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Processing Random and Systematic Experimental Uncertainties in Replicate Tests of Stochastic Phenomena for Real-Space Model Validation*

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Albuquerque, NM

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Definition of Random and Systematic Uncertainties

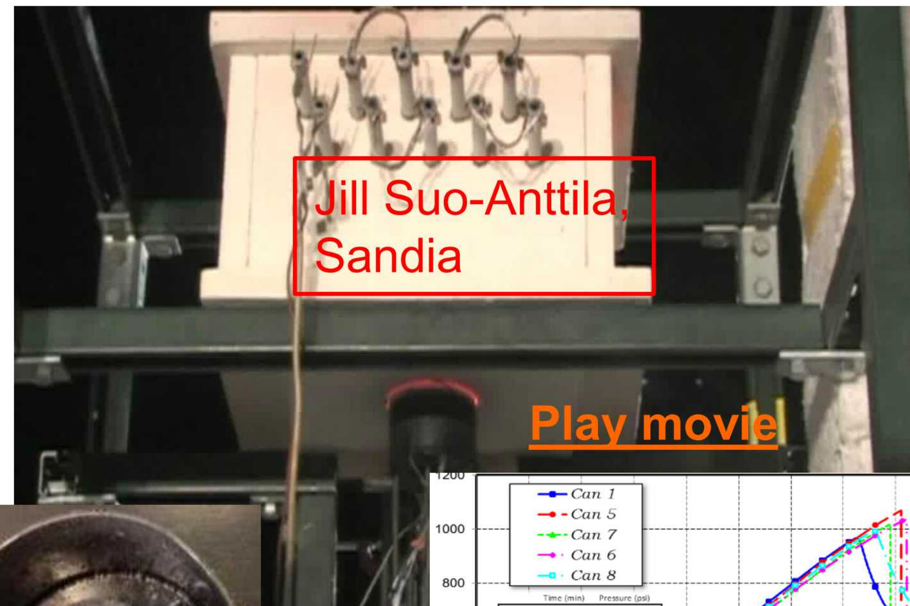
- **Random Errors**
  - errors that differ from test to test in an uncorrelated random manner
- **Systematic Errors**
  - errors that are effectively the same (perfectly correlated) from test to test
- **Uncertainty regarding the actual values of random and systematic errors in multiple tests are commonly called Random and Systematic Uncertainties**
  - Commonly used and expressive terminology, but arguably improper in a strict sense
  - **Alternate terms:**
    <u>Aleatory Uncertainty</u> re. the random values of error in the tests
    <u>Epistemic Uncertainty</u> re. the single but uncertain value of an error that is consistent across the tests

Validation Application

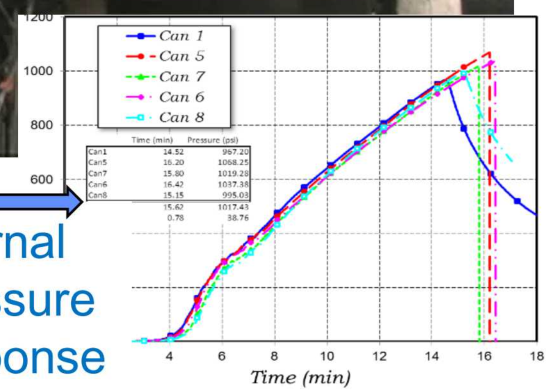
Coupled Thermal-Chemical-Mechanical Response and Structural Failure

Project Goal: assess predictiveness of thermal transport, foam thermal-chemical pyrolysis, can pressurization, and failure of lid weld

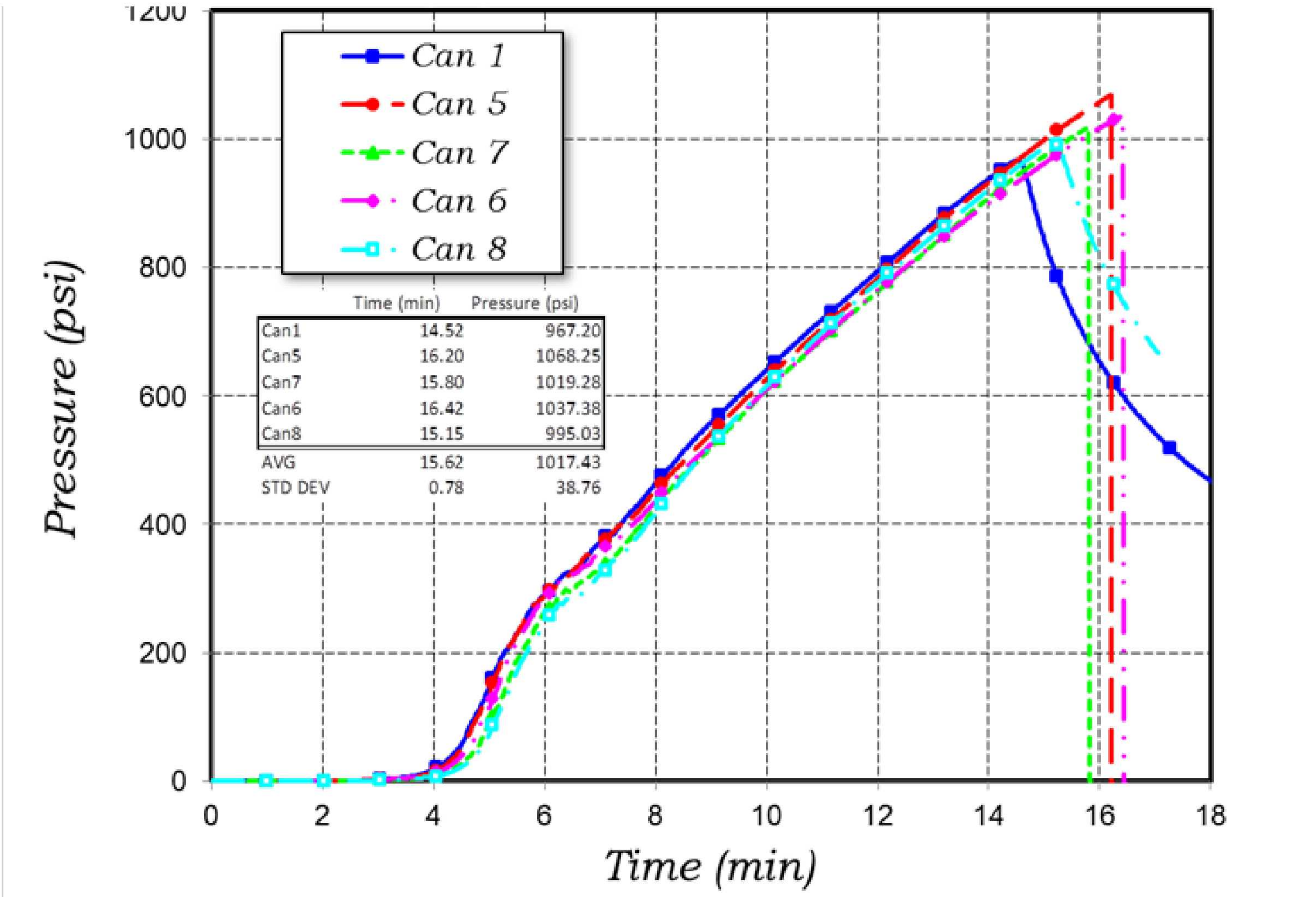
simplified geometry for V&V of phenomena modeling



internal pressure response

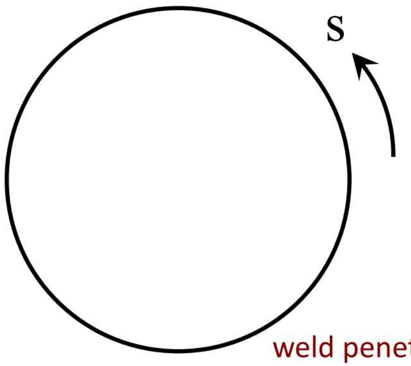


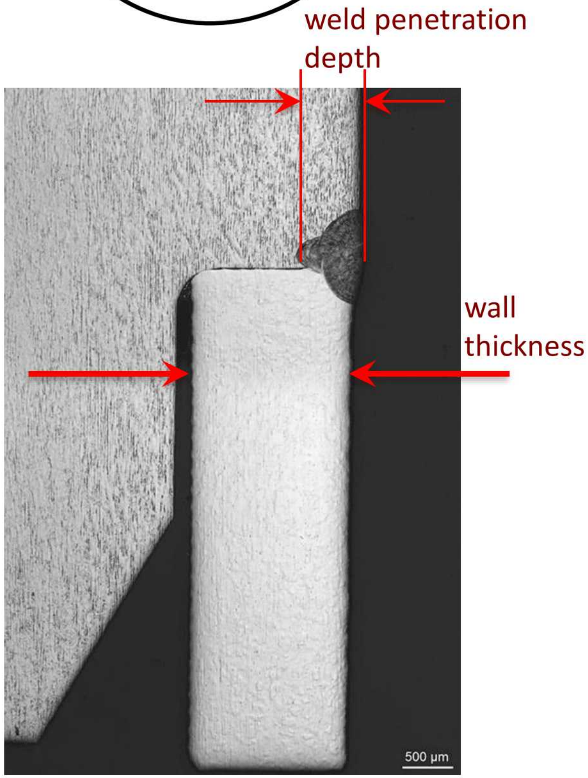
Experimental Variation of Can Failure Pressures

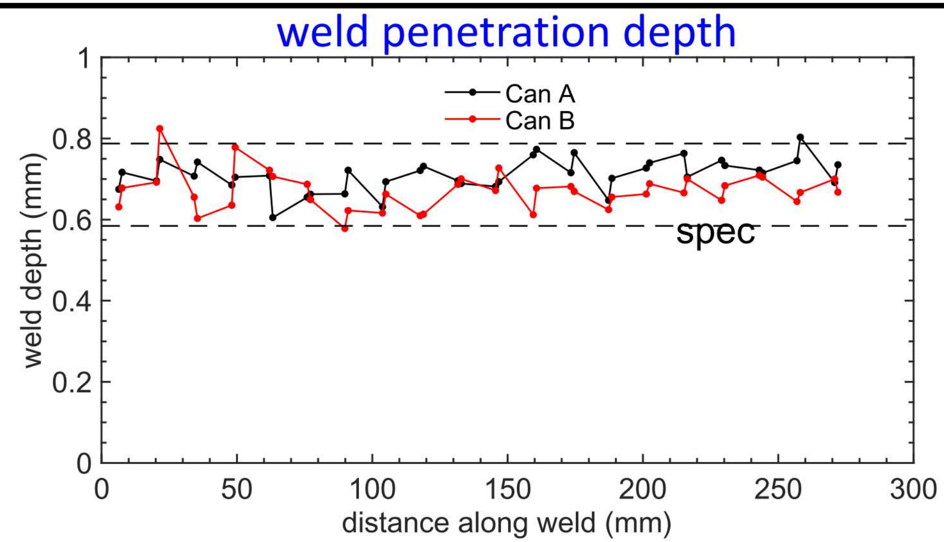


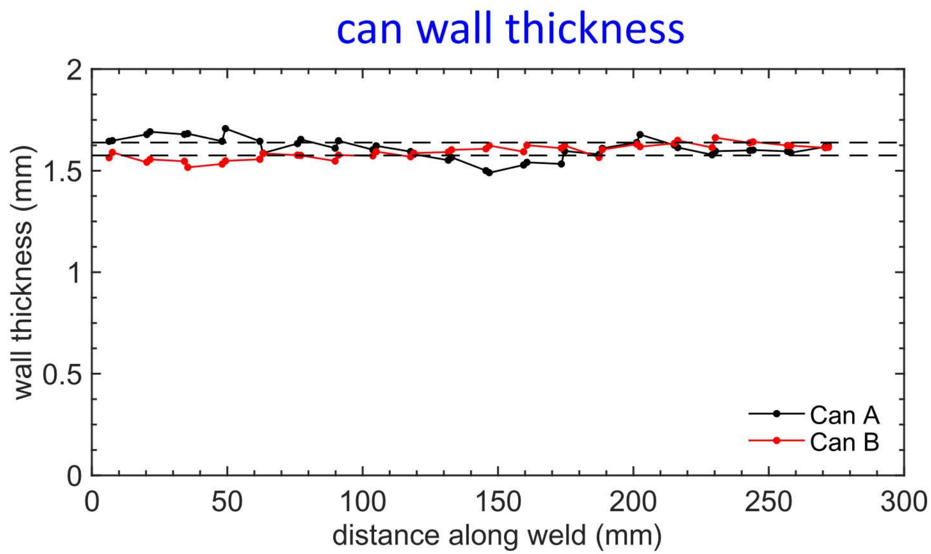
Unit-to-Unit Variations in Weld Depth and Can-Wall Thickness — lead to variations in can failure pressures

Bonnie Antoun, Sandia









Test-to-Test Variations of Initial Conditions and Heating Boundary Conditions

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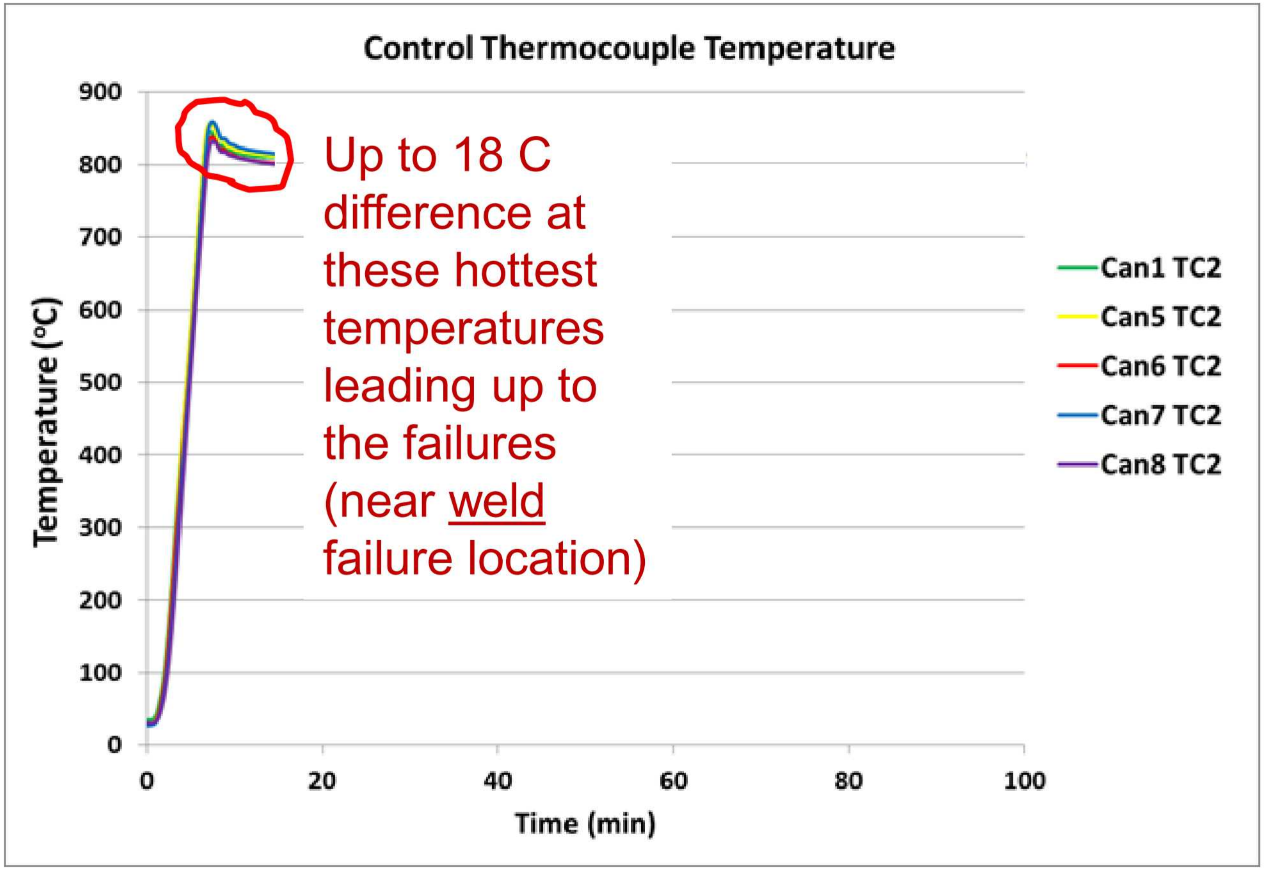
Upright Test	Can Initial Temperature (K)
Can 1	306.23
Can 5	302.69
Can 6	302.06
Can 7	300.17
Can 8	303.08



Normalize Experimental Output Data (experimental samples of Can failure pressure)

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- **Subtract-out variability in response data due to test-to-test differences of experimental inputs (inexact experimental control)**
  - more legitimate response variability to compare model predictions against ("Apples-to-Apples" basis)
  - more accurate estimate of prediction bias due to model-form error
- **Normalize all test results to a set of reference input conditions** (perturb outputs as though the test occurred at the ref. conditions)
- **Typically use the median test's input conditions as reference**
  - produces Independent and Identically Distributed (IID) response samples for legitimate statistics from the experimental data
- **In normalizing, also account for random and systematic uncertainties in measurements of experimental inputs & outputs**
  - **This part is equivalent to ASME VV20 procedure in certain cases**

Measurement and Estimation Uncertainties in model validation problem

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Non-Traveling Uncertainties

Experimental Test/Test Random

- lid TC measurement/redundancy test-test variations: I[±2%]
- ss304 emissivity can-can variations: I[±0.03]
- ambient temperature test-test variations I[±10C]
- pressure measurement/redundancy test-test variations: I[±2%]

Experimental Test/Test Systematic

- ss304 emissivity effective value over time, space: 0.69 + I[±20%]
- effective temperature for radiative, convective losses: 29C + I[±15C]
- convection coeff. effective value over time, space: $10 W/m^2$-K + I[±40%]

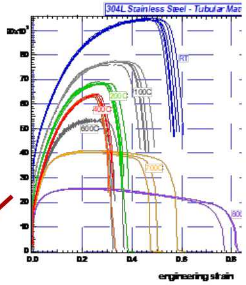
Model Epistemic

- mesh size error
- solver error

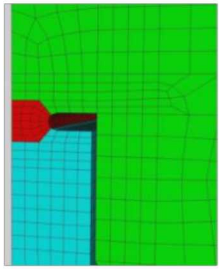
Traveling Uncertainties

Model Aleatory

- material stress-strain curves for lid, weld, & wall



- lid thermal contact: I[20%, 90%] of distance between modeled extremes of no heat transfer and perfect-contact heat transfer



- wall thickness: I[0.062,0.0645]in.
- weld depth: I[0.023, 0.031]in. (next slide shows measured values)

Model Epistemic

- foam conductivity: *f(temp.)* + I[±20%]
- foam specific heat: *f(temp.)* + I[±20%]
- foam activation energy: value + I[±4%]
- foam pressure multiplier: I[0.5, 2.64]
- ss304 conductivity: *f(temp.)* + I[±20%]
- ss304 specific heat: *f(temp.)* + I[±20%]

5 Levels of Increasing Rigor in Treatment of Experimental and Simulation Uncertainties in Model Validation

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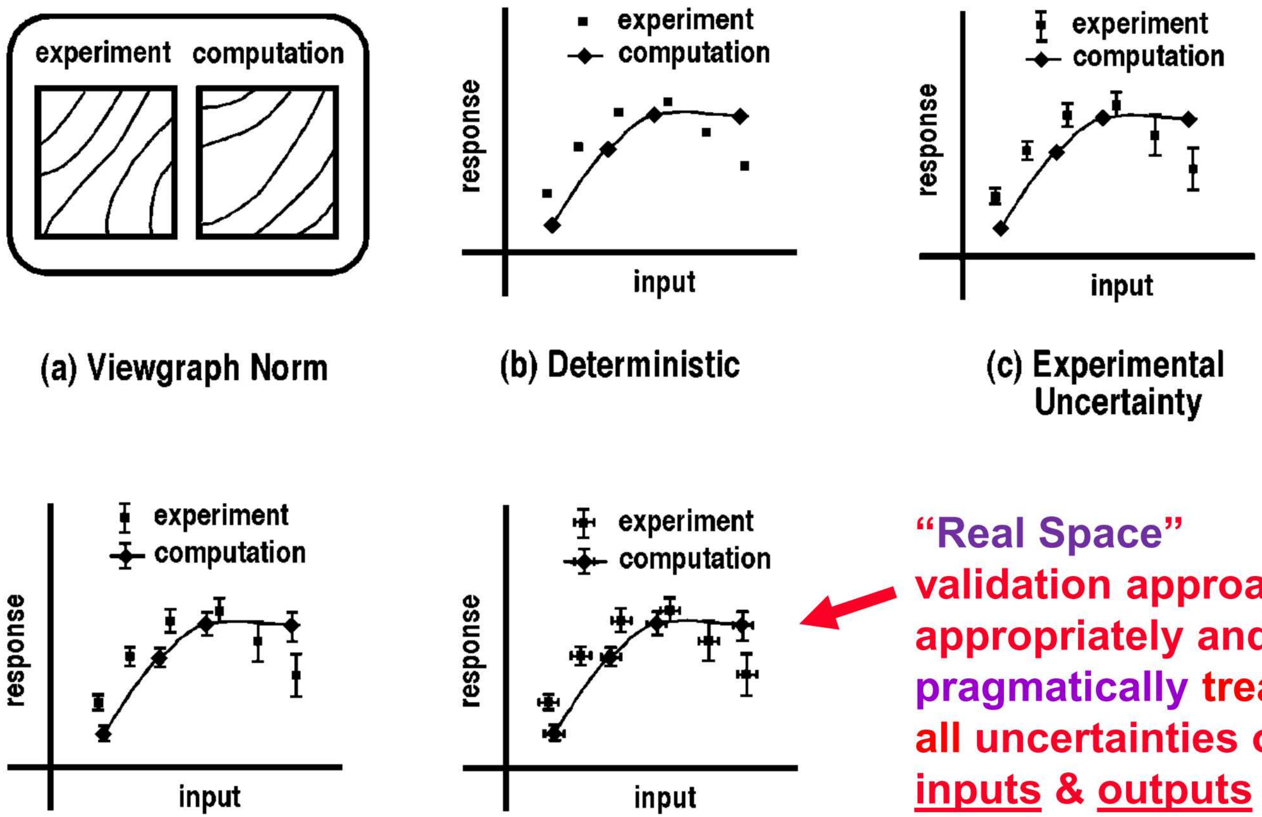


(a) Viewgraph Norm

(b) Deterministic

(c) Experimental Uncertainty

(d) Numerical Error

(e) Nondeterministic Computation

"Real Space" validation approach appropriately and pragmatically treats all uncertainties on <u>inputs</u> & <u>outputs</u> of experiments and simulations

Figs from "Increasing Quality of Validation Metrics," Sandia National Laboratories report SAND2003-3769, Oberkampf, Trucano, & Hirsch

Procedure to Normalize Experimental Results

<u>Taylor Series approach</u> (linear example)

temperature BC in reference test

$$Pfail_{Can1}(\vec{x}_{refCan6}) \cong Pfail_{Can1}(\vec{x}_{Can1}) + \sum \frac{\partial(Pfail_{mod/sim})}{\partial(x_i)} \bullet (x_{i\_refCan6} - x_{i\_Can1})$$

Normalized Failure Pressure for Can1

Measured Failure Pressure for Can1

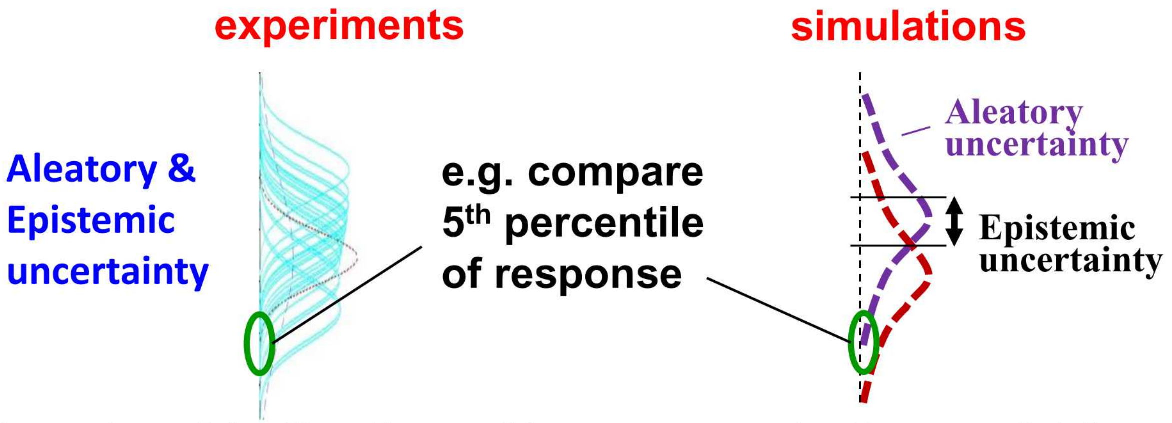
Failure Pressure change per change in temperature BC
- **FROM empirical relationship (experimental)**
- **OR from model simulations**

temperature BC in test whose results are being normalized

- **Random and Systematic uncertainties in most RHS quantities result in Random and Systematic components of uncertainty in LHS quantity**
- **Linear and Quadratic Taylor Series with Monte Carlo propagation of RHS uncertainties are transformed to MC sampling and propagation through Linear and Quadratic polynomial response surfaces of** $Pfail_{mod/sim}(\vec{x}_i)$

Real Space comparison for Stochastic Experimental and Simulation Results

- **Compare decision-intuitive statistical measures of response, not CDFs**



- **Intuitive visual indication of how accurate the model is, on several fronts:**
  - **Means** of the predicted and experimental populations
  - **Variances**
  - **Percentiles**
  - **Range of response %age, e.g. the "central" 95% between 2.5 and 97.5 percentiles**

  (These last two account for combined uncertainty in mean, variance, and possible higher moments of stochastic response and are found to be the most useful in practice)

- **Percentile comparisons are particularly useful for validation of models to be used for analysis of performance and safety margins, e.g. QMU.**

Dimension- and Order- Adaptive Response Surface for Monte Carlo Propagation of Experimental Uncertainties

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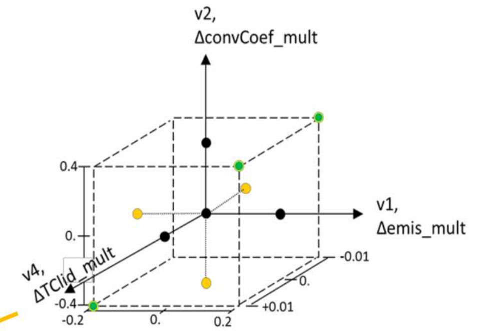
Uncertain Experimental Input Variables

- emissivity multiplier:
- convection coeff. mult.
- ambient temperature mult:
- Can lid thermocouple multiplier

4D Staged Mixed-Order Polynomial Surrogate Model based on 11 model runs



quadratic main effects identify best corners to sample for interactn. effects

quadratic interaction terms in dominant 3 factors

Linear terms in all 4 factors

Linear sens. analysis →

higher-order in dominant 3 factors— Quadratic main-effects terms →

translated coordinates where local origin is at reference point from which main-effects perturbations are taken in the uncertainty space														
f(v1,...,v4) = b0 + b1*v1 + b2*v2 + b3*v3 + b4*v4 + b1,1*v1*v1 + b2,2*v2*v2 + b4,4*v4*v4 + b1,2*v1*v2 + b1,4*v1*v4 + b2,4*v2*v4														
row	Const	v1	v2	v3	v4	v1*v1	v2*v2	v4*v4	v1*v2	v1*v4	v2*v4	coeffs. {b}	= y_predic	True Y
1	1	0	0	0	0	0	0	0	0	0	0	974.9308	974.93077	974.939
2	1	0.2	0	0	0	0.04	0	0	0	0	0	103.2241	992.5232	993.332
3	1	0	0.4	0	0	0	0.16	0	0	0	0	26.29418	985.72013	986.529
4	1	0	0	0.03	0	0	0	0	0	0	0	-12.6419	974.55151	974.549
5	1	0	0	0	0.01	0	0	0.0001	0	0	0	-1861.94	956.97387	956.169
6	1	-0.2	0	0	0	0.04	0	0	0	0	0	-76.3096	951.23357	950.427
7	1	0	-0.4	0	0	0	0.16	0	0	0	0	1.698033	964.68478	963.879
8	1	0	0	0	-0.01	0	0	0.0001	0	0	0	6624.772	994.21262	995.020
9	1	0.2	0.4	0	-0.01	0.04	0.16	0.0001	0.08	-0.002	-0.004	6.42673	1018.8304	1018.023
10	1	-0.2	-0.4	0	0.01	0.04	0.16	0.0001	0.08	-0.002	-0.004	427.8135	919.26669	920.073
11	1	0.2	0.4	0	0.01	0.04	0.16	0.0001	0.08	0.002	0.004	855.6242	990.14792	990.147

Spreadsheet Sampling of Experimental Random and Systematic Uncers.

- Interval treatment via Monte Carlo sampling of uniform distributions and appropriate <u>processing and interpretation</u> of propagation results

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<u>Systematic</u> uncertainties; correlated across the 5 replicate experiments

<u>Random</u>; uncorrelated across experiments

	A	B								
1										
2		RAND# =	6734							
3										
4			realization	v1sys = ΔemisMult = Unif[-0.2, 0.2]	v2sys = ΔconvCoeffMult = Unif[-0.4, 0.4]	v3sys = ΔTambMult = Unif[-0.03, 0.03	v4sys = ΔTlidTCmult = Unif[-0.003, 0.]	v3ind = ΔTambMult = Unif[-0.02, 0.02	v4ind = ΔTlidTCmult = Unif[-0.01, 0.01]	v5ind = ΔmeasPres = Unif[-10, 10]psi
5	RNGseeds ->			5301	4105	6999	9724	7490	52	4485
6			1	0.011786	-0.07179	0.011921	-8.9E-05	0.009904	-0.00987	-1.03732
7			2	-0.18207	0.190814	-0.02911	-0.00043	-0.01718	-0.00415	-2.313
8			3	0.040376	0.060903	-0.0119	-0.00032	0.019232	0.009941	4.824061
9			4	0.1541	0.078237	0.019105	-0.0002	-0.00455	-0.00478	3.046663
10002			9997	0.118528	0.117203	0.012582	-0.00156	0.004796	-0.00029	-2.00415
10003			9998	0.132505	-0.21164	0.009023	-0.00195	-0.00206	0.006737	-6.05335
10004			9999	0.107163	0.179485	0.028414	-0.00137	-0.01185	0.008592	-0.78829
10005			10000	0.177795	-0.02533	-0.01103	-3.6E-05	0.004812	-0.00551	0.653401
10006										
10007										
10008	stats		mean =	0.0011	0.0005	0.0001	-0.0015	-0.0001	0.0000	-0.0317
10009	from		max =	0.2000	0.3999	0.0300	0.0000	0.0200	0.0100	9.9969
10010	10000		min =	-0.2000	-0.4000	-0.0300	-0.0030	-0.0200	-0.0100	-9.9988
10011	samples		stdev =	0.1156	0.2323	0.0173	0.0009	0.0115	0.0058	5.7716
10012										

- samples of random and systematic components of uncertainty of a given measurement X_i are added to it to obtain a perturbed value X_i' that is propagated to response surface evaluation: $\mathbf{P}\mathit{\mathbf{fail}}_{\mathbf{Can\_j}}(\vec{X}_i') =$ a response sample

- Response samples $\mathbf{P}\mathit{\mathbf{fail}}_{\mathbf{Can\_j}}$ are correlated across Cans according to systematic components of uncertainty for X_i variables

95/90 Statistical Tolerance Intervals from Realizations of Normalized Failure Pressures

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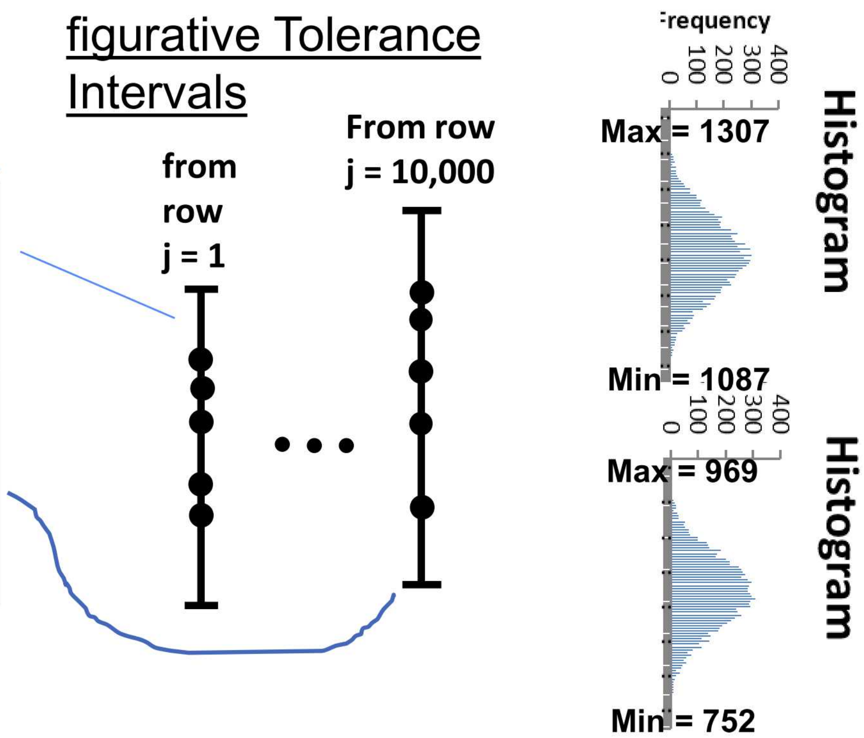
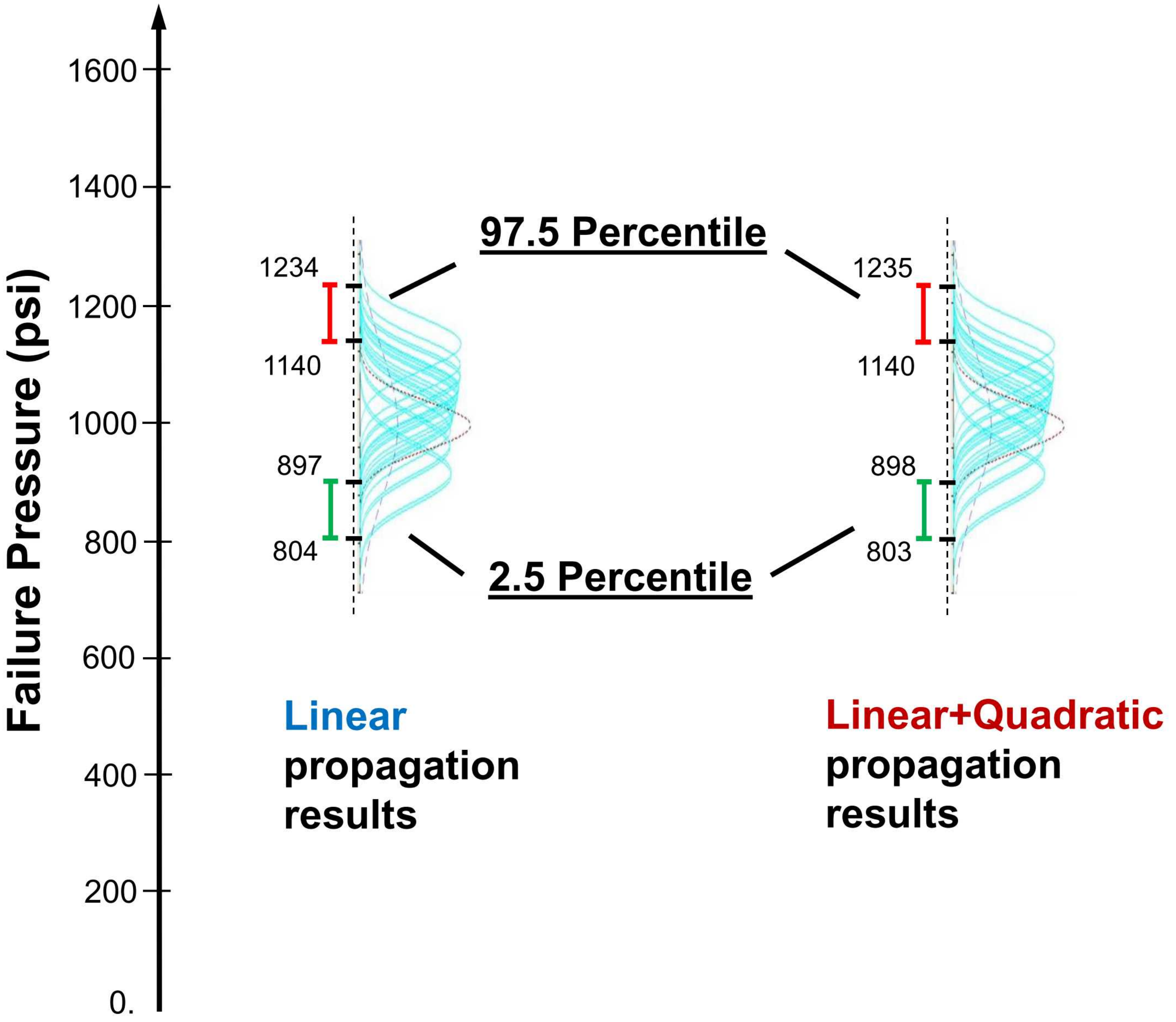
realization	Pfail-Exp6	Pfail-Exp5	Pfail-Exp7	Pfail-Exp8	Pfail-Exp1
1	1029.50	1054.015	1020.72	1015.175	966.478
2	1064.82	1077.199	1031.47	995.1603	990.9597
3	1040.20	1079.222	995.88	972.7477	951.9825
9998	1031.89	1079.139	997.55	977.3928	978.2092
9999	1020.46	1066.808	1007.25	971.7379	946.5493
10000	1049.55	1045.07	1014.45	1001.597	958.3771



- A 95/90 TI is 90% confident to capture 95% of failure pressures of an asymptotically large population of cans tested at the reference conditions IF the true population is Normally distributed and the 5 Normalized failure pressures are 5 possible random samples from it.
- High credibility that the true confidence is > 75%, based on testing over 144 Non-Normal distributions.

Effectively Converged ~Same Results from Linear and Linear+Quadratic Response Surfaces



Closing Remarks

- **A detailed methodology was summarized for processing experimental data from replicate tests of stochastic phenomena**
- **The methodology accounts for:**
  - realistically few replicate tests and data samples
  - experimental control variability over the tests
  - random and systematic measurement errors and uncertainties
- **Standard EXCEL spreadsheet functions are used for constructing Taylor Series response surfaces, MC propagation, Sensitivity Analysis, statistical processing**
- **Detailed paper in review for submission to *ASME J. VVUQ***