 3a reports an example of stress distribution in the PCM system at temperature $T_{\Gamma} = 200\text{ }^{\circ}\text{C}$.
 272 The stress distribution in the steel container is similar to that in a cylindrical vessel under internal
 273 pressure. The radial stress σ_r is compressive within the whole PCM system; it is constant in the
 274 aluminium, continuous at the aluminium/steel interface, while it decreases to zero at the outer radius of
 275 the container. The tangential stress σ_{θ} is also compressive in the aluminium (where it overlaps to radial
 276 stress), while it becomes tensile in the steel container (i.e. a discontinuity occurs at aluminium/steel

277 interface). The compressive stresses inside the aluminium are then balanced by the tensile tangential
278 stresses in the steel container. The axial stress σ_z is almost zero in the whole domain.

279 The stress distribution in Figure 3a, which occurs in start-up and switch-off phases, can be explained by
280 the mismatch in mechanical properties of aluminium and steel (e.g. coefficient of thermal expansion and
281 elastic modulus). The aluminium has a coefficient of thermal expansion greater than that of steel, which
282 leads aluminium to expand more than the container. This thermal expansion, however, is hindered by
283 the steel container, because of its much higher elastic modulus at any temperature (see Table 3). The
284 stress distribution then depends on the mechanical properties of the steel grade used for the container.
285 Figure 3a also plots the distribution of the equivalent Von Mises stress:

$$\sigma_{vm} = \sqrt{\sigma_r^2 + \sigma_\theta^2 - \sigma_r\sigma_\theta} \quad (17)$$

286 in which the axial stress σ_z has been neglected. The maximum Von Mises stress is located at the inner
287 radius of the steel container, where plastic strain is then expected to occur. This is the most critical point
288 in the PCM system, which has to be monitored in the design. Similarly to the overall stress distribution,
289 also the maximum Von Mises stress depends on the steel type, as shown in Figure 3b.

290 To understand the mechanical behaviour of PCM system during the start-up and switch-off phases, it is
291 of interest to plot the maximum Von Mises stress $\sigma_{vm,max}$ at each temperature T_Γ reached in such phases
292 ($T_\Gamma = 100\div 660$ °C).

293 Figure 3b shows that Von Mises stress has a nearly parabolic profile, with a peak around 450°C, where
294 the combination of thermal expansion and mechanical constraint reaches its maximum effect.

295 The analysis also highlights how the Von Mises stress in AISI410S steel is more than double to that
296 generated into AISI316 steel. This stress difference can be explained by considering that AISI410 steel
297 has a lower coefficient of thermal expansion and a higher elastic modulus than those of AISI 316 steel
298 (see Table 3). Figure 3b also compares the maximum Von Mises stress to the yield stress σ_y of each steel
299 type considered as container material; it can be observed that, at any temperature, the AISI 316 steel has
300 a yield stress lower than that of AISI410S steel. Yielding occurs at the temperature T_y where the
301 maximum Von Mises stress $\sigma_{vm,max}$ reaches the yield stress $\sigma_y(T)$. Figure 3b shows that yielding occurs
302 at $T_y = 150^\circ\text{C}$ for the AISI410S (point B) and at $T_y = 225^\circ\text{C}$ for the AISI316 (point A). For temperatures

303 $T > T_y$ plastic strain begins and, of course, the Von Mises stress calculated by the elastic model is no
304 longer representative of the state of stress in the container. Therefore, the most suitable stainless steel
305 for the container is AISI 316, because its lower stress levels allow the container to behave elastically
306 over a temperature range wider than that of AISI410S.

307 The mechanism that generates thermal stresses in PCM system can be interpreted and further explained
308 by using the simple two-bars model in Figure 2b, which has been suggested by Manson [17]. This
309 mechanical model exemplifies the tangential (hoop) displacements of two small elementary elements of
310 aluminium and steel, located at the interface between aluminium and steel in the PCM system. The two
311 bars, connected at both ends, expand under a temperature increase ΔT .

312 In the model, the total strain is $\varepsilon_{\text{tot}} = \varepsilon_{\text{th}} + \varepsilon_{\text{mec}}$, where $\varepsilon_{\text{th}} = \alpha \Delta T$ is the thermal strain for a temperature
313 variation $\Delta T = T_{\Gamma} - T_{\text{ref}}$ and ε_{mec} is the mechanical strain, which is responsible for the stress $\sigma = E \varepsilon_{\text{mec}}$.

314 In the simplified two-bars model, the amount of thermal strain $\varepsilon_{\text{th}} = \alpha \Delta T$ is proportional to the
315 temperature change ΔT and to the coefficient of thermal expansion of the material α . The thermal strain
316 induces a thermal expansion of the system, which, however, can be limited partially, depending on the
317 imposed amount of mechanical constraint.

318 A free thermal expansion occurs when no mechanical constraint is imposed, which in turn gives no
319 mechanical strain and stress in the system. The amount of mechanical constraint imposed on thermal
320 strain depends, of course, on the mechanical stiffness of the system (e.g. elastic modulus and geometry).

321 It is then clear that the mechanical strain ε_{mec} (which generates the stress) depends on the relative
322 contribution of thermal expansion and imposed mechanical constraint. Two limiting cases exist: i) free
323 thermal expansion with no mechanical constraint (which gives a stress-free situation) and ii) totally
324 constrained thermal expansion (which gives rise to the maximum stress). In the case of no mechanical
325 constraint on thermal expansion, the total strain equals the thermal strain $\varepsilon_{\text{tot}} = \varepsilon_{\text{th}}$ and the mechanical
326 strain is zero $\varepsilon_{\text{mec}} = 0$, with no stress on the system; this situation describes the free thermal expansion
327 without any mechanical stress. Conversely, in the case of totally constrained thermal expansion, the total
328 strain is zero $\varepsilon_{\text{tot}} = 0$ and all the thermal strain is converted into mechanical strain $\varepsilon_{\text{mec}} = -\varepsilon_{\text{th}} = -\alpha \Delta T$,
329 which then becomes directly proportional to the temperature variation (the higher the temperature, the
330 higher the stress).

331 In the PCM system, both aluminium and steel container tend to expand for an imposed temperature
332 variation. The constraint on the free thermal expansion of the aluminium is imposed by the surrounding
333 steel container; this constraint, however, is partially relaxed by the thermal expansion of the steel
334 container itself. On the other hand, the imposed constraint also depends on the stiffness (i.e. elastic
335 modulus) of both materials, which in turn decreases with temperature. As a result, the PCM system is in a
336 halfway condition between the two limit cases explained above and the amount of thermal stress depends
337 on several parameters of the PCM system, as well as on temperature.

338 The governing equations of the two-bars model and the resulting thermal stresses are derived in
339 Appendix C. Based on the stress equations (C.4) and (C.5), all the relevant parameters that control the
340 amount of thermal stress in the steel container can be conveniently summarised in the following stress
341 index:

$$i = \frac{(\alpha_a - \alpha_s)\Delta T}{1 + \xi} \quad (18)$$

342 which is obtained from the expression (C.5) by assuming an equal area ($A_a = A_s$) for the two bars. In
343 expression (18), $\Delta T = T_\Gamma - T_{\text{ref}}$ is the imposed temperature variation, α_a , E_a and α_s , E_s are, respectively, the
344 coefficient of thermal expansion and elastic modulus for aluminium and steel, evaluated at temperature
345 T_Γ .

346 The assumption of equal area is justified by considering that the two-bars model represents two small
347 elementary elements (see Figure 2b) of same geometry: this allows the index i to evaluate the effect of
348 material properties on the coupling at the interface, regardless of the particular geometry of the PCM
349 system.

350 The stress index i can provide a simple, although approximate, estimate of the severity of thermal
351 stresses that could develop in the PCM steel container, depending on the materials used. The higher the
352 index i , the higher the thermal stresses expected in the system. An index $i = 0$ means that no thermal
353 stress would develop in the steel container.

354 Quite intuitively, the stress index i is proportional to the difference ($\alpha_a - \alpha_s$) in thermal expansion
355 coefficients, to quantify that thermal stress is proportional to the mismatch in thermal strain that occurs
356 in different materials subjected to the same temperature change ΔT . The higher the difference ($\alpha_a - \alpha_s$)

357 is, the higher the thermal strain mismatch and thus the resulting thermal stresses. If both materials had
 358 identical thermal strains (which occurs when $\alpha_a = \alpha_s$), the stress index would be $i = 0$ and no stress would
 359 virtually develop in the system, irrespective of the values of the elastic moduli E_a, E_s of both materials.
 360 The stress index i also depends on the ratio $\zeta = E_s/E_a$, to quantify that thermal stress depends on the
 361 mechanical constraint imposed on thermal strain.
 362 The ratio ζ is also a function of temperature. For example, when aluminium approaches its melting
 363 temperature $T_{m,a}$, its elastic modulus E_a becomes so small compared to E_s , that the ratio ζ diverges to
 364 infinity and the stress index $i \rightarrow 0$, with no stress in the steel container (see Figure 4). Conversely, at
 365 lower temperature the ratio ζ is higher, which means that steel container is so stiff to prevent the thermal
 366 expansion of the contained aluminium, and a higher thermal stresses develop, see Figure 4.

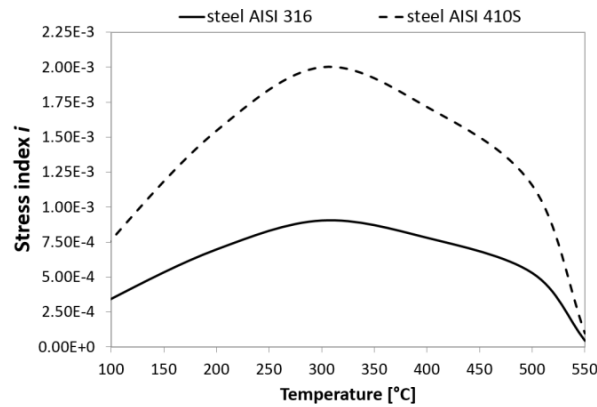


Figure 4. Comparison of the stress index i for the steels AISI 316 and AISI 410S.

367 Owing to its simple expression, the stress index i can be very useful for a sensitivity analysis on materials
 368 properties, which allows a preliminary comparison among different materials in the choice of the best
 369 material for the PCM container. As an example, Figure 4 shows the comparison of the stress index i
 370 calculated for the AISI316 and AISI 410S steels, with the materials properties in Table 3. The similarity
 371 of the trends in Figure 4 with the results in Figure 3 is evident, which confirms the validity of the two-
 372 bars model.

373

374 5. ELASTIC-PLASTIC MODEL

375 The results in the previous section has shown that the stresses in the container exceed the yield point of
 376 the considered steels for temperature higher than 120°C for the AISI410S and higher than 200°C for

377 AISI316 respectively. An elastic-plastic model of the container is then required to study the behaviour
378 of the component during the whole start-up phase and to estimate the extension of the plastic zone.

379 The finite element method is used to analyse the thermo-mechanical elastic-plastic behaviour of the thin
380 circular disk model. The results of the elastic model identified the AISI 316 steel as the most suitable
381 containment material among the considered steels and justified the hypothesis of plane stress, which can
382 thus be employed also in the elastic-plastic model.

383 The one quarter finite element model, shown in Figure 5a, adopts 4-nodes isoparametric linear elements
384 to discretise both aluminium and steel parts. A mapped mesh is used for the container domain and the
385 aluminium close to the interface, a free mesh is used elsewhere. The thermal analysis is first carried out
386 to compute the temperature in each node; the calculated nodal temperatures are then input as thermal
387 loads in the next mechanical analysis.

388 A numerical uncertainty analysis has initially been performed to assess the approximation errors of the
389 finite element solution. In particular, a convergence analysis on the element size has been carried out to
390 identify at which element size the solution of the finite model in Figure 5(a) becomes grid independent.
391 On the other hand, it has to be noted that the model has a very simple geometry (without notches or
392 geometrical discontinuities), that a refined mesh is not necessary. Subsequently, the correctness of the
393 finite element solution has also been verified by comparison with the results of the theoretical model of
394 Section 4 (an error of less than 1% was observed, which is fully acceptable). Unfortunately, a
395 comparison with experimental data is not possible, as to our knowledge experimental data for this type
396 of PCM configuration are not available.

397 As evidenced in Section 3, it is possible to consider the system at uniform (steady state) temperature at
398 any given time instant. This consideration allows simulating the thermo-mechanic behaviour of the
399 component by a sequence of steady state analyses. In the thermal analysis, the applied thermal load is
400 simply a uniform temperature on the whole finite element model. In the mechanical analysis, symmetry
401 boundary conditions are applied as shown in Figure 5a; the hypothesis of plane stress is considered. An
402 elastic-perfectly plastic material model has been used for aluminium and steel. A small positive value
403 of the hardening modulus has been set to obtain convergence of the numerical solution. All thermal and
404 mechanical properties are considered to be temperature dependent, as in Table 3.

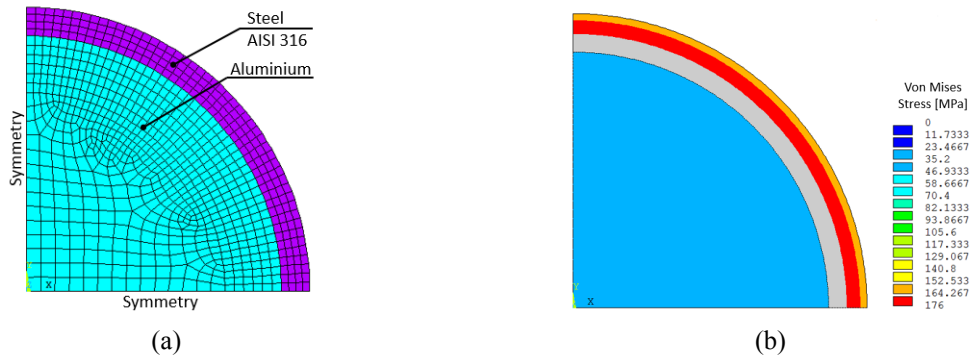


Figure 5. (a) Finite element model and (b) plastic strain (grey colour) of the container at 250 °C

405 Figure 5b shows the Von Mises stress distribution; the colour scale is bounded by the value of the yield
 406 stress of AISI316 stainless steel at 250°C. Therefore, the grey colour represents the region where plastic
 407 strain occurs, while the remaining parts are only subjected to elastic strain. Figure 6a reports the profile
 408 of the Von Mises stress distribution of Figure 5b along a radial direction; the distribution of radial,
 409 tangential and axial stresses are also shown. The trends in Figure 6a are actually similar to those in
 410 Figure 3a. In the elastic-plastic results, however, a lower tangential stress σ_θ is observed at the inner
 411 radius, where the maximum Von Mises stress is equal to the yield stress.

412 The comparison between the Von stress calculated by the FEM model and the elastic analytical model
 413 is reported in Figure 6b. In particular, the maximum Von Mises stress at the inner radius r_i and the Von
 414 Mises stress at the outer radius r_o of the container are reported in Figure 6b; the yield stress of the
 415 stainless steel AISI 316 is also shown.

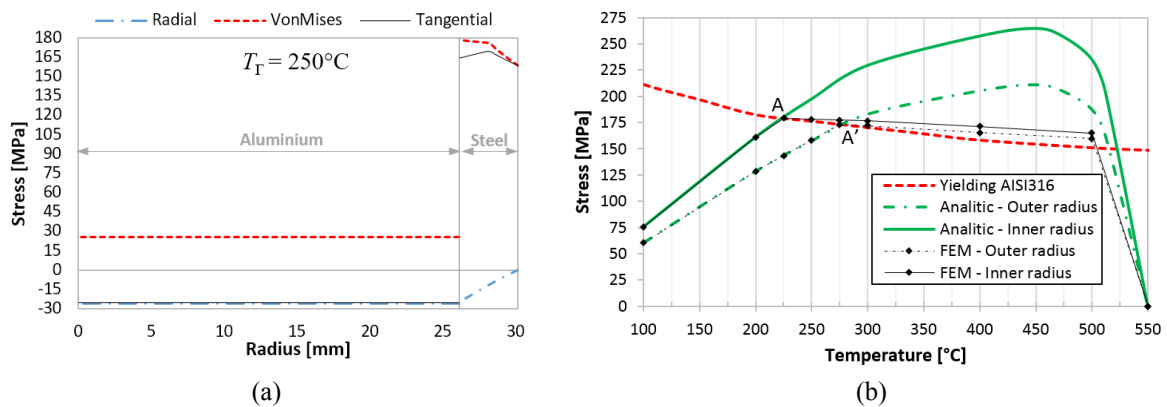


Figure 6. (a) Stress distribution as radius function and (b) comparison between Von Mises stress distribution of the elastic analytical model and the elastic-plastic FEM model

416
 417 Figure 6b shows that the plastic deformation of the container starts at 225 °C (point A) from the inner
 418 radius and it expands along radial direction as the temperature increases; the complete plastic

419 deformation of the whole thickness is reached at 275°C (point A'). In the elastic-plastic model, a
 420 preliminary evaluation of component structural integrity can be performed by comparing the maximum
 421 elastic-plastic strain to the material fracture strain. The graph in Figure 6b allows considering that at a
 422 temperature of about 500 °C the maximum elasto-plastic strain is 1.79e-3, which is far below the fracture
 423 strain $\varepsilon_f = 0.4$ of AISI316 at 500 °C [10]. It can be concluded that the component can resist to a single
 424 phase of start-up.

425

426 6. ALTERNATIVE DESIGN OF PCM CONTAINER

427 The previous analysis highlighted that the proposed PCM container geometry, sketched in Figure 1b,
 428 leads to plastic deformation of the considered steel. However, it is desirable to individuate a PCM
 429 container geometry that allows the steel to work within the elastic field. The design of the alternative
 430 configuration has also to be as simple as possible to guarantee a low manufacturing cost.

431 The proposed alternative configuration (Figure 7a) consists of two concentric cylindrical containers
 432 (pipes) in stainless steel AISI316, where the hollow cavity is filled by PCM.

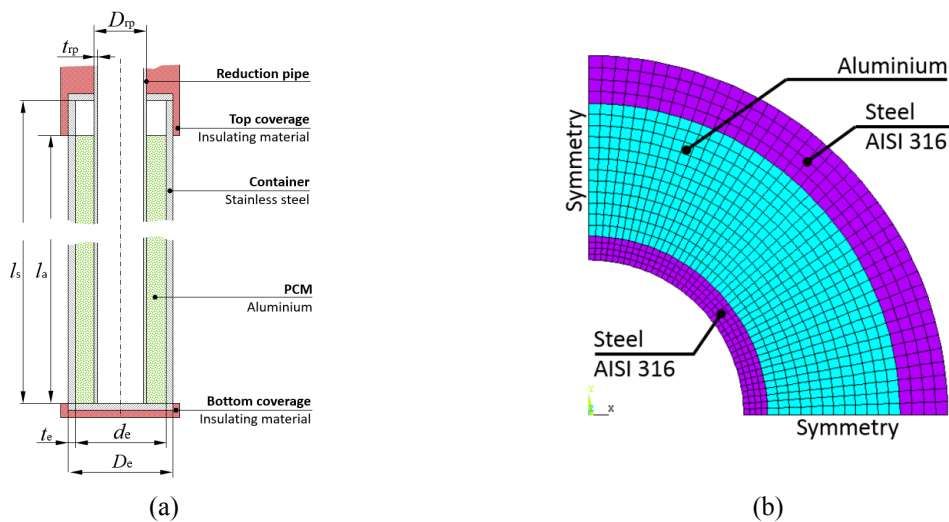


Figure 7. (a) Alternative configuration with concentric pipes and (b) its finite element model

433 For a sake of comparison, the diameter of the external pipe is maintained equal to the diameter $D_e = 60.3$
 434 mm of the initial configuration. The internal pipe is named as *reduction pipe*, as its purpose is to reduce
 435 the volume available to PCM, and it can be used to hang the container to the settling chamber roof. The
 436 dimensions of the reduction pipe (outer diameter and thickness) are design parameters that are
 437 investigated by a sensitivity analysis. The new geometrical configuration is studied by exploiting the

438 elastic-plastic finite element model developed in Section 5. A mapped mesh is now used in the whole
 439 domain (see Figure 7b).

440 First, a sensitivity analysis by varying the diameter of the reduction pipe, in the range $D_{rp} = 20\div 40$ mm,
 441 has been carried out, to find that diameter that allows the steel of the external pipe to work within the
 442 elastic field. In the sensitivity analysis, the reduction pipe has a thickness $t_{rp} = 2$ mm, while the external
 443 pipe maintains the same thickness $t_e = 4$ mm of the initial configuration of Figure 1b.

444 Figure 8a shows the maximum Von Mises stress as a function of temperature, for different values of
 445 diameter D_{rp} of the reduction pipe; the yield stress of AISI 316 is also reported. For diameters $D_{rp} < 30$
 446 mm, plastic deformation still occurs in steel of the external pipe; for diameters $D_{rp} > 30$ mm, instead,
 447 yielding does not occur at any temperature and the steel of the external pipe works in the elastic field.
 448 For each diameter $D_{rp} > 30$ mm, Figure 8a allows individuating the temperature at which the maximum
 449 Von Mises stress is reached in the elastic domain; this temperature is defined as “critical temperature”
 450 T_{crit} and, for all diameters, it is equal to 400 °C.

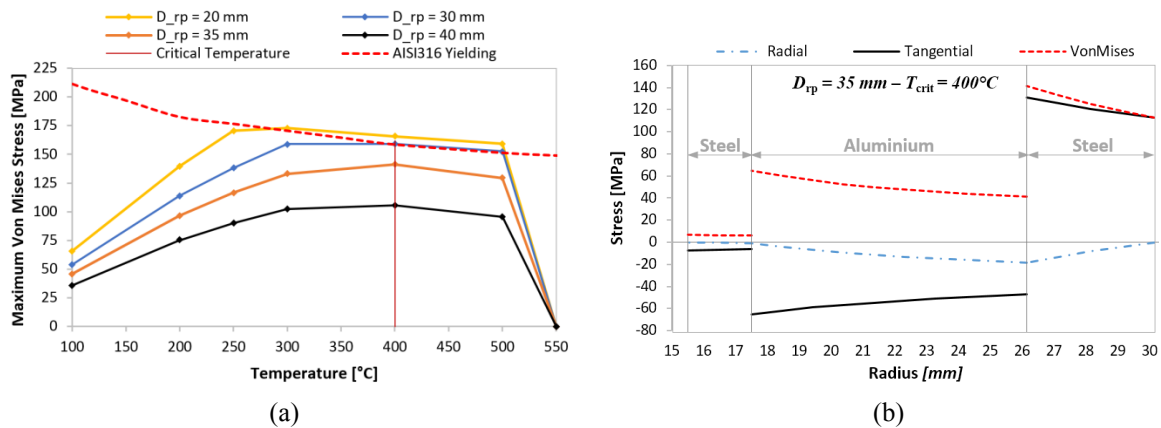


Figure 8. (a) Maximum Von Mises stress at different temperature and reduction diameter D_{rp} ; (b) stress distribution as a function of radius, for $D_{rp} = 35$ mm and $T_{crit} = 400$ °C

451 Figure 8b reports the stress distribution in the configuration with diameter $D_{rp} = 35$ mm, at the critical
 452 temperature $T_{crit} = 400$ °C. It can be seen that the maximum stress is located at the interface between the
 453 PCM and the external pipe, while the stress in the reduction pipe is negligible.

454 The previous analysis has shown that the reduction pipe becomes a fundamental element of the PCM
 455 system as it allows the steel to work within the elastic field. A further sensitivity analysis at the critical
 456 temperature 400 °C has been carried out by varying the thickness t_{rp} , t_e of the reduction pipe and external
 457 pipe.

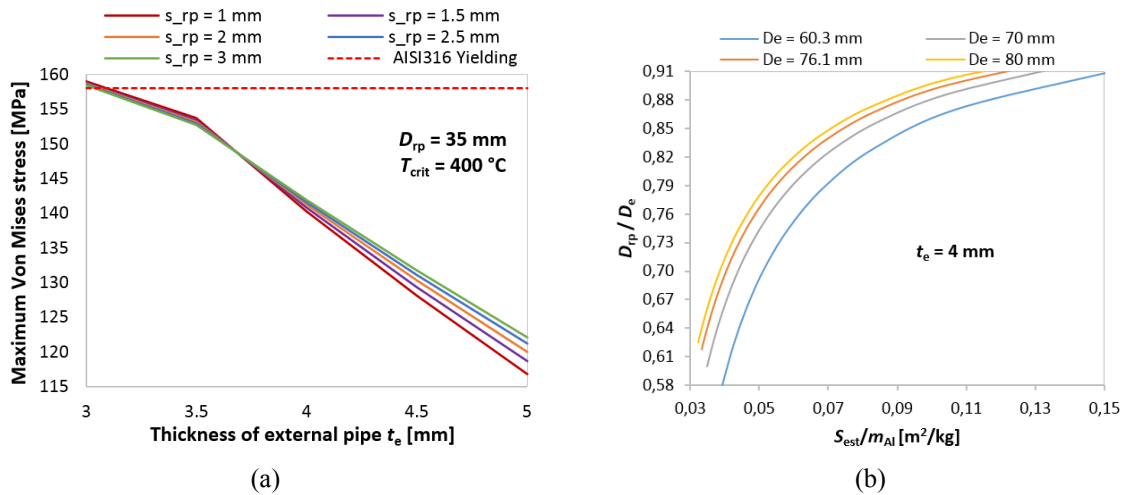


Figure 9. (a) Sensitivity analysis by varying reduction pipe t_{rp} and external pipe t_e thickness and (b) possible configuration as function of the ratio A_{est}/m_{Al} and of D_e to $t_e = 4$ mm

458 Figure 9a shows an example of sensitivity analysis for the configuration with diameter $D_{rp} = 35$ mm of
 459 the reduction pipe. The plot shows that the thermal stress is mainly influenced by the thickness t_e of the
 460 external pipe, while the effect of the thickness t_{rp} of reduction pipe is actually negligible.

461 The smallest thickness $t_{rp} = 1$ mm of the reduction pipe is chosen as it gives the lighter weight of the
 462 structure while assuring low stresses (axial stress due to the component weight $\sigma_z < 0.5$ MPa and stress
 463 generated by the aluminium expansion $\sigma_{vm,max} < 10$ MPa). The thickness of 1 mm has then been used as
 464 a reference value to define the “allowable configurations”, which are all the geometrical configurations
 465 where the container works in the elastic field.

466 The design of the whole PCM system is first based on thermo-physical parameters, mainly represented
 467 by the ratio of external surface of heat exchange A_{est} to the aluminium mass m_{Al} . Figure 9b shows an
 468 example of allowable configurations for the external thickness $t_e = 4$ mm in terms of diameter ratio D_{rp}
 469 $/D_e$ and as a function of the ratio A_{est}/m_{Al} . Figure 9b shows a typical design chart to identify the allowable
 470 configurations; in particular, the figure reports the diameter ratio D_{rp}/D_e as a function of A_{est}/m_{Al} for a
 471 given external thickness $t_e = 4$ mm and for different external diameters D_e .

472

473 7. CONCLUSIONS

474 This article presented an analytical and numerical approach to evaluate thermal stress in a phase change
 475 material (PCM) system, used for temperature smoothing of waste gas of Electric Arc Furnace. Thermal
 476 analysis showed that the Biot number of the PCM system is less than 0.1 and therefore the PCM system

477 can be assumed, with a negligible error, to be at uniform temperature at any time instant. This isothermal
478 condition allowed the thermo-mechanical behaviour of the system to be simulated by a sequence of
479 steady-state analyses.

480 The mechanical analysis based on axialsymmetric plane analytical model allowed to compare elastic
481 thermal stress distribution for AISI410S and AISI316 stainless steels and to identify the latter as the
482 most suitable material for the PCM container. The simple two-bars model and a stress index are used to
483 explain the thermal stress distribution in the PCM system and the nearly-parabolic profile of Von Mises
484 stress over temperature. Mechanical analysis showed that thermal stresses exceed the yield point of both
485 stainless steels used in the container. Therefore, a FEM analysis has been carried out to evaluate the
486 elastic-plastic behaviour of the component. The results showed that a total plastic deformation of the
487 container can occur even during a single start-up phase, where the PCM system is heated from room
488 temperature up to the melting point of PCM. An alternative geometrical configuration with concentric
489 cylindrical containers (pipes) has finally been designed to avoid plastic deformation in the steel
490 container. A sensitivity analysis on some design parameters allowed identifying diameter of the
491 reduction pipe D_{rp} and thickness of the external pipe as the main design parameters that control the
492 amount of thermal stress in the PCM system.

493 **8. APPENDIX A – TRANSIENT THERMO-MECHANICAL SIMULATION OF PCM SYSTEM**
494 **RESPONSE**

495 This Appendix presents the distribution of temperature and thermal stresses calculated by a transient
496 thermo-mechanical simulation, which also includes the phase change (melting) of the PCM. The purpose
497 of this simulation is to confirm how the hypothesis of steady state analysis and uniform temperature
498 distribution in the PCM system is a very good approximation of transient analysis. Secondly, the
499 simulation results will also show how the modelling of phase change of PCM is actually not necessary
500 in the computation of thermal stresses, as the highest stress occurs only at the start-up phase when the
501 PCM is solid, whereas much lower stresses occur when the PCM is liquid, or even when it is still solid
502 at temperatures far below the melting point.

503 The transient thermo-mechanical simulation adopts the same mesh distribution used in the one quarter
504 finite element plane model of Figure 5a, although 8-nodes elements are preferred here to improve
505 solution accuracy. The model is under ‘plane stress’ condition (i.e. zero axial stress), which is also
506 justified in Appendix B. In transient simulations, thermal analysis is carried out first to compute the
507 time-varying temperature in each node, which is next applied as a load thermal input in the mechanical
508 analysis.

509 In thermal analysis, to replicate as close as possible the operating condition in the settling chamber (see
510 Figure 1a), the PCM system is subjected to a convection boundary condition, with a film coefficient h_{ext}
511 = 126 W/m²K and a waste gas temperature (bulk temperature) that increases linearly from 200 °C to
512 950 °C over a time interval of 20 min, then back to 200 °C over the next 20 min, and then kept constant
513 over the final 20 min.

514 The phase change (melting) of the PCM (aluminium) is simulated by defining an enthalpy vs.
515 temperature curve, which increases by the latent heat $H_a=396$ kJ/kg (see Table 2) at the melting
516 temperature.

517 In mechanical simulation, an elastic material model is used, with temperature-dependent mechanical
518 properties as per Table 3; note how the elastic modulus of the PCM (aluminium) rapidly goes to zero
519 for temperatures approaching 660 °C (for example, from 20 °C to 400 °C the elastic modulus is halved).

520 In simulations the AISI 316 steel is used for the container, but similar conclusions would be obtained
521 by using AISI 410S as well.

522 In transient simulation, a Newmark time integration scheme is adopted, with a very small integration
523 time step to assure numerical convergence.

524 Figure 10 shows the temperature and stress over time, monitored at four different locations in the PCM
525 system: i) outer surface of steel container (labelled 'surface'), ii) inner surface of steel container, at the
526 PCM/steel interface (labelled 'interface'), iii) at a point in PCM part, 4 mm underneath the PCM/steel
527 interface (labelled 'sub-interface'), iv) at the centre of PCM.

528 Figure 10a shows that the temperature distribution within the PCM systems is almost uniform at any
529 time instant (the four lines in the graph are overlapped). Melting of PCM starts after about 20 minutes
530 and lasts for about 18 minutes; the temperature of PCM system then decreases as the bulk temperature
531 goes down to 250 °C. It can be concluded that the hypothesis of uniform temperature distribution within
532 the PCM system is fully justified by the results of transient thermal analysis shown in Figure 10a.

533 Figure 10b shows the change over time of radial and tangential (hoop) thermal stresses at some locations
534 in the PCM system. The radial stress at 'surface' is always zero, as expected. For more clarity, the graph
535 does not show the lines of radial σ_r and hoop σ_θ stresses at 'centre' and 'sub-interface' locations, because
536 they are practically overlapped to the radial stress σ_r at 'interface', which is compressive in the time
537 intervals 0÷15 min and 38÷60 min (while it is almost zero elsewhere). In the same time intervals where
538 σ_r is compressive, tensile hoop stresses are observed at 'surface' and 'interface' locations. Finally, the
539 graphs in Figure 10b also shows the change over time of Von Mises stress at 'interface' locations, as
540 calculated by Eq. (17).

541 The results of Figure 10b show the following important findings. The Von Mises stress has a maximum
542 after about 11 min, when the PCM system is at 400 °C and the PCM is still in solid phase, see Figure
543 10a (melting only starts after 20 min). The maximum Von Mises stress is slightly higher than 250 MPa,
544 which is a value in close agreement to the estimation in Figure 3b given by the analytical model of
545 Section 4.

546 For time values larger than 11 min, the Von Mises stress (as all other stress components) rapidly
547 decrease; they become almost zero at about 15 min (i.e. when the PCM is still in solid phase). This sharp

548 decrease of stress is explained by the drop in elastic properties of PCM material, which at temperatures
 549 above 400 °C actually has a very low value of its elastic modulus (see Table 3). Negligible stresses are
 550 then maintained up to 18 min (when melting of PCM starts) and later on, up to 38 min (when the PCM
 551 comes back to solid state). The results in Figure 3b then show that melting of PCM actually does not
 552 contribute in an increase in calculated stresses, as compared to the values estimated by the analytical
 553 model in Section 4.

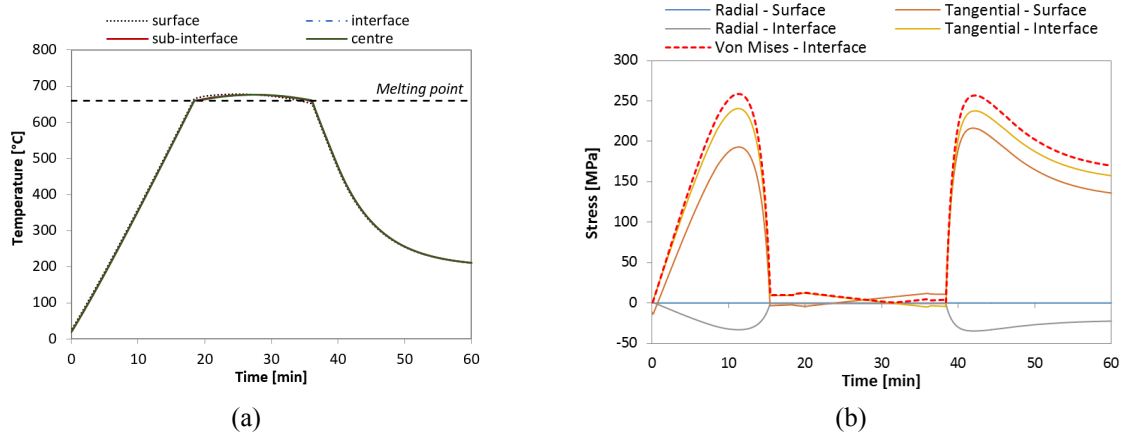


Figure 10. Results of transient numerical analysis with melting of PCM, monitored at four different locations in the PCM system: (a) temperature evolution; (b) stresses.

554

555 9. APPENDIX B – NUMERICAL STUDY WITH A PLANE AXISYMMETRIC MODEL

556 A small longitudinal portion of the PCM system in Figure 1(b) is analysed by a plane axisymmetric
 557 finite element model. Both aluminium and steel regions are discretised by 4-nodes elements with
 558 axisymmetric option, arranged in a mapped mesh over the whole domain. Contact elements are also
 559 placed at the interface between aluminium and steel container, to simulate the separation and then to
 560 allow a relative sliding between the two materials. Two values of the friction coefficient μ were used to
 561 simulate two limiting situations: $\mu=0$ for perfect sliding (i.e. no constraint to aluminium thermal
 562 expansion), $\mu=0.65$ (a typical value for aluminium/steel coupling) to simulate a constrain to thermal
 563 expansion of aluminium. Both aluminium and steel materials are assumed to be linear elastic, with
 564 mechanical properties listed in Table 2.

565 The whole model is subjected to a uniform temperature increase (to simulate the start-up phase described
 566 in Section 2), which induces a thermal expansion of the contained aluminium. Figure 11 shows the

567 distribution of stresses (radial σ_r , hoop σ_θ , axial σ_z and shear τ_{rz}) resulting from the analyses with the
 568 two values of friction coefficient. The figures also compare the equivalent Von Mises stress:

$$\sigma_{vm} = \sqrt{\sigma_r^2 + \sigma_\theta^2 + \sigma_z^2 - \sigma_r\sigma_\theta - \sigma_r\sigma_z - \sigma_\theta\sigma_z + 3\tau_{rz}^2} \quad (B.1)$$

569 to the von Mises stress calculated by Eq. (17) under the plane stress hypothesis ($\sigma_z=\tau_{rz}=0$).

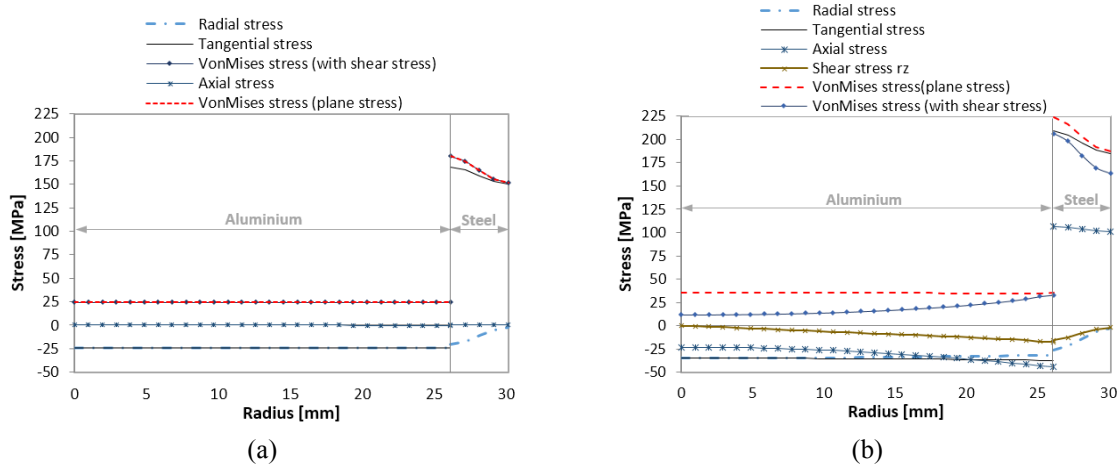


Figure 11. Stress distribution as a function of radial coordinate for two values of friction coefficient at the aluminium/steel interface: (a) zero friction ($\mu=0$); (b) $\mu=0.65$.

570 With no friction at the interface ($\mu=0$), there is no constraint to thermal expansion and only radial σ_r and
 571 hoop σ_θ stresses develop, while, as expected, the axial and shear stresses are zero ($\sigma_z=\tau_{rz}=0$). Instead,
 572 with a high friction coefficient ($\mu=0.65$) the free thermal expansion of aluminium is prevented and both
 573 axial σ_z and shear stress τ_{rz} appear, along with radial σ_r and hoop σ_θ stresses. In aluminium the axial
 574 stress is compressive, while it is discontinuous at the interface and then tensile in the steel. The figures
 575 show that the axial stress has a small influence on the von Mises stress in the steel container. At the
 576 inner radius, the equivalent von Mises stress under plane stress, see Eq. (17), is about 14% higher than
 577 the von Mises stress of Eq. (B.1), which considers instead all stress components. Remarkably, the plane
 578 stress model is then over-conservative. As known from the theory of strength of materials, there would
 579 actually be no difference in equivalent stresses, if they were calculated by using the Guest-Tresca
 580 criterion (i.e. maximum shear stress), which computes the equivalent stress $\sigma_{gr} = |\sigma_\theta - \sigma_r|$ as the
 581 difference of maximum principal stresses.
 582 These results allow one to conclude that the plane stress hypothesis is a reasonable assumption for the
 583 analytical model of the PCM system.

584 **10. APPENDIX C – SIMPLE TWO-BARS MECHANICAL MODEL**

585 The two-bars model in Figure 2b exemplifies two elementary elements at the aluminium/steel interface
 586 in the PCM system. The two elements are attached at two rigid plates at both ends. One end plate is
 587 fixed, while the plate at the opposite side can translate. No rotations are allowed and the bars can only
 588 deform along the longitudinal direction (i.e. this is a one-dimensional model). The two bars, which
 589 represent aluminium and steel, have, respectively, areas A_a, A_s , elastic modulus E_a, E_s and coefficient of
 590 thermal expansion α_a, α_s . Both bars are subjected to a temperature increment $\Delta T = T - T_{ref}$, with respect
 591 to a reference temperature T_{ref} .

592 The thermal expansion of the system is partially constrained by the different longitudinal elongation of
 593 the two bars, which are then subjected to thermal stresses. The value of thermal stresses can be computed
 594 analytically by the expressions.

595 The total strain in each bar is the sum of thermal strain and mechanical strain:

$$\varepsilon_{tot} = \varepsilon_{th} + \varepsilon_{mec} \quad (C.1)$$

596 Thermal strain is caused by the temperature increase, $\varepsilon_{th} = \alpha \Delta T$, while the mechanical strain ε_{mec} gives the
 597 thermal stress $\sigma = E \varepsilon_{mec}$. The response of the two-bar model in Figure 2b is governed by the following
 598 equations (equilibrium and compatibility):

$$\begin{cases} \varepsilon_{tot,a} = \varepsilon_{tot,s} \\ \sigma_a A_a + \sigma_s A_s = 0 \end{cases} \quad (C.2)$$

599 The first equation states that the elongations of both bars must be equal, because the bars are attached
 600 to the same rigid end plate; the second equation specifies the equilibrium of forces transmitted by the
 601 two bars to the top rigid plate. By using Eq. (C.1), the first of previous equations can be rewritten as:

$$\alpha_a \Delta T + \frac{\sigma_a}{E_a} = \alpha_s \Delta T + \frac{\sigma_s}{E_s} \quad (C.3)$$

602 After rearranging, and by using the second equation in (B.2), the stress in the steel bar is obtained as:

$$\sigma_s = \frac{(\alpha_a - \alpha_s) E_s \Delta T}{1 + \frac{E_s A_s}{E_a A_a}} \quad (C.4)$$

603 while the stress in the aluminium bar is:

$$\sigma_a = - \frac{(\alpha_a - \alpha_s) E_a \Delta T}{1 + \frac{E_a A_a}{E_s A_s}} \quad (C.5)$$

604 Equations (C.4) and (C.5) show that thermal stresses are directly proportional to the temperature change
605 and, of course, no stress would develop without a temperature variation ($\Delta T = 0$). No stress is also
606 generated (even with a temperature change $\Delta T \neq 0$) if both materials have identical thermal expansion
607 coefficients ($\alpha_a = \alpha_s$), because the two bars elongate with identical thermal expansions. For the
608 aluminium/steel system (where $\alpha_a > \alpha_s$), the equations (C.4)-(C.5) correctly predict a tensile stress in the
609 steel bar and a compressive stress in the aluminium bar, as also shown by the results in Figure 3.
610 Equations (C.4) and (C.5) also show that thermal stress is controlled by the stiffness values of aluminium
611 and steel elements (summarised by the elastic moduli E_a, E_s), other than by the relative ratio of stiffness
612 (summarised by the ratios E_a/E_s and E_s/E_a).

613

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617

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