Model Validation Challenge Problems: Thermal Problem

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Introduction

Here we present a carefully defined challenge problem which incorporates features that represent the practical realities that are often imposed on modelers and experimentalist in the development and execution of a validation exercise. The sources of difficulty in a validation exercise include the uncertainties in model validation experiments due to unit-to-unit variability in the physical properties and the consideration that most models for complex systems contain approximation.

The specific task of this validation exercise is to develop statements (or measures) of confidence that the provided model can be applied to a specified set of conditions (intended application), given a set of validation tests. In the exercise, participants are invited to quantify the accuracy of the model through comparisons with experimental data, and, if deemed necessary, provide error compensation methodology for the application to the specified conditions.

The physical process chosen for this challenge problem is transient, heat conduction through a slab (1D heat flow). This application was chosen because a) it has many features associated with a broader class of transport phenomena such as the transport of mass, momentum, energy, and chemical species; b) the governing differential equation, which is based on conservation of energy and Fourier's law, is familiar to many engineers, mathematicians, and physicists; c) exact solutions to the corresponding governing equations are available in the form of Fourier series; and d) temperatures measured as a function of time from such a system results in multivariate, correlated data.

The challenge problem consists of four distinct activities characteristic of many real world situations:

1. Use material characterization data to estimate the uncertainty in physical properties associated with the mathematical model.
2. Make an assessment of model accuracy within an available database consisting of a number of experiments (exploring design and/or operation factors) that are clearly related to, but may not fully relevant to the intended application.
3. Make an assessment of model accuracy for limited number of tests, which are nearly representative of the application parameter space, but at a point outside the parameter space of the previously available database.
4. Assess regulatory compliance using all available information from the previous validation activities.

The first activity is a precursor to validation. The value of the physical properties, and associated uncertainty, are derived from the material characterization for use in the mathematical model in the subsequent validation activities. The next two activities represent quantifying the accuracy of the model for a suite with limited number of experiments over a database. The fourth activity brings the quantification into a (regulatory) decision context.

In reality, adequacy of models can only be judged in an application context; which for the purpose of discussion, is taken to be a high-consequence regulatory decision. It is this perspective that drives the need for validated models; consequently, the framework for a regulatory decision is described next.

A HIGH-CONSEQUENCE REGULATORY DECISION FOR AN INTENDED APPLICATION

We have an ensemble of safety-critical devices that exhibit unit/unit variability due to manufacturing processes. The device is a material layer of thickness L that is exposed to a heat flux. In the intended application the devices are exposed to environments that are well characterized, $q = 3500\ W/m^2$ and thickness $L = 1.90\ cm$, neither having uncertainty.

The regulatory requirement states that at a specified time $t' = 1000$ sec, the surface temperature (T_s) is not to exceed a failure temperature $T_f = 900^o C$ in a specified fraction of the units ($p_f = 0.01$). Specifically,

$$p\left(T_s(t = t') > T_f\right) < p_f \tag{1}$$

It is prohibitively expensive to assess regulatory compliance though lot sample testing of the safety devices; consequently, it is expected that the validated model, discussed next, will play a critical role in the assessment of regulatory compliance. ***Participants are asked to assess whether the device meets the regulatory requirement using the model and their confidence in the assessment.***

The same processes are used for preparing the samples for testing in validation (described later) as is used in the intended application. Hence, unit-to-unit variability in the intended application is the same as investigated in the material characterization and validation activities discussed in the following sections.

Mathematical Model for the Intended Application

The temperature response of the device in the intended application is modeled by one-dimensional heat conduction through a slab (Figure 1). The boundary conditions are specified flux on the *x=0* face and adiabatic on the *x=L* face. Furthermore, the thermal properties, k and ρC_p and initial condition, T_i, are described by constants. The analytical solution for the temperature in the body (for $t>0$) can be written as

$$T(x,t) = T_i + \frac{qL}{k}\left[\frac{\left(k/\rho C_p\right)t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2}\left(\frac{x}{L}\right)^2 - \frac{2}{\pi^2}\sum_{n=1}^{6}\frac{1}{n^2}e^{-n^2\pi^2\frac{\left(k/\rho C_p\right)t}{L^2}}\cos\left(n\pi\frac{x}{L}\right)\right] \quad (2)$$

The solution is a truncated infinite series. Sufficient accuracy for the challenge problem exercise can be obtained with six terms (for $t>0$) in the series. The solution at $t=0$ is $T(x,t=0) = T_i$; Eq. (2) should not be evaluated at $t=0$. Eq. (2) is the mathematical model to assess the regulatory decision for the intended application in the previous section. This model will also be compared to experimental data as part of the validation exercises described later.

To verify each participant's implementation of the analytical solution in Eq. (2), numerical values for the temperature at $x=0$ are provided for the parameter values listed in Table 1. The temperature solution is provided in Table 2. The values are an accurate solution to Eq. (2) for the number of significant digits provided in the table.

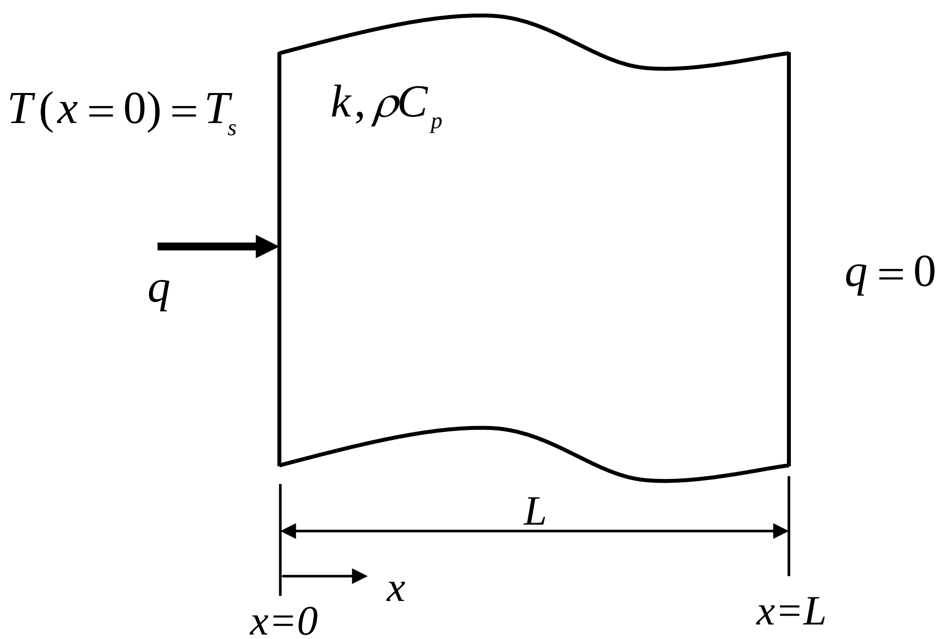

Figure 1. Schematic of heat conduction problem

Table 1. Model parameters for checking the implementation of Eq. (2)

Parameter Name	**Parameter Symbol**	**Value**
Thermal conductivity (W/m^{o}C)	k	0.05
Volumetric Heat Capacity (J/m^{3o}C)	ρC_p	0.4E+06
Heat Flux (W/m^2)	q	3000
Thickness (m)	L	0.0127
Initial Temperature (^{o}C)	T_i	25

Table 2. Temperature values from with Eq. (2) using the property values in Table 1

Time (sec)	**Temp (^{o}C), x=0**
100	264.365410
200	363.582289
300	440.597591
400	507.977177
500	570.904767
600	631.761990
700	691.655773
800	751.101191
900	810.337947
1000	869.477597

Validation Activities

The intended application requires the model to predict the surface temperature given the thermal properties, *k* and ρCp, applied heat flux, *q*, thickness, *L*, and initial temperature, T_i. Specifically, we need to assess whether the model can be used to assess compliance with the regulatory requirement given in Eq. (1). Three experimental activities are planned to understand the accuracy of the model for the intended application. These activities are discussed next.

Material Characterization. Thermal properties, *k* and ρCp, required for the model are characterized. Material characterization is a precursor to validation and does not involved the mathematical model. The material characterization is performed on samples representative of the intended application, but does not require a mathematical model.

Ensemble Validation. A suite of experiments is conducted over a range of thicknesses, *L* and heat flux magnitudes, *q*. The suite of experiments was selected based on 1) concerns that the model's accuracy may be sensitive to *L*, 2) experimental issues make experiments at higher heat flux values more costly, and 3) the intended application is an extrapolation from the heat fluxes studied here. Experiments are conducted at the four heat flux/ thickness points shown in Figure 2 . As discussed later, multiple experiments may be conducted at each point in the parameter space (*L*/*q*). These experiments are related, but not fully relevant to the conditions of the intended application and regulatory requirements.

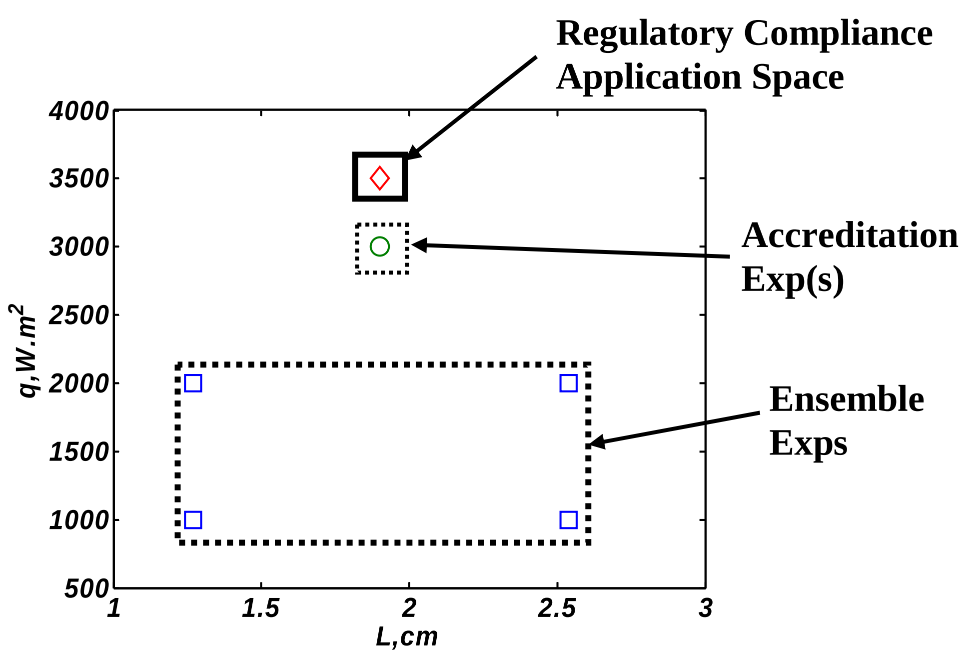

Figure 2. Parameter space for the validation activities

Accreditation Validation. Limited experiments are conducted for conditions more representative of the intended application. The number of experiments is limited by cost and schedule. As shown in Figure 2, the conditions for the experimental activity are closer to the conditions associated with the regulatory requirement, but have a lower heat flux magnitude.

Regulatory Compliance. After considering the comparison of the model for the three experimental activities, participants are asked to assess regulatory compliance for the intended application. Conditions for the intended application require an extrapolation from heat flux magnitudes studied in the accreditation and ensemble validation (Figure 2).

Participants are asked to address each experimental activity for a different number of experiments. Consider three levels to describe the number of experiments: low, medium, and high. The number of experiments associated with each level is shown in Table 3. For the ensemble and accreditation validation varying numbers of experiments are provided at points identified in Figure 2. For example, a low-level of experimental information has six experiments to characterize the material, one experiment at each point in the parameter space (configuration) for a total of four for the ensemble validation, and one accreditation experiment. We are asking participants to provide three solutions. The first solution uses "Low" experimental information, 6 experiments for the material characterization, 4 experiments (1 per configuration) for the ensemble validation, and 1 experiment for the accreditation. The second solution would use "Medium" experimental information identified in the middle row of Table 3 and the third solution would used "High" experimental information identified in the last row of Table 3. The intent is to see how the conclusions are impacted by more experimental data. If a participant wishes to provide only one solution, the "Medium" experimental information should be used.

The following sections describe the experimental data provide for each experimental activity. The participants are asked to use the experimental data provided in the following sections to address questions in the Tasking document.

Table 3. Number of experiments for each experimental activity

Exp runs	**Material Characterization (N_c)**	**Ensemble Validation (N_v)**	**Accreditation (N_a)**
Low	6	1 per Config./ 4 total	1
Medium	20	2 per Config./ 8 total	1
High	30	4 per Config./ 16 total	2

MATERIAL CHARACTERIZATION

The project manager is concerned that the available model applies only to the specialized case of constant material properties. The project manager funds a materials characterization study over the temperature range of the validation database and the intended application. The material characterization is performed on specimens that have nominal dimensions that are representative of the intended application and specimens are manufactured with the same processes used in the intended application.

The material characterization provides an estimate of both thermal conductivity and volumetric heat capacity for a (randomly) selected specimen at a given temperature. Each pair of property estimates (thermal conductivity and volumetric heat capacity) is from the characterization of a different randomly selected sample. It is reasonable to assume that 1) diagnostic variability or uncertainty is negligible compared to specimen-to-specimen variability, 2) estimates of thermal conductivity and volumetric heat capacity are independent, and 3) estimates for a given property at different temperatures are independent (i.e., from characterizing a different sample).

The material characterization data are provided in Table 4. The low-level of experimental information provides six (N_c=6) thermal conductivity/volumetric heat capacity estimates at one of three temperatures (20, 500, and 1000 ^{o}C). Higher-levels of experimental information add additional values and include values at more temperatures. For example, the medium-level (N_c=20) includes the 6 values from the low-level and adds 14 more values, including values at additional temperatures.

Table 4. Material characterization of the thermal properties

Thermal Conductivity, *k(T)*, W/m^{o}C				
***k*(20^{o}C)**	***K*(250^{o}C)**	***k*(500^{o}C)**	***k*(750^{o}C)**	***k*(1000^{o}C)**
		N_c = 6		
0.0496	-	0.0602	-	0.0631
0.0530	-	0.0546	-	0.0796
		N_c = 20		
0.0496	0.0628	0.0602	0.0657	0.0631
0.0530	0.0620	0.0546	0.0713	0.0796
0.0493	0.0537	0.0638	0.0694	0.0692
0.0455	0.0561	0.0614	0.0732	0.0739
		N_c = 30		
0.0496	0.0628	0.0602	0.0657	0.0631
0.0530	0.0620	0.0546	0.0713	0.0796
0.0493	0.0537	0.0638	0.0694	0.0692
0.0455	0.0561	0.0614	0.0732	0.0739
0.0483	0.0563	0.0643	0.0684	0.0806
0.0490	0.0622	0.0714	0.0662	0.0811
Volumetric Heat Capacity, ρCp(T), J/m^{3o}C				
ρCp(20^{o}C)	**ρCp(250^{o}C)**	**ρCp(500^{o}C)**	**ρCp(750^{o}C)**	**ρCp(1000^{o}C)**
		N_c = 6		
3.76E+05	-	4.52E+05	-	4.19E+05
3.38E+05	-	4.10E+05	-	4.38E+05
		N_c = 20		
3.76E+05	3.87E+05	4.52E+05	4.68E+05	4.19E+05
3.38E+05	4.69E+05	4.10E+05	4.24E+05	4.38E+05
3.50E+05	4.19E+05	4.02E+05	3.72E+05	3.45E+05
4.13E+05	4.28E+05	3.94E+05	3.46E+05	3.95E+05
		N_c = 30		
3.76E+05	3.87E+05	4.52E+05	4.68E+05	4.19E+05
3.38E+05	4.69E+05	4.10E+05	4.24E+05	4.38E+05
3.50E+05	4.19E+05	4.02E+05	3.72E+05	3.45E+05
4.13E+05	4.28E+05	3.94E+05	3.46E+05	3.95E+05
4.02E+05	3.37E+05	3.73E+05	4.07E+05	3.78E+05
3.53E+05	3.77E+05	3.69E+05	3.99E+05	3.77E+05

VALIDATION EXPERIMENTS

The experimental data provided in this section to assess the model are simulated. As explained below, the process to generate the simulated experimental data has taken into account the variability between nominally identical test specimens that one encounters in an actual experiment.

An experimental apparatus for the configuration shown in Figure 1 is the basis for generating the experimental data. In the ensemble validation, a suite of experiments is conducted for a range of thicknesses and heat flux magnitudes with replicate experiments. The accreditation conducts a limited number of experiments for a specified thickness and heat flux which is different from the values investigated during the ensemble validation. A description of the process to conduct the (simulated) experiment follows.

Each experiment is conducted on a randomly selected specimen. Our knowledge of the effect of variability between experimental specimens on their thermal properties is reflected in the data provided in the Material Characterization section. All data associated with the experiment is assumed to be "perfect". The applied heat flux (at x=0) and specimen thickness are measured without error. The temperature (at selected locations) is measured without error. While real applications will exhibit experimental measurement errors, we neglect these effects in the challenge problems to simplify the analysis.

Ensemble Validation over a Database

A suite of experiments is conducted with the experimental process described previously over two specimen thicknesses, for two heat flux magnitudes (Figure 2). Replicate experiments are conducted for each configuration (for medium-level and high-level experimental information). Design values for the specimen thicknesses and applied fluxes are listed in Table 5. Experimental limitations only allow for conducting these experiments at heat fluxes of $1000 W/m^2$ and $2000 W/m^2$ which is lower than expected in the intended application.

Table 5. Experimental configurations for ensemble validation

Exp Configuration	**Heat Flux, *q* (W/m^2)**	**Thickness, *L* (cm)**
1	1000	1.27
2	1000	2.54
3	2000	1.27
4	2000	2.54

The measured transient temperature response at x=0 for experiments of each configuration is listed in Table 6. The thickness of the specimen and heat flux applied for each experimental configuration is as given in Table 5. The experimental data have no measurement errors. The model predictions of the experimental data should be made using Eq. (2) for x=0, with the provided heat flux, thickness, and thermal properties based on the data provide in the previous section on Material Characterization.

The analysis should be conducted for the three levels of experimental information; Low, Medium, and High as identified in Table 3. The analysis for a "Low" level of experimental information would include N_c=6 data from the Material Characterization (Table 4) and only Exp 1 from each configuration in Table 6 for the ensemble validation. Analysis for a "Medium" level of experimental information would include N_c=20 from the Material Characterization (Table 4) and Exp 1 and Exp 2 from each configuration in Table 6 for the ensemble validation. The "High" level of experimental information includes N_c=30 and all (4) experiments from each configuration in Table 6 for the ensemble validation.

Table 6. Experimental data for ensemble validation

Time, sec	**T(x=0), ^oC**							
	Configuration 1				**Configuration 2**			
	Exp 1	**Exp 2**	**Exp 3**	**Exp 4**	**Exp 1**	**Exp 2**	**Exp 3**	**Exp 4**
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
100.0	105.5	109.0	96.3	111.2	99.5	106.6	96.2	101.3
200.0	139.3	143.9	126.0	146.9	130.7	140.4	126.1	133.1
300.0	165.5	170.5	148.7	174.1	154.4	165.9	148.7	157.2
400.0	188.7	193.5	168.5	197.5	174.3	187.2	167.7	177.2
500.0	210.6	214.6	186.9	219.0	191.7	205.8	184.3	194.8
600.0	231.9	234.8	204.6	239.7	207.3	222.4	199.3	210.6
700.0	253.0	254.6	222.0	259.9	221.7	237.6	213.0	225.0
800.0	273.9	274.2	239.2	279.9	235.0	251.7	225.7	238.4
900.0	294.9	293.6	256.4	299.9	247.6	264.9	237.6	251.0
1000.0	315.8	313.1	273.5	319.8	259.5	277.4	248.9	262.9
	Configuration 3				**Configuration 4**			
	Exp 1	**Exp 2**	**Exp 3**	**Exp 4**	**Exp 1**	**Exp 2**	**Exp 3**	**Exp 4**
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
100.0	183.1	177.8	187.2	171.3	173.4	178.9	179.3	188.2
200.0	247.4	240.2	254.2	231.6	234.2	241.9	242.6	254.6
300.0	296.3	287.4	306.1	277.6	279.7	289.1	290.1	304.2
400.0	338.7	327.8	351.9	317.4	317.4	328.4	329.6	345.4
500.0	378.0	364.8	395.4	354.2	350.2	362.6	363.9	381.1
600.0	416.0	400.2	437.9	389.7	379.5	393.2	394.7	413.1
700.0	453.5	434.8	480.0	424.5	406.3	421.1	422.8	442.1
800.0	490.8	469.1	522.1	459.1	430.9	446.9	448.8	469.0
900.0	528.2	503.3	564.1	493.7	454.0	471.1	473.3	494.0
1000.0	565.6	537.6	606.2	528.2	475.6	493.9	496.4	517.6

Accreditation Validation Experiment

After the assessment noted above for the ensemble validation over the database, the project manager deems it prudent to conduct a limited number of accreditation tests with actual hardware at a single representative point in the application parameter space. The test(s) will be conducted for conditions near those specified for the regulations. The test conditions are summarized in Table 7.

Table 7. Experimental configuration for accreditation test

Exp Configuration	**Heat Flux, *q* (W/m^2)**	**Thickness, *L* (cm)**
5	3000	1.90

The relevant experimental data are provided in Table 8. For the accreditation experiments, measurements were taken at three locations. Temperature at the surface (x=0), in the middle of the specimen (x=L/2), and at the back of the specimen (x=L) were collected. The heat flux and thickness are as shown in Table 7. The model predictions of the experimental data should be made using Eq. (2), with the provided heat flux, thickness, and thermal properties based on the data provide in the previous section on Material Characterization. As before, consider three levels of experimental data in the analysis; Low, Medium, and High experimental information as described in Table 3.

Table 8. Experimental data for accreditation

Time, sec	***T(x)*, °C**					
	Exp-1			**Exp-2**		
	x=0	**x=L/2**	**X=L**	**x=0**	**x=L/2**	**x=L**
0.0	25.0	25.0	25.0	25.0	25.0	25.0
50.0	183.8	26.3	25.0	179.2	25.9	25.0
100.0	251.3	34.0	25.1	243.9	32.2	25.1
150.0	302.2	47.7	26.0	292.2	44.2	25.6
200.0	344.6	64.9	28.3	332.3	59.9	27.3
250.0	381.7	83.9	32.7	367.1	77.5	30.6
300.0	414.9	103.7	39.3	398.3	96.2	35.8
350.0	445.4	124.0	48.1	426.7	115.3	42.9
400.0	473.6	144.4	58.7	452.9	134.7	52.0
450.0	500.0	164.9	71.1	477.4	154.2	62.7
500.0	525.0	185.4	84.9	500.5	173.6	74.9
550.0	548.8	205.9	100.0	522.4	193.1	88.4
600.0	571.7	226.3	116.1	543.4	212.5	103.1
650.0	593.8	246.8	133.0	563.5	231.8	118.7
700.0	615.2	267.2	150.7	583.0	251.1	135.0
750.0	636.1	287.6	169.0	602.0	270.3	152.1
800.0	656.6	307.9	187.8	620.4	289.5	169.7
850.0	676.7	328.3	207.0	638.5	308.7	187.8
900.0	696.4	348.6	226.5	656.3	327.8	206.3
950.0	716.0	369.0	246.3	673.9	346.9	225.1
1000.0	735.4	389.3	266.3	691.2	366.0	244.2