Estimating Error for Numerical Evaluation of the Arrhenius Integral

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The Arrhenius Integral model for thermal damage requires the evaluation of the integral[1]

$$\Omega(\tau) = \int_0^\tau A e^{\frac{-Ea}{RT(t)}} dt. \tag{1}$$

For all but the simplest thermal profiles, this integral must be numerically evaluated. We would like to estimate the error accumulated during numerical evaluation.

Assume that we have a thermal profile sampled at discrete times $\{t_i\}$. If the temperature between any two times is a monotonic function between the temperature at each time, then the accumulated damage between the two times must be greater than the damage that would accumulate at minimum temperature over the time interval, and the damage that would accumulate at the maximum temperature over the time interval.

Let T_i be the temperature at the time t_i. The accumulated damage over the interval $[t_i, t_{i+1}]$ will satisfy

$$A e^{\frac{-Ea}{R\min(T_i,T_{i+1})}} \tau \geq \Omega \geq A e^{\frac{-Ea}{R\max(T_i,T_{i+1})}} \tau \tag{2}$$

A numerical implementation will need to check for the case that $T_0 = T_1$ and use the constant temperature quadrature. If T_0 and T_1 are stored as floating point numbers, then we will probably need to check that they are "close", rather than "equal". Note that, for a linear temperature rise from T_0 and T_1, evaluating Equation **??** will to give a numerical value between $Ae^{-E_a/RT_0}(t_1 - t_0)$ and $Ae^{-E_a/RT_1}(t_1 - t_0)$. We can therefore write a limit on the maximum error in incurred by any numerical approximation to integral over duration $t_1 - t_0$.

$$\epsilon \leq \frac{\left|Ae^{-E_a/RT_1}(t_1 - t_0) - Ae^{-E_a/RT_0}(t_1 - t_0)\right|}{Ae^{-E_a/RT_0}(t_1 - t_0)} = \left| e^{-\frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_0}\right)} - 1 \right| \tag{3}$$

This gives a metric for deciding if T_1 and T_0 are "close enough". Given a tolerance, or maximum allowed error, we

$$\frac{R}{E_a} \ln(\epsilon + 1) \leq \left| \frac{1}{T_1} - \frac{1}{T_0} \right| \tag{4}$$

For small ϵ, $\ln(\epsilon + 1) \approx \epsilon$,

$$\frac{1}{T_1} - \frac{1}{T_0} \geq \frac{R}{E_a}\epsilon \tag{5}$$

References

[1] A.J. Welch and M.J.C van Germert, editors. *Optical-Thermal Response of Laser-Irradiated Tissue*. Plenum Press, 2nd edition, 2011.