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Calculation of relative thermal elongation of structural steels

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Abstract In the recent past, there have been a number of studies toward predicting the thermal and structural behavior of components subjected to elevated temperature due to an exposure to fire. Numerical modeling has been applied quite extensively toward this end. An accurate numerical model requires the use of appropriate thermophysical properties of the materials such as steels, concretes etc. Recent investigations into the collapse of World Trade Center building 7 showed that thermal expansion played an important role in the generation of stresses at elevated temperatures in components that are restrained structurally [Structural fire response and probable collapse sequence of World Trade Center Building 7, NIST NCSTR 1-9, November 2008]. In this article, relative thermal elongations of structural steels are computed using an approach similar to the one proposed by Andres et al. [Scr Mater 39:791, 1998] but with a novel method of computing volume phase fractions using a thermodynamic database in conjunction with Thermo-Calc [Thermo-Calc Software (2009) http://www.thermocalc.com, Stockholm Technology Park, Björnnäsvägen 21, SE-113 47 Stockholm, Sweden], a software that performs standard equilibrium calculations and calculation of thermodynamic quantities based on thermodynamic databases. Thermal expansion coefficient values were computed for a steel of eutectoid composition and an ASTM A572 Grade 50 steel. While the volume fractions of phases for A572 steel were computed using the thermodynamic approach, those for the eutectoid steel were computed using an approach similar to the one proposed in reference [Scr Mater 39:791, 1998]. The computed values of relative thermal elongation were compared with the values obtained from Eurocode. While the match was reasonable for the most part, there are significant differences in the values obtained during the phase transformation range (967–1,086 K for ASTM A572 Grade 50 steel). Also, the computed values were compared against those recommended during the NIST (National Institute of Standards and Technology) World Trade Center failure investigation. Reasonable agreement was achieved in the temperature range between room temperature and 600 °C (873 K).

Introduction

In the recent past, there have been many analytical studies aimed at predicting the thermal and structural behavior of components subjected to elevated temperatures due to an exposure to fire [1]. Numerical modeling has been applied greatly toward this end. A combination of models, e.g., fire growth model, heat transfer model, and structural models were used to predict the behavior of components accurately. These models can be used in a sequential manner as opposed to a coupled model, which is computationally challenging and somewhat unnecessary as the selection of elements varies greatly among these models. For example, the transfer of temperature data from a heat transfer model to a structural model, or the transfer of nodal deflection data from a structural model to a heat transfer model can be done using compatible elements in a commercial software.

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An accurate model requires the use of appropriate thermophysical properties of the materials such as steels, concretes, etc. One of the important parameters in accounting for the expansion behavior is the thermal expansion coefficient. Recent investigation into the collapse of World Trade Center 7 building showed that thermal expansion played an important role in the generation of stresses at elevated temperatures [1].

The *thermal expansion coefficient* is a thermodynamic property of a substance. With the increase in the temperature of a material, the energy that is stored in the intermolecular bonds between atoms increases. As the stored energy increases with temperature, it results in an increase in the length of the intermolecular bonds. Solids typically expand when heated and usually contract on cooling. This dimensional response to temperature change is expressed by the coefficient of thermal expansion. Different coefficients of thermal expansion can be defined: linear thermal expansion, area thermal expansion, and volumetric thermal expansion.

The linear thermal expansion can only be defined for solids, and is common in engineering applications. It is a quantity that correlates the change in temperature of a material to its linear dimensions. It is defined as the ratio of the change in length over the original length per unit degree of temperature change:

$$\alpha = \frac{1}{L_0}\frac{\Delta L}{\Delta T}, \tag{1}$$

where L_0 is the original length and ΔL is the change in length due to a change in temperature of ΔT (unit can be in °C, °F, or K). Since the strain, ε_T, is defined as $\Delta L/L_o$, Eq. 1 can be written as:

$$\varepsilon_T = \alpha\,(\Delta T). \tag{2}$$

In order to compute the stress created by a temperature change in an axially restrained member, the following equation is written from Hooke's law:

$$\varepsilon = \frac{\sigma}{E} = \frac{P}{AE}, \tag{3}$$

where σ is the tensile stress, E the elasticity modulus, P the axial load and A the cross-sectional area. For a restrained component, since the total deformation must be zero, we can obtain the following expression by combining Eqs. 2 and 3:

$$P = -AE\alpha(\Delta T). \tag{4}$$

Since the axial force generated due to thermal expansion at elevated temperature is directly proportional to the thermal expansion coefficient, it is important to obtain accurate values of this thermal expansion coefficient of the material as a function of temperature. Note that the thermal expansion coefficient is a function of temperature.

In this article, a modified model based on the original model described by Andres et al. [2] is used to examine the dilatometric behavior of typical structural steel. Thermal expansion coefficients are computed using (a) the equilibrium phase fraction for a steel of eutectoid composition using binary phase diagram data and (b) phase fractions obtained as a function of temperature using the CALPHAD method [3] for an ASTM A572 Grade 50 steel. The computed data will be compared against the Eurocode approach [4].

Mathematical model

The room temperature microstructure of typical steel contains pearlite, a two phase mixture consisting of ferrite and cementite. On heating, the microstructure would change once the transformation temperature is reached. After heating to a single phase region (based on the composition of the steel), the microstructure would be fully austenitic if sufficient time is allowed for the diffusion process to come to completion. On heating, the temperature at which the steel becomes fully austenitic decreases with increase in carbon equivalent for a hyopeutectoid steel (e.g., steel with carbon equivalent <0.83 wt%). On the other hand, the temperature at which the steel becomes fully austenitic increases with increase in carbon equivalent for a hypereutectoid steel (e.g., steel with carbon equivalent >0.83 wt%). The austenitizing temperature for an eutectoid steel (carbon equivalent = 0.83 wt%) is 996 K. For a multicomponent steel, the following empirical equations can be written for Ac_1 and Ac_3 (Ac_1 is the temperature at which austenite begins to form during heating, Ac_3 is the temperature at which transformation of ferrite to austenite is completed during heating) as a function of concentration [5] (the element concentrations are given in mass%).

$$\begin{aligned} Ac_1 = {} & 723 - 10.7\ \mathrm{Mn} - 16.9\ \mathrm{Ni} + 29.1\ \mathrm{Si} + 16.9\ \mathrm{Cr} \\ & + 290\ \mathrm{As} + 6.38\ \mathrm{W} \end{aligned} \tag{5a}$$

$$\begin{aligned} Ac_3 = {} & 910 - 203\ \mathrm{C}^{1/2} - 15.2\ \mathrm{Ni} + 44.7\ \mathrm{Si} + 104\ \mathrm{V} \\ & + 31.5\ \mathrm{Mo} + 13.1\ \mathrm{W} \end{aligned} \tag{5b}$$

For isotropic expansion on heating, the following expression is valid for small changes:

$$\frac{\Delta L}{L_0} = \frac{V - V_0}{3\,V_0}, \tag{6}$$

where L_0 and V_0 are the length and volume at room temperature, respectively, and V the volume at a temperature greater than the room temperature. The relative change in length, $\Delta L/L_0$, can be computed from the volumes of the unit cells and the volume fractions of phases following [2]. Since unit cells of ferrite, cementite, and austenite contain 2, 12, and 4 iron atoms, respectively, the volume of the steel at a given temperature can be written as:

$$V = 2\,V_\alpha\,a_\alpha^3 + \frac{1}{3}\,V_\theta\,a_\theta\,b_\theta\,c_\theta + V_\gamma\,a_\gamma^3, \tag{7}$$

where V_α, V_θ, and V_γ are the volume fractions of ferrite, cementite, and austenite, respectively, and a_α and a_γ are the lattice parameters for ferrite and austenite, respectively. The lattice parameters for cementite are denoted as a_θ, b_θ, and c_θ.The lattice parameters are an approximately linear function of temperatures. For example, the lattice parameter of ferrite at a given temperature, a_α, is given by the following equations:

$$a_\alpha = a_{\alpha_0}\,[1 + \beta_\alpha\,(T - 300)], \tag{8}$$

where β_α is the linear thermal expansion coefficient of ferrite and T is temperature in K. Similar expressions are valid for cementite and austenite. Table 1 lists the lattice parameters and linear thermal expansion coefficients of each of the phases. The ferrite room temperature lattice parameter is assumed to be that of pure iron.

The lattice parameter of austenite at room temperature is obtained using the following equation [6, 7]:

$$\begin{aligned} a_{\gamma_0} &= 0.357 + 0.003\,w_{\mathrm{C}} + 0.000095\,w_{\mathrm{Mn}} - 0.00002\,w_{\mathrm{Ni}} \\ &\quad + 0.00006\,w_{\mathrm{Cr}} + 0.0003\,w_{\mathrm{Mo}} + 0.0002\,w_{\mathrm{V}}, \end{aligned} \tag{9}$$

where the lattice parameter a_{γ_0} is in nm and the mass fraction of the chemical composition is given as %. Here, w_{C}, w_{Mn}, w_{Ni}, w_{Cr}, w_{Mo}, and w_{V} are the compositions of carbon, manganese, nickel, chromium, molybdenum, and vanadium, respectively.

The linear thermal expansion coefficient of cementite is obtained using the following expression following Ridley [6] (temperature T is in K):

$$\begin{aligned} \beta_\theta &= 6 * 10^{-6} + 3 * 10^{-9}(T - 273) \\ &\quad + 1 * 10^{-11}(T - 273)^2. \end{aligned} \tag{10}$$

The volume at room temperature, V_0, can be determined using the same expression as given in Eq. 7 but using the room temperature coefficients as given in Table 1. Then the relative thermal elongation can be obtained by using Eq. 6 above.

When the temperature reaches the eutectoid transformation temperature, Ac_1, the austenite formation begins and with time pearlite structure disappears. The isothermal transformation of pearlite into austenite can be obtained using an Avrami type equation [8]. In the approach outlined in reference [2], no discussion is provided on how the volume fractions of ferrite and cementite are determined once the temperature exceeds the temperature at which eutectoid transformation begins.

In this article, for the case of the eutectoid steel used in reference [2], the volume fractions of phases are obtained using the Fe–$\mathrm{Fe_3C}$ phase diagram. When the temperature exceeds the transformation temperature, the relevant lines in the phase diagram are extrapolated. For the case of ASTM A572 Grade 50 steel, the volume fractions of phases are computed using the CALPHAD method [3].

For the case of the eutectoid steel, we use a modified Avrami type equation to obtain the fraction transformed in a constant rate heating mode. The transformed fraction of austenite at a temperature, T is obtained using the following classic equation:

$$x = 1 - \exp \int_{Ac_1}^{T} \frac{4\pi}{3\,\dot{T}^4}\,\dot{N}\,G^3\,\Delta T^3\,\mathrm{d}T, \tag{11}$$

where $\dot{T}$ is the heating rate, $\dot{N}$ and G are the nucleation and growth rates of austenite, respectively, and $\Delta T = T - \mathrm{Ac}_1$ (T, Ac_1 in K). Following Roosz et al. [9], the nucleation and growth rates depend on the pearlitic microstructure characteristics and the amount of heating beyond the transformation temperatures as expressed below:

$$\dot{N} = \frac{1.378 * 10^{-12}}{[(a^{\mathrm{P}})^2\,S_0]^2}\,\exp\left(\frac{-25.4}{T - \mathrm{Ac}_1}\right), \tag{12}$$

$$G = \frac{7 * 10^{-11}}{S_0^2}\,\exp\left(\frac{-29.7}{T - \mathrm{Ac}_1}\right), \tag{13}$$

where S_0 is the pearlite interlamellar spacing and a^{P} is the edge length of pearlite colonies. The units of nucleation and growth rates are in $\mathrm{mm}^{-3}\,\mathrm{s}^{-1}$ and mm/s, respectively. For the purpose of this study, S_0 is taken as 1.0×10^{-4} mm [10] and a^{P} is assumed to be $2.1\mathrm{e}^{-3}$ mm following [9]. A slow heating rate of 0.05 K/s is considered.

The relative change in length as computed by the model is shown in Fig. 1. Also, plotted on the same graph are the values computed using Eurocode equations for structural

Table 1 Lattice parameters and thermal expansion coefficient of phases

Phase	Lattice parameter	Room temperature value (nm)	Linear thermal expansion coefficient of phases (β)	Value (K^{-1}) (K = temperature in kelvin)
Ferrite	a_α	0.2866	β_α	1.244×10^{-5}
Austenite	a_γ	Eq. 8	β_γ	2.065×10^{-5}
Cementite	a_θ	0.45246	β_θ	Eq. 9
	b_θ	0.50885	β_θ	Eq. 9
	c_θ	0.67423	β_θ	Eq. 9

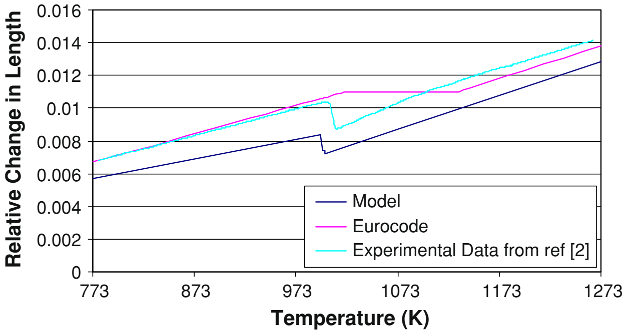

Fig. 1 Relative change in length for a steel of eutectoid composition

steel [4] and the experimental data from reference [2]. The Eurocode approach is comprised three equations: (1) from room temperature to 750 °C (1,023 K) (quadratic function of temperature), (2) from 750 °C (1,023 K) to 860 °C (1,133 K) (the relative change in length is constant), and (3) from 860°C (1,133 K) to 1,200°C (1,473 K) (linear function of temperature). The data computed using the model is similar to the one in reference [2]. The graph shows a linear increase in the relative change in length with increase in temperature until the phase transformation begins. Since there is volumetric contraction with formation of austenite, the relative change in length decreases until the transformation is completed. After this point, there is linear increase in the relative change in length with increase in temperature. The computed values from the model are slightly lower than the experimental values reported in reference [2] (Fig. 1). However, the trend is very similar including the magnitude of the contraction. The approximate values of parameters such as lattice parameters could be instrumental in causing this discrepancy. The Eurocode values are higher than those predicted by the model. The Eurocode predicts a constant value of the relative change in length during the phase transformation temperature range, which is considered to be rather large. This is not true for steel of eutectoid composition, which is the case here.

Next, an ASTM A572 Grade 50 steel was studied to determine the thermal expansion behavior. The mass fractions of the steel composition as % are given in Table 2.

Table 2 Chemical composition of ASTM A572 Grade 50 steel

Element	Mass fraction (%)
C	0.23
Nb	0.005
Mn	1.35
P	0.04
Si	0.4
S	0.05
V	0.11

Phase equilibria calculations

For the calculation of phase equilibria using the CALPHAD method [3], the Gibbs energy functions of each phase in a system are described as functions of temperature, compositions, and, if needed, pressure. The Gibbs energy functions are developed by fitting the adjustable parameters to experimental data of the constituent binary and ternary sub-systems and are collected in a so-called thermodynamic database. Thermodynamic extrapolation methods are then used to extend the thermodynamic functions into higher order systems. The phase equilibria, i.e., fractions of the stable phases and their compositions, are calculated by minimizing the overall Gibbs energy for a given composition, temperature, and pressure. The present calculations were carried out with the Thermo-Calc[1] software [11, 12] and a thermodynamic database for HSLA (high strength low alloy) steels [A. Kusoffsky, 2004, personal communication, SIMR].

The composition of the ASTM A572 Grade 50 steel was used for an equilibrium heating exercise. At each temperature, the fraction of phases present and the fractions of solutes in each phase were obtained. The following expressions are used to obtain the volume fraction of phases from molar fraction of phases and compositions of phases.

The molar volume of a phase, V_M^j, can be written as:

$$V_M^j = \sum_i x_i V_m^i, \tag{14}$$

where x_i is the atomic fraction of element i and V_m^i is the molar volume of element i. Then, the volume fraction of phase j, v_j, can be written as:

$$v_j = \frac{n_j V_M^j}{\sum_k n_k V_M^k}, \tag{15}$$

where n_j is the mole fraction of phase j obtained from Thermo-Calc and k varies from phase 1 to phase n present in the system.

The volume fractions of phases were computed for this steel by converting the phase fraction and composition data from Thermo-Calc [11] using expressions (14) and (15) and using values listed in Table 3. Figure 2 shows the variation of fraction of phases as a function of temperature. Small quantities of minor phases are not shown in this figure.

It can be seen that the room temperature microstructure contains mainly ferritic phase with a very small amount of cementite. Austenite starts forming at about 694 °C

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[1] Commercial products are referenced in this article as examples. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that it is necessarily the best available for the purpose.

Table 3 Data used for obtaining volume fraction phases

Element	Atomic mass, A_i (g/mol)	Molar volume, V_m^i (10^{-6} m^3/mol)	V_m^i/A_i (10^{-6} m^3/g)
C	12.011	5.3145	0.4424694
Nb	92.90638	10.841	0.11668736
Mn	54.93805	7.3545	0.133868967
Si	28.0855	12.054	0.4291894
S	32.066	16.36	0.5102
V	50.9415	8.3374	0.16366617
Fe	55.847	7.0923	0.1269952

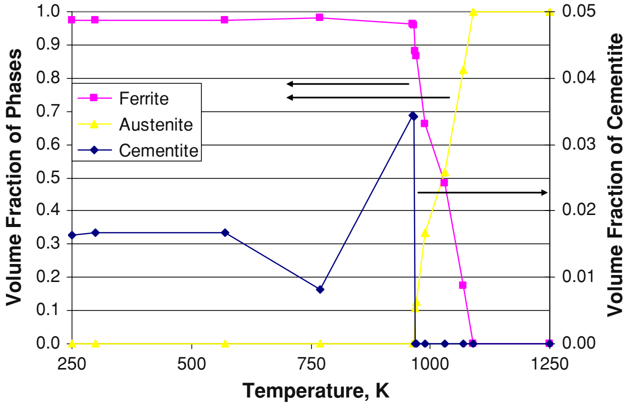

Fig. 2 Calculated volume fraction of an A572 Grade 50 Steel as a function of temperature

(967 K) and fully austenitic microstructure is obtained at 813 °C (1,086 K).

The variation of thermal elongation of the A572 Grade 50 steel was computed using the same model following Eq. 6 but using the volume fraction of phases as computed with thermodynamic databases as shown in Fig. 3. Also plotted on the same figure are the values computed using the Eurocode. In addition, the data recommended by the NIST (National Institute of Standards and Technology) World Trade Center (WTC) investigation report [13] are plotted in Fig. 3. It can be seen that the model predicts the contraction as expected during the formation of austenite. There is a reasonable agreement of model data with Eurocode except during the phase transformation. The Eurocode assumes a constant value during the phase transformation. It does not capture the contraction associated with the austenite formation. The model values compare reasonably well with values recommended by the NIST WTC investigation, especially in the temperature range from room temperature to about 600 °C (873 K). The present approach using a realistic phase fraction data computed with the actual chemical composition of steel can provide accurate values of the relative thermal elongation ($\Delta L/L$) of steel over a broad range of temperature.

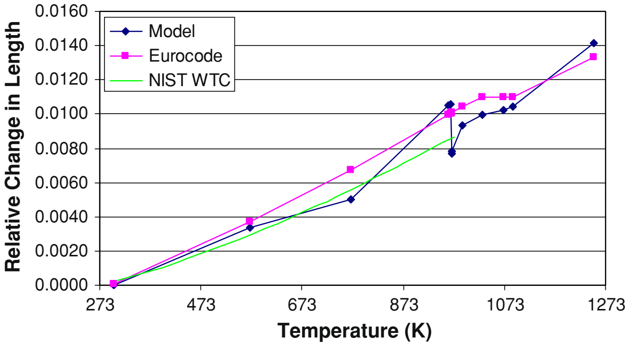

Fig. 3 Dilatation curves of an A572 Grade 50 steel computed with the model using thermodynamic databases, with Eurocode, and from NIST WTC report [13]

Summary

1. Relative thermal elongation of an eutectoid steel was computed using an Avrami equation for phase transformations following functions proposed by Roosz et al. [9] and a model for dilatometric behavior for steels proposed by Andres et al. [2], which was modified to compute phase fractions using extrapolated equilibrium phase diagram lines. The computed data were compared with those calculated using the Eurocode approach [4]. The trend was mostly similar except in the phase transformation region, where the model data lag those from Eurocode but correctly predict the contraction as expected during the phase transformation.
2. Relative thermal expansion for an ASTM A572 Grade 50 steel was computed with the same model but using the realistic volume fraction obtained by the CALPHAD approach and the thermodynamic databases in Thermo-Calc [3]. The computed data were compared against Eurocode values and the match was quite good except in the phase transformation region, where the Eurocode assumes a constant value. The model correctly predicts the contraction during the phase transformation. This approach can be readily used for any structural steel using the chemical composition and a thermodynamic package such as Thermo-Calc. The computed relative thermal elongation can then be used for an accurate modeling of the structural behavior of steel components under fire-induced heating.
3. The model assumes some characteristics of the pearlitic microstructure that can be varied based on actual data. Also, the model can be improved by obtaining more accurate lattice parameter values and linear thermal expansion coefficients of individual phases at elevated temperatures.

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