USING RESIDUALS IN THE EVALUATION OF COMPETING MODELS



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Overview:

Experimental Measurements Mathematical Models Insight from sensitivity coefficients Insight from Residuals Selecting Competing Models Various Applications



To Start: Experimental Measurements



Temperature measurements from a 1mm thick carbonbonded carbon-fiber material (CBCF) at 1000°C in a laser flash diffusivity experiment.

Method first used by Parker, et al. (1961)



Mathematical Model:

Temperature response on the unheated surface from a heat pulse of magnitude q_o (in Joules per square meter). This assumes pure Fourier diffusion of heat with a convective surface on each face.

Three parameters: α , q_o and Bi

$$T(L, t) = \frac{2q_o \alpha}{Lk} \sum_{m=1}^{\infty} e^{-\beta_m^2 \alpha t/L^2} \frac{\beta_m [\beta_m \cos(\beta_m) + Bi \sin(\beta_m)]}{\beta_m^2 + Bi^2 + 2Bi}$$
$$\tan(\beta_m) = \frac{2\beta_m Bi}{\beta_m^2 - Bi^2}$$



Accounting for penetration of the flash heating:



New model for the initial condition: $T(x,0) = e^{-x/a}$

"Mean free path" of a photon as fourth parameter "a"



Sensitivity coefficients:

- Derivative of temperature with respect to the parameters
- Plot with respect to time for insight into experiment design





Residuals: The error between the measurements and the model



If we plot the measurements and the model, the results should line up on one another as in the graph above.



Analysis of Residuals:

•"Diamond" plot is desired

"Square" plot has a signature indicating something is not accounted for in the physics of the problem.
Residual standard deviation drops from 0.032 to 0.011

by adding fourth parameter.









Residual Analysis

Test 3 has a definite signature

This sample became de-laminated during





Residual analysis

The model appears to be valid over a 100 second period but breaks down subsequent to that, presumably due to thermal damage to the sample.





Flash Diffusivity – thin highly conductive samples - Assumed Pulse Shape





Four Parameters Simultaneously Estimated

Using least squares in nonlinear regression

- 1. Thermal diffusivity
- 2. Magnitude of heat pulse
- 3. Pulse start time (t_1)
- 4. Pulse end time (t_2)



Plot of Residuals

Greatest impact during early portion of experiment





Results from Three Sample Thicknesses

Stainless steel NIST SRM-1461

Published diffusivity $4.62 \pm 0.42 \text{ mm}^2/\text{s}$





Application of the "F" Test

•Uses the "F" Statistic to determine whether an additional parameter is statistically significant in a more sophisticated model.

•95% confidence region is normally used

Procedure:

- 1. Find sum of squares of residuals (R) resulting from each model being compared.
- 2. Subtract the two sums of squares from each other (ΔR).
- 3. Divide ΔR by mean square error sum of refined model (s²).
- 4. Compare this quotient to the "F" statistic.
- 5. If $\Delta R/s^2 > F$ then the additional parameter is valid.



Example Application of the "F" Test

(a) One-dimensional conduction assuming surface heating only (Parameters: α ,q, Bi; R=2.042).

- (b) Two-dimensional conduction assuming surface heating only (Parameters: α ,q, Bi; R=1.122).
- (c) One-dimensional conduction assuming penetration of the flash (Parameters: α ,q, Bi, a; R=0.172).
- (d) Two-dimensional conduction assuming penetration of the flash (Parameters: α ,q, Bi, a; R=0.062).

(e) Two-dimensional conduction assuming penetration of the flash and a nonuniform distribution of the flash over the face of the sample

(Parameters: α ,q, Bi, a, r_h; R=0.043).

Comparison	ΔR	$\Delta R/s^2$	"F" Statistic	Additional Parameter Valid
Models (a) and (c)	1.87	1911	3.95	yes
Models (b) and (d)	1.06	2854	3.95	yes
Models (d) and (e)	0.0184	70.6	3.95	yes



Conclusions

- •Three examples were considered
- •An analysis of the residuals allowed a comparison of competing models
- •A signature in the residuals indicated an inadequacy in the model
- •The "F" Test can be used to determine whether additional parameters are statistically significant



