Mysteries behind the Coefficient of Thermal Expansion (CTE) Revealed

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Which calculation is correct?
Your job is to calculate the final length of a 1 meter long metal rod heated from 20C to 1020C. The coefficient of thermal expansion is α = 5.e-04 m/mC.

You use the formula $\dfrac{L - L_0}{L_0} = \alpha\left(T - T_0\right)$

And calculate $L = 1 + (1)(5.e - 04)(1020 - 20) = 1 + 0.5 = 1.5 \;\; m$

In checking your work, a colleague uses the thermodynamic definition for the coefficient of thermal expansion

$$\alpha = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_P \qquad \text{or} \qquad \frac{dL}{L} = \alpha dT$$

Integrating $\displaystyle\int_1^L \frac{dL}{L} = 5.e - 04 \int_{20}^{1020} dT$

He gets $\ln(L) - \ln(1) = (5.e - 04)(1020 - 100) = 0.5$

$$L = \exp[\ln(1) + 0.5] = 1.65 \;\; m$$

There is a large difference between the two answers. Which one is correct?

Both are correct plus 1 other is also correct
The difference is related to the definition of the CTE – there are 3. When using a CTE from a reference publication, you must determine how the CTE is defined. The 3 definitions for CTE are:

1. Tangent CTE using current length $\alpha_t = \dfrac{1}{L}\left(\dfrac{\partial L}{\partial T}\right)_P$ (eq. 1)
2. Tangent CTE using reference length $\alpha_{t,r} = \dfrac{1}{L_r}\left(\dfrac{\partial L}{\partial T}\right)_P$ (eq. 2)
3. Secant (or, mean) CTE $\alpha_s = \dfrac{L - L_r}{L_r\left(T - T_r\right)}$ (eq. 3)

These are shown graphically in figure 1. The thermodynamic defined coefficient, α_t, is the slope of the tangent to the curve at a specific temperature, T. The secant coefficient, α_s, is the slope of the line between two points on the curve. One point is taken as the reference state (T_r, L_r). The subscript, r, means reference state. The thermal strain is zero at the reference temperature, T_r , and reference length, L_r. The reference temperature is usually 20C.

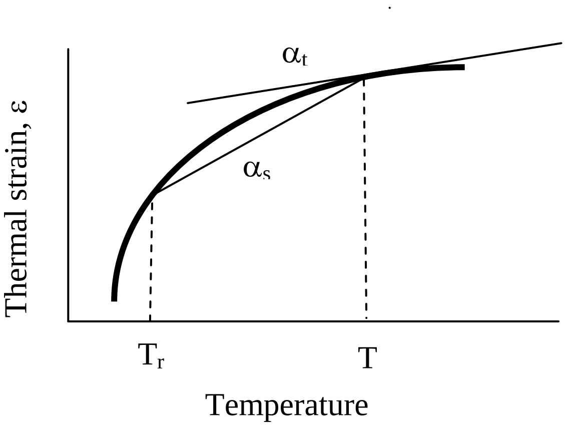

Figure 1: Shown is the graphical representation of the tangent, α_t, and secant, α_s, coefficient of thermal expansion.

The CTEs can also be interpreted as representing the:

- "natural (logarithmic)" strain $\bar{\varepsilon} = \frac{dL}{L} = \alpha_t dT$ using eq. 1.
- "engineering (linear)" strain $\varepsilon = \frac{L - L_r}{L_r} = \alpha_s (T - T_r)$ using eq. 3.

Integrating $\int_{L_r}^{L} \frac{dL}{L}$, we obtain the logarithmic strain $\bar{\varepsilon} = \ln\left(\frac{L}{L_r}\right)$.

This can also be expressed as $\bar{\varepsilon} = \ln\left(1 + \frac{L - L_r}{L_r}\right) = \ln(1 + \varepsilon)$

If $\alpha_s (T - T_r) << 1$, then $\bar{\varepsilon} \cong \varepsilon$. CTE values for metals and alloys are in the range of 10x10^{-6} to 30x10^{-6} /K. The difference in the thermal strain calculation if you use a tangent or secant CTE for reasonable temperature changes is very small for metals. However, using the correct CTE definition becomes more important for plastics with a typical CTE around 1x10^{-4} K.

The tangent coefficient of thermal expansion (default CTE definition in LS-DYNA)

The tangent coefficient of thermal expansion, $\alpha_t = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_P$, is a very convenient value to use in an explicit finite element code. An explicit analysis is an incremental method where calculations are based on the instantaneous properties of the material. A reference state (e.g., reference temperature, reference length) is not required. The same tangent CTE values are applicable for heating an object up from room temperature or, cooling it down from an elevated temperature (e.g., hot stamping, casting). This is not true for secant CTEs which have different values for heating and cooling because the secant CTE is a function of a strain free reference state. The secant CTE values depend on whether the strain free reference state is at room temperature or at the elevated temperature.

A thermodynamic relation defines the tangent CTE. It is therefore compatible with thermodynamic defined equations of state. This makes solid-solid and liquid-solid volume changes during phase transition easy to calculate.

A main difficulty is finding values for tangent CTEs. They are much less reported in the literature than secant values. However, they can be easily calculated. An excellent source for CTE values is the reference book, <u>Thermophysical Properties of Matter, Thermal Expansion</u>, Vol. 12., ed. Y.S. Touloukin. Thermal expansion data is presented as polynomial curve fits, such as:

$$\frac{L - L_{293}}{L_{293}} = a + bT \quad + cT^2 + dT^3 \qquad \text{(eq. 4)}$$

To obtain the tangent CTE, we can simply take the derivative of this polynomial, dL/dT, and then divide by the current length, L, at a specific temperature, T.

The tangent coefficient of thermal expansion using a reference length

The tangent coefficient of thermal expansion using a reference length, $\alpha_{t,r} = \frac{1}{L_r}\left(\frac{\partial L}{\partial T}\right)_P$, is presented as tabulated data in the reference book, <u>Thermophysical Properties of Matter, Thermal Expansion</u>, Vol. 12., ed. Y.S. Touloukin. I'm not aware of any FE codes that use this definition. However, this definition gets confused with the tangent coefficient, α_t, in the literature. You will find the statement in the literature that, "if the CTE is not a function of temperature, then the tangent CTE equals the secant CTE". This is only true for $\alpha_{t,r}$ and not for α_t.

Integrating eq. 2 $$\int_{L_r}^{L} \frac{dL}{L_r} = \int_{T_r}^{T} \alpha_{t,r}\, dT \qquad \text{(eq. 5)}$$

We obtain $$\frac{L-L_r}{L_r}=\int_{Tr}^{T}\alpha_{t,r}\,dT \qquad \text{(eq. 6)}$$

Equation 3 can be written as $$\frac{L-L_r}{L_r}=\alpha_s\left(T-T_r\right) \qquad \text{(eq. 7)}$$

Then, equating equations 6 and 7 we obtain: $$\alpha_s=\frac{1}{\left(T-T_r\right)}\int_{T_r}^{T}\alpha_{t,r}\,dT \qquad \text{(eq. 8)}$$

We can see from equation 8 that if $\alpha_{t,r}$ is not a function of temperature, then $\alpha_s=\alpha_{t,r}$. Equation 8 also shows that α_s is the mean value of $\alpha_{t,r}$ over the temperature interval.

The secant coefficient of thermal expansion (optional CTE definition for MAT_106 in LS-DYNA)

Another definition for the coefficient of expansion exists which is called the secant value, α_s. These are easily obtained in the laboratory and I'm sure many of you performed this experiment in a college physics lab. Take a rod at room temperature (i.e. reference temperature), T_r, and measure its length, L_r. Then uniformly (usually by an electric current) heat the rod and measure its new length, L, (or, change in length) and temperature, T. Then,

$$\alpha_s=\frac{L-L_r}{L_r\left(T-T_r\right)} \qquad \text{(eq. 9)}$$

Note that a reference temperature, T_r, must be specified when using the secant value of thermal expansion. α_s is also referred to as the "mean" or "effective" coefficient of thermal expansion.

Historically, the specification of α_s as a function of temperature allowed modeling the nonlinear influence of temperature on thermal strain in linear finite element codes. This specification carried over to many of the current nonlinear codes. For linear and nonlinear incremental material analysis, the increment in thermal strain can be calculated by

$$\Delta\varepsilon=\frac{\Delta L}{L_r}=\alpha_{s,T+\Delta T}\left(T+\Delta T-T_r\right)-\alpha_{s,T}\left(T-T_r\right) \qquad \text{(eq. 10)}$$

This is an exact calculation and therefore is not dependent on the incremental time step size. This expression is used in implicit finite element calculations.

The main disadvantage in using α_s is the requirement of a reference state. If the part initial temperature is different from the material reference state temperature, then the α_s values are no longer valid. They must be adjusted to account for the new strain free condition at the part initial temperature.

How do you adjust α_s values at a new reference state?

If the part initial temperature state (P_1), is different from the material reference temperature state (P_0), then the α_s values must be modified. The subscript RM means ‘reference material’, and the subscript RP means ‘reference part’. Figure 2 graphically depicts the computational method.

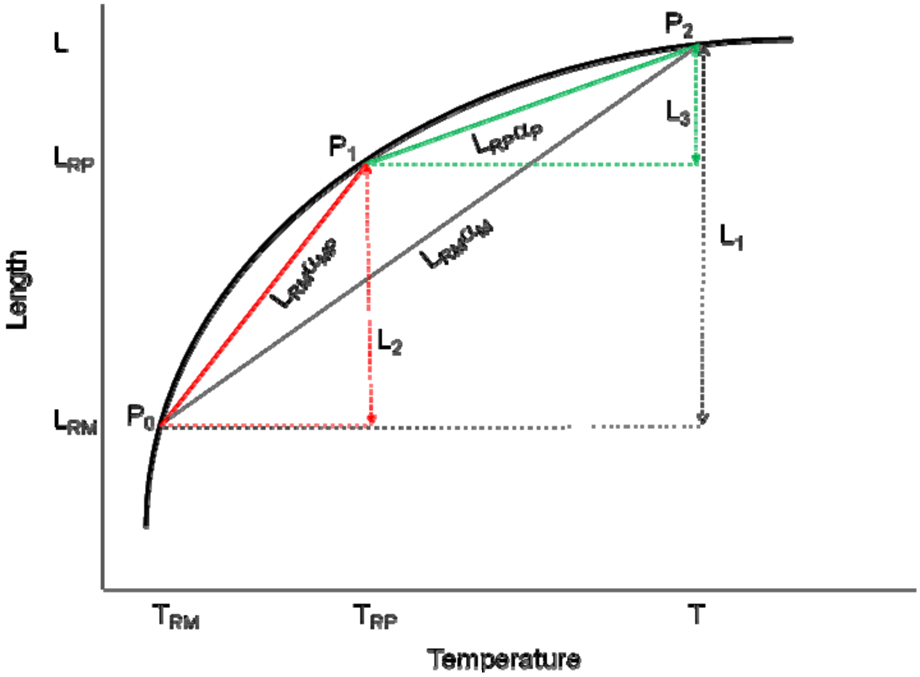

Figure 2: This figure shows graphically the parameters used in eq. 11 to shift the CTE reference state.

(T_{RM}, L_{RM}) is the material reference state at point P_0. This is the reference state for the material data. α_M is the secant CTE at the temperature, T. α_{MP} is the secant CTE at the temperature T_{RP}. α_M and α_{MP} are obtained from the literature.

(T_{RP}, L_{RP}) is the part reference state at point P_1. This is the initial temperature for the part at which the thermal strain is 0. We want to calculate α_P.

$L_{RM}\alpha_M$ is slope of the line from point P_0 to P_2.

$L_{RM}\alpha_{MP}$ is the slope of the line from point P_0 to P_1.

$L_{RP}\alpha_P$ is the slope of the line from point P_1 to P_2.

$$L_1 = L - L_{RM} = L_{RM}\alpha_M\left(T - T_{RM}\right)$$

$$L_2 = L_{RP} - L_{RM} = L_{RM}\alpha_{MP}\left(T_{RP} - T_{RM}\right)$$

$$L_3 = L - L_{RP} = L_{RP}\alpha_P\left(T - T_{RP}\right)$$

$$L_3 = L_1 - L_2$$

$$\alpha_P = \left(\frac{L_{RM}}{L_{RP}}\right)\frac{\alpha_M\left(T - T_{RM}\right) - \alpha_{MP}\left(T_{RP} - T_{RM}\right)}{\left(T - T_{RP}\right)} \qquad \text{(eq. 11)}$$

How do you calculate α_t from α_s?

The secant lines can be used to approximate the tangent. The slope of a secant line (e.g., α_p in figure 2) approaches the slope of the tangent line as the secants' 2nd point (i.e., P_2) approaches the 1st point (i.e., P_1). The problem of finding the tangent line to a graph was one of the main problems that originated calculus. In calculus this problem is solved using Newton's difference quotient.

$$f'(a) = \lim_{h \to 0}\frac{f(a+h) - f(a)}{h}$$

This equation is similar to eq. 11. Also, by observation, the secant α_P in figure 2 appears to represent the slope of the tangent to the curve at the point $(T+T_{RP})/2$. The input to most FE codes is by piecewise linear data tables. If we have 2 data pairs (α_{s1},T_1) and (α_{s2}, T_2), we can calculate α_t at the midpoint temperature (T1+T2)/2 using eq. 11. Remember that this calculation is approximate and becomes more accurate in the limit as $\lim(T-T_{RP}) \rightarrow 0$.

How do you calculate α_s from α_t?

We can use equation (1) to calculate the thermal strain, $\varepsilon = \frac{dL}{L_r} = \int_{T_r}^{T} \alpha_t dT = \alpha_t\ (T - T_r)$ for the case α_t = constant. The input to most FE codes is by piecewise linear data tables in which the tangent coefficient of thermal expansion is considered constant over the temperature increment. For example, $\alpha_{t,1}$ is constant between T_r and T_1, $\alpha_{t,2}$ is constant between T_1 and T_2, etc. Then

$$\varepsilon_1 = \alpha_{t,1}(T_1 - T_r)$$

$$\varepsilon_2 = \varepsilon_1 + \alpha_{t,2}(T_2 - T_1)$$

$$\varepsilon_3 = \varepsilon_2 + \alpha_{t,3}(T_3 - T_2)$$

Secant values of the coefficient of thermal expansion can then be calculated from:

$$\alpha_{s,1} = \varepsilon_1/(T_1 - T_r)$$

$$\alpha_{s,2} = \varepsilon_2/(T_2 \quad T_r)$$

$$\alpha_{s,3} = \varepsilon_3/(T_3 - T_r)$$

CTE Data for Aluminum

Temperature [K]	Length [m]	α_{tan} [μm/m K]	α_{tan_r} [μm/m K]	α_{sec} [μm/m K]
293	1.000000	23.59	23.59	23.59
300	1.000165	23.63	23.64	23.61
325	1.000759	23.84	23.86	23.72
350	1.001359	24.08	24.11	23.84
375	1.001965	24.35	24.40	23.97
400	1.002579	24.65	24.71	24.10
425	1.00321	24.98	25.06	24.25
450	1.003833	25.34	25.44	24.41
475	1.004474	25.73	25.85	24.58
500	1.005126	26.15	26.29	24.76
525	1.005789	26.61	26.76	24.95
550	1.006465	27.09	27.26	25.15
575	1.007153	27.60	27.80	25.37
600	1.007855	28.14	28.36	25.59
625	1.008572	28.71	28.95	25.82
650	1.009304	29.31	29.58	26.06
675	1.010052	29.94	30.24	26.31
700	1.010817	30.60	30.93	26.58
725	1.011599	31.28	31.65	26.85
750	1.012400	32.00	32.40	27.13
775	1.013220	32.74	33.18	27.43
800	1.014060	33.52	33.99	27.73