SAND2011-9035P

Fire CFD Model Validation Case Study

—Chapter VII in JANNAF Simulation Credibility Guide

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Albuquerque, NM

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JANNAF Simulation Credibility Guide Workshop VI

Dec. 6, 2011, Huntsville, AL

National Nuclear Security Administration

*Sandia National Laboratories document SAND2011-YYYYP (unlimited release)

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An <u>Operational</u> Definition of model validation (for computational phys. engr. models)

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<u>Model Validation</u> is the compilation of useful indicators regarding the accuracy and adequacy of a model's predictive capability for particular output quantities (possibly filtered and transformed) that are important to predict for an identified purpose,
where meaningful comparisons of experiment and simulation results are conducted at points in the modeling space that present significant prediction tests for the model use purpose.

A Pragmatic “Real Space” approach to model validation will be presented here

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- The approach evolved from working many industrial scale validation problems featuring a broad variety of real-world conditions and difficulties
- Philosophy and rationale underlying the Real Space approach were presented and discussed at the last JANNAF workshop
- This talk will concentrate on illustrating processes and procedures of the approach

- **Caveats**
  - No overwhelming consensus yet exists for how to approach model validation—the Real Space approach is just one possible approach
  - Model validation theory and methodology are still being actively researched, developed, debated, and refined in the experimental, V&V, and M&S communities
  - the Real Space methodology itself is still under development, testing, and evaluation, and continues to evolve

Real Space accuracy/discrepancy measure and Model Adequacy criterion

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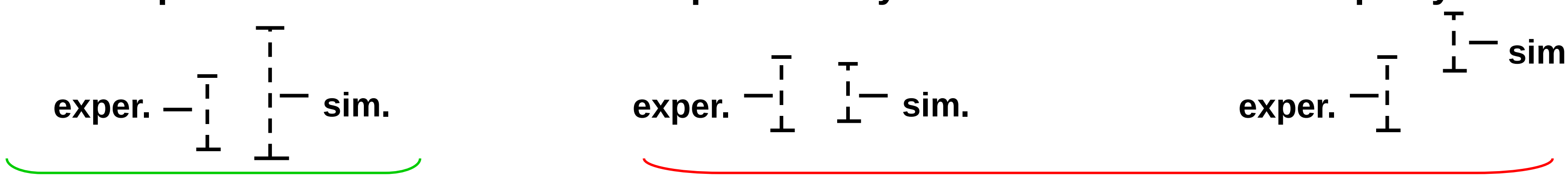
- "<u>Real Space</u>" – involves no subtractive difference of results from simulation and experiment, or other transform discrepancy measures
- Simple criterion for zeroth-order preliminary indication of model adequacy



This case meets "<u>Zeroth-order</u>" conditions for model adequacy

- **model prediction bounds experimental uncertainty bar** (as the best available evidence of where "reality" lies)
- **If the data/model relationship remains <u>consistent</u> in extrapolation (*the hope in all modeling*), the predictions will bound reality in the extrapolation conditions**

☑**Reality lying w/in the predictions is what a designer or decision maker wants***

*assuming non-excessive (acceptable) sim. uncer. range as assessed by propagation to system level

<u>Greater prediction risk in above cases</u>

- **much of reality lies outside the model predictions**
- **If data/model relationship remains consistent in extrapolation then much of reality will lie outside predictions**

Adequacy in any of the 3 cases shown above can be assessed more definitively <u>if</u> can propagate errors to system level & assess whether errors are acceptably small (<u>jointly</u>, for all lower-level validation results considered <u>together</u>)

- Requires system-level model & parametric map to "traveling model" at validation setting

Equations for Constructing Net Experimental & Simulation Uncertainty Bars for Real-Space Comparisons

(I don't expect you to read these!)

– Fire CFD val. example only involves a few of these terms

Experiment

$$Intvl\_d\left\{\hat{r}_{e\_adjusted_{(1)}},\cdots,\hat{r}_{e\_adjusted_{(k)}},\cdots,\hat{r}_{e\_adjusted_{(K)}}\right\}$$

$$;\ \hat{r}_{e\_adjusted_{(k)}} =$$

$$\hat{r}_{e\_observed_{(k)}} \quad \text{(A)}$$

$$-\left[\sum_{j}^{\#rand\_correlMeas\_I.A} \Delta\hat{r}_{e_{j(k)}}\right] \quad \text{(B)}$$

$$-\left[\sum_{i}^{\#rand\_correlMeas\_II.2,NonTrav\ II.1.a} \Delta\hat{r}_{e_{i(k)}}\big|_{\Delta\hat{x}_{i(k)}}\right] \quad \text{(C)}$$

$$+$$

$$\bigcup_{j}^{\#syst\_I.B} U[r_e]_{I.B_j} \quad \text{(D)}$$

$$+$$

$$\bigcup_{i}^{\#syst\_nonTrav\ IV} U[(r_e^L, r_e^U)|_{U[X_i\ \ nonTrav]}] \quad \text{(E)}$$

$$= \boxed{\Delta r_{e\_net}}$$

—Experimental uncertainty bar (net)

Model

$$\text{(F)} \quad Intvl\_d\left\{\hat{r}_{m_{(1)}},\cdots,\hat{r}_{m_{(k)}},\cdots,\hat{r}_{m_{(K)}}\right\}$$
$$;\ \hat{r}_{m_{(k)}} = \overline{r}_m + \sum_{n}^{\#rand\_correlMeas\_Trav\ II.1.a} \Delta\hat{r}_{n(k)}\big|_{\Delta\hat{x}_{n(k)}}$$

$$+$$

$$\text{(G)} \quad \bigcup_{i}^{\#syst\_nonTrav\ IV} U[r_m|_{U[X_i\ \ nonTrav]}]$$

$$+$$

$$\text{(H)} \quad \bigcup_{i}^{\#syst\_Trav\ IV} U[r_m|_{U[X_i\ \ Trav]}]$$

$$+$$

$$\text{(I)} \quad \bigcup_{k}^{\#model\_intrinsic\_Trav} U[r_m|_{U[\theta_k\_Trav]}] - \bigcup_{k}^{\#model\_intrinsic\_nonTrav} U[r_m|_{U[\theta_k\_nonTrav]}]$$

$$+$$

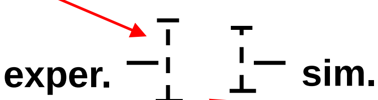
$$\text{(J)} \quad \bigcup_{k}^{\#postprocessing\_Trav} \Delta r_{m\_postproc\_Trav_k} - \bigcup_{k}^{\#postprocessing\_nonTrav} \Delta r_{m\_postproc\_nonTrav_k}$$

$$+$$

$$\text{(K)} \quad \bigcup_{k}^{\#discretization\_Trav} \Delta r_{m\_discr\_Trav_k} - \bigcup_{k}^{\#discretization\_nonTrav} \Delta r_{m\_discr\_nonTrav_k}$$

$$= \boxed{\Delta r_{m\_net}}$$

—Simulation uncertainty bar (net)



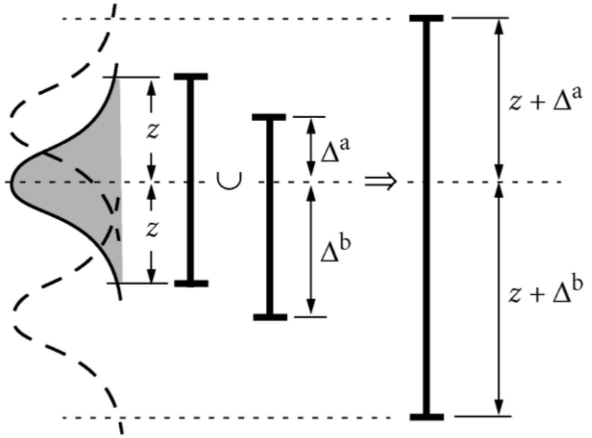
Different Types of Uncertainties within Terms of Equation Set

Uncertainties in various Terms of the Equation Set can be <u>interval and/or distributional</u>,

e.g. <u>interval and distributional subterms</u> in Term D of Master Equation Set:

$$\bigcup_{j}^{\#I.B\_sources} U[r_e]_{I.B_j} = \bigcup_{j=1}^{\#I.B\_\boxed{intvl\_sources}} U[r_e]_{I.B_j} + Intvl\_c\left\{ \bigcup_{j=1}^{\#I.B\_\boxed{PDF\_sources}} U[r_e]_{I.B_j} \right\}$$

- **<u>Interval</u> uncertainties seem to be much more prevalent in real model validation settings than are uncertainty <u>distributions</u>**



Aggregation of Interval and PDF uncertainties

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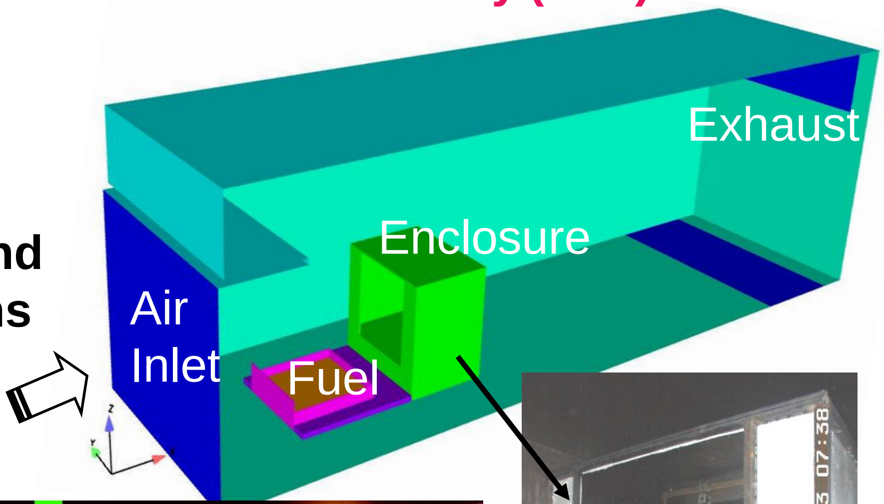
Case Study example:
Validation of Fire CFD model

- **Validate fire CFD simulations of radiative and convective heating of a weapon-like calorimeter in wind-driven fire.**

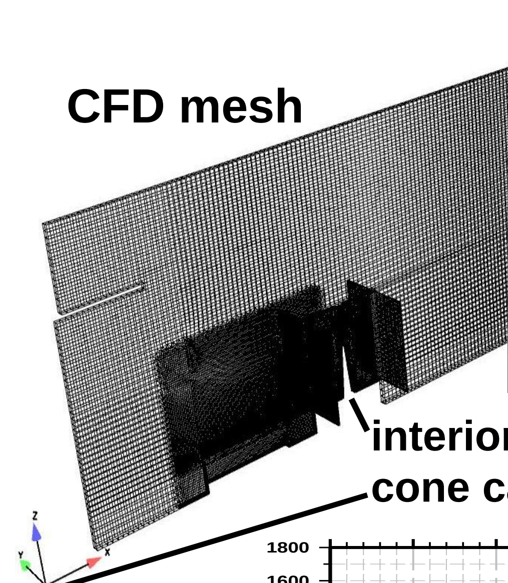
Cross-Wind Test Facility (XTF)

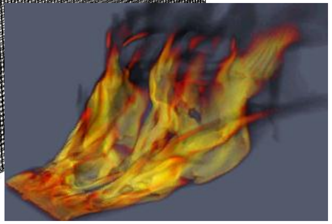
wind fans



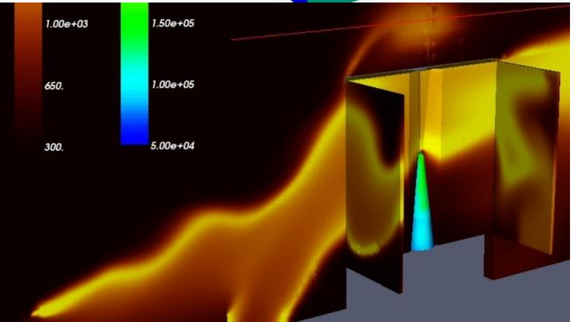
CFD mesh

movie

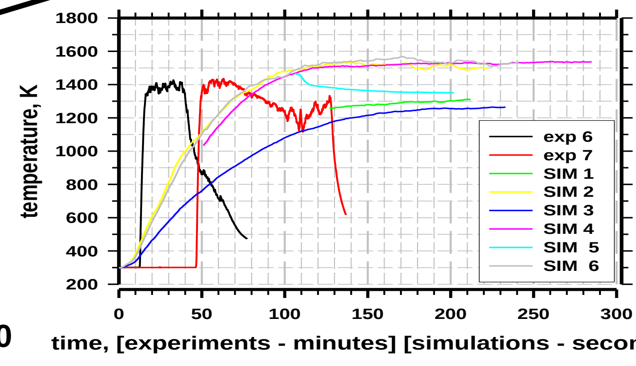




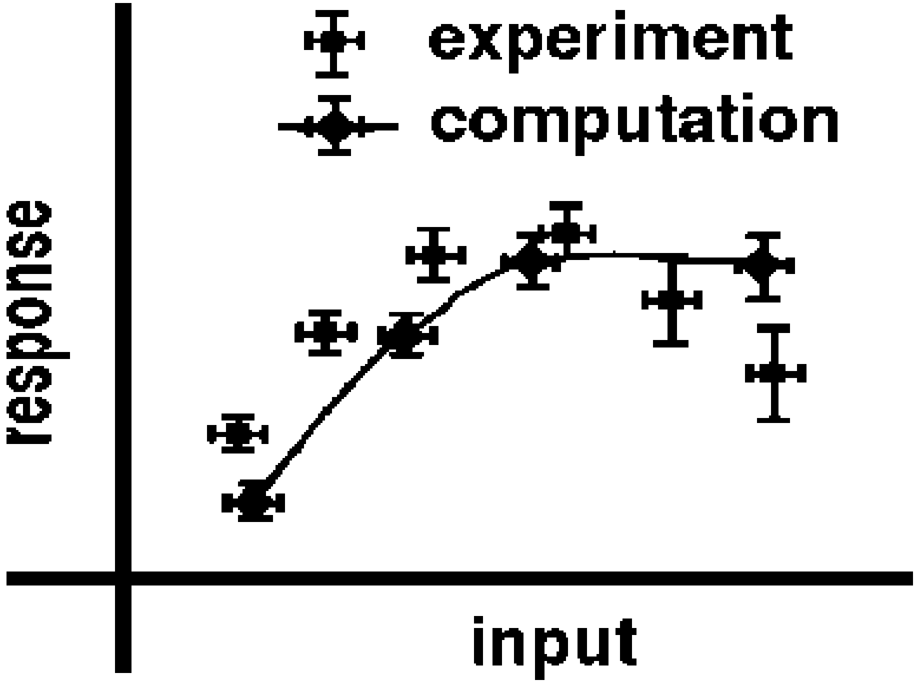
interior of cone calorimeter



Calorimeter Response at location 10



Construction of Uncertainty Bars on Experimental Results



Fire Fluctuation-induced uncertainty on experim. sustained high-mean temperature

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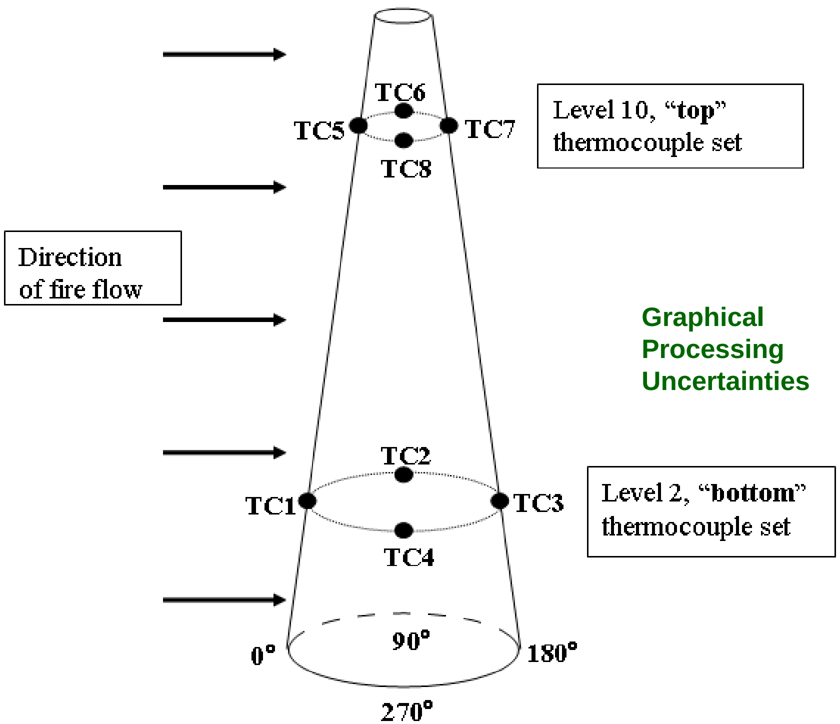
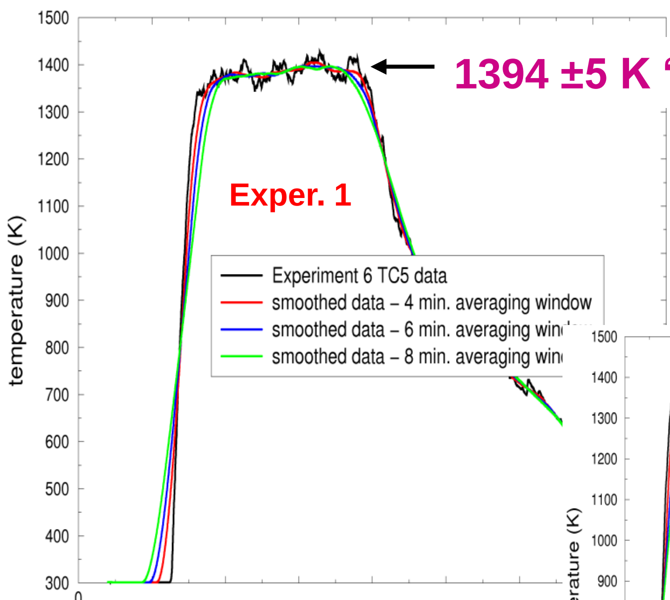
- Sustained high steady-state temperature is the Quantity of validation interest

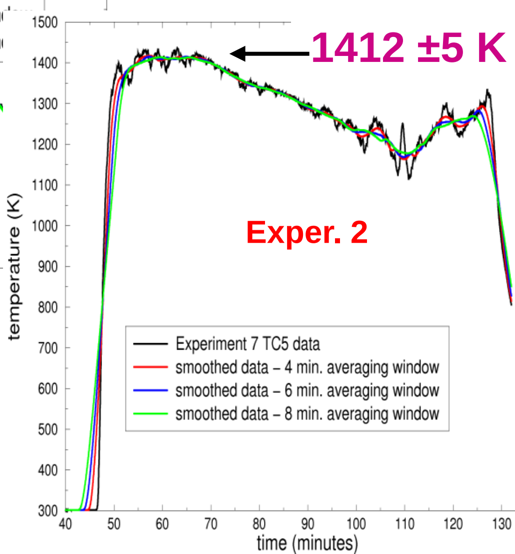
- Validation comparisons at 8 TCs diversely and representatively spaced on calorimeter

These sample results are for TC #5



Graphical Processing Uncertainties





- different averaging time-windows (4, 6, 8 min.) give steady-state high temps. within ±5K

Possible sources of Uncertainty in experimental processed results

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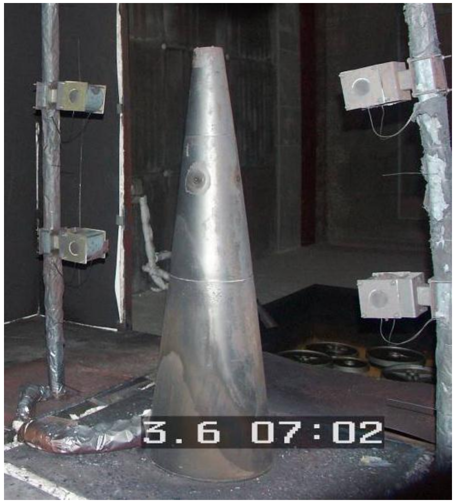
- **error/uncertainty in processing of measurement sensor results**
  - **e.g. spatial interpolation and/or integration or averaging of sensor data**
  - **±5 K for fire example**

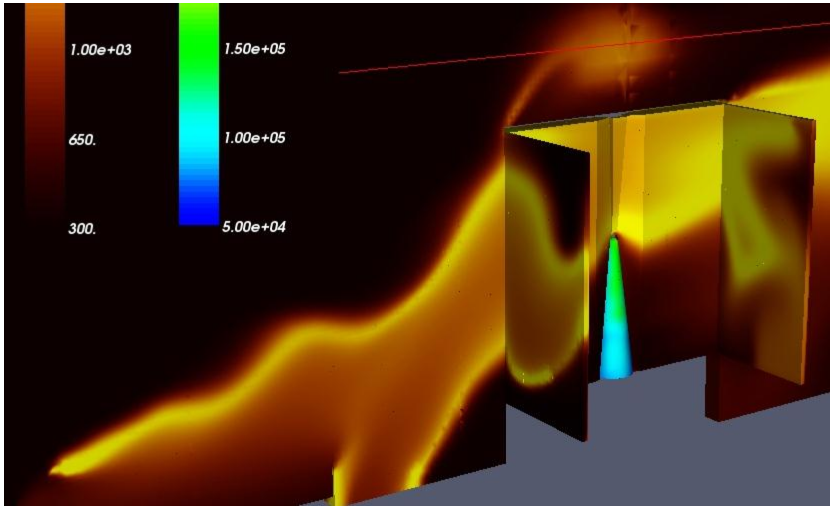
- **sensor reading bias-errors, e.g.**
  - **thermocouple transducer bias error (±11 K for fire example)**
  - **bias error in calibration standard used to calibrate data acquisition system (to correct for transducer bias error)**
  - **sensor mounting effects like contact resistance between a thermocouple and the surface it is mounted to (~0 for fire example, averages out of mean)**

- **error/uncertainty in** *Data Reduction Equations* **(DREs) used to calculate "derived" measurements from other quantities, e.g.**
  - *Speed* **is not measured directly, is calculated by** *distance ÷ elapsed_time*
  - Gas velocity **is calculated from Bernoulli Equation, Ideal Gas Law, and measured atmospheric pressure and local temperature and pressure drop in a Pitot tube**
- **uncertainty in measured quantities input to DREs**
- **uncertainty in experimental conditions like BCs, ICs, & item next slide**

"Data Conditioning" of Experimental Results to account for Uncertain Experimental Input Factor

Emissivity of painted black surface of calorimeter in fire experiments was a prominent experimental uncer. (systematic, not random, over expers.)

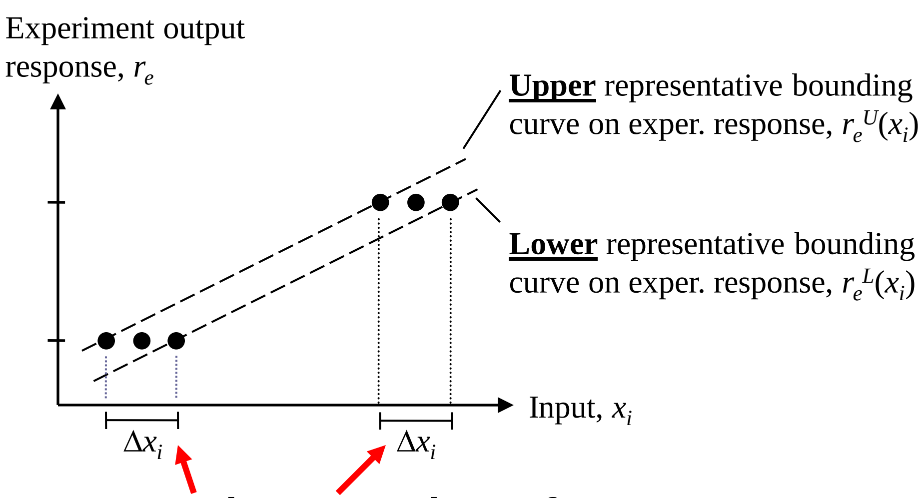




- uncertainty of the black paint's emissivity is a non-traveling systematic uncertainty (0.86 ± 0.1) in the validation experiments
- this emissivity strongly affects the validation response quantities (temperatures at the thermocouples) in the experiments
- Since there is significant uncertainty in this experimental input factor, and the experimental output results of validation interest (TC temperatures) are sensitive to this input, the output results must be conditioned to reflect this input uncertainty.
- "horizontal" input factor uncer. ➡ vertical uncer. bar on output result from model, emis. uncer ± 0.1 ➡ ± 33K at TC#5

Data Conditioning of Experimental Results to account for Systematically Uncertain <u>Input</u> Factor –Term E, 1-D case

- **Input uncertainty in the experiment should be reflected by uncertainty on the output result, but does not automatically show up without “conditioning” the data**

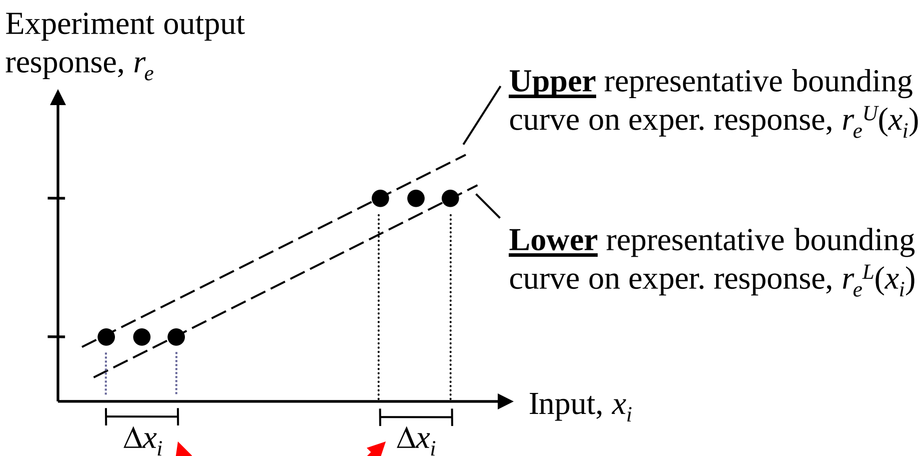


Systematic uncertainty of input to an experiment, *e.g.* a load or boundary condition

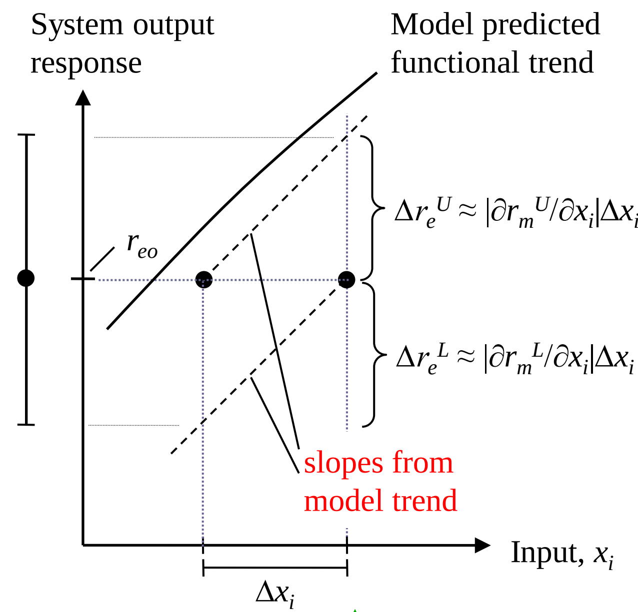
- **Systematic input uncertainties can be:**
  - **intervals**
  - **uncertainty distributions**
  - **combination of both**

Data Conditioning of Experimental Results to account for Systematically Uncertain Input Factor –Term E, 1-D case

- **Input uncertainty in the experiment should be reflected by uncertainty on the output result, but does not automatically show up without "conditioning" the data**



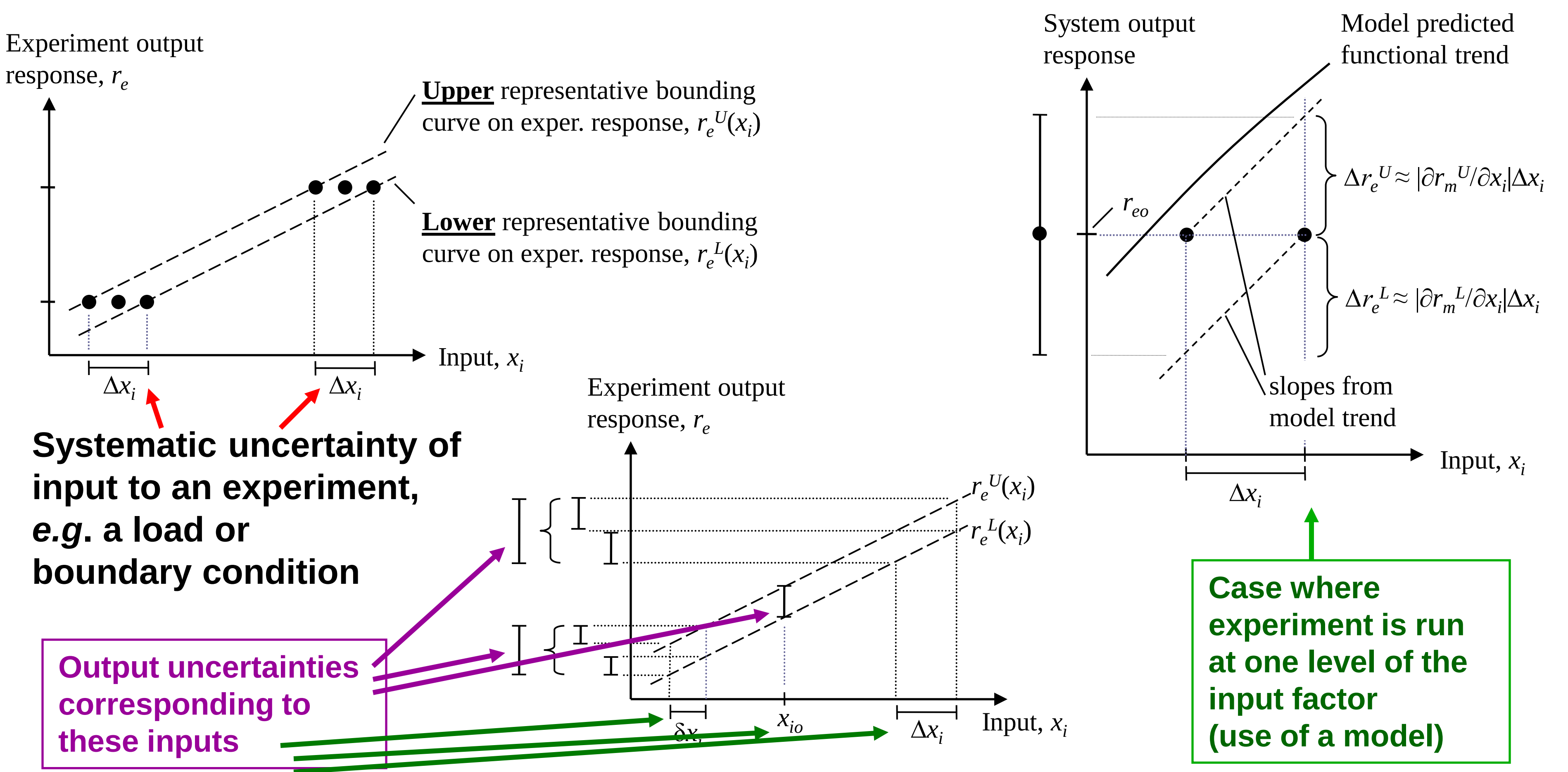
Systematic uncertainty of input to an experiment, *e.g.* a load or boundary condition



Case where experiment is run at one level of the input factor, + use of a model

Data Conditioning of Experimental Results to account for Systematically Uncertain <u>Input</u> Factor –Term E, 1-D case

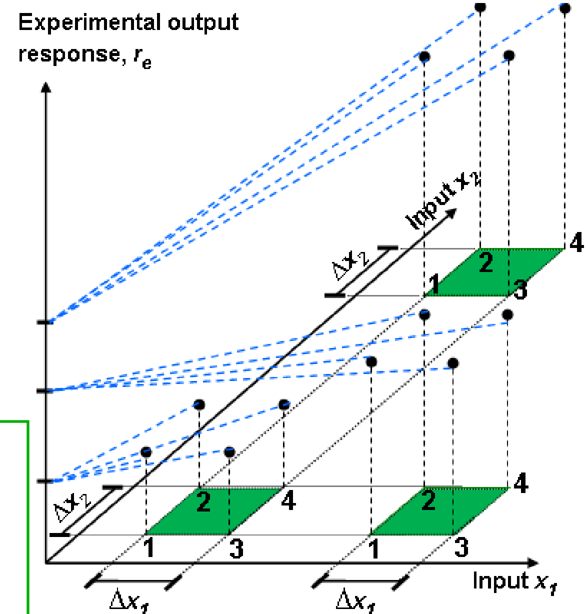
• **Input uncertainty in the experiment should be reflected by uncertainty on the output result, but does not automatically show up without "conditioning" the data**



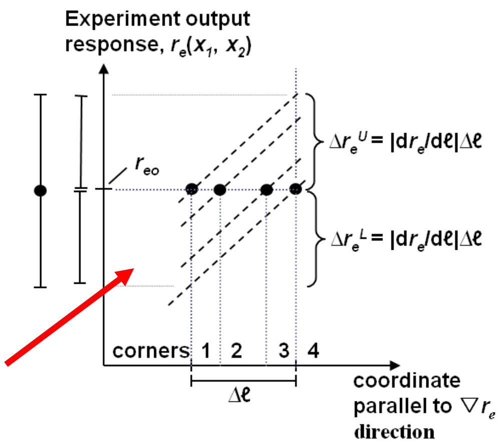
Data Conditioning of Experimental Results

–Term E, multivariate case (2D example)

- **Multivariate treatment is much more involved than 1-D univariate case**



2-D example of multivariate case where experiment is run at sufficient level combinations of the input factor (model not used)



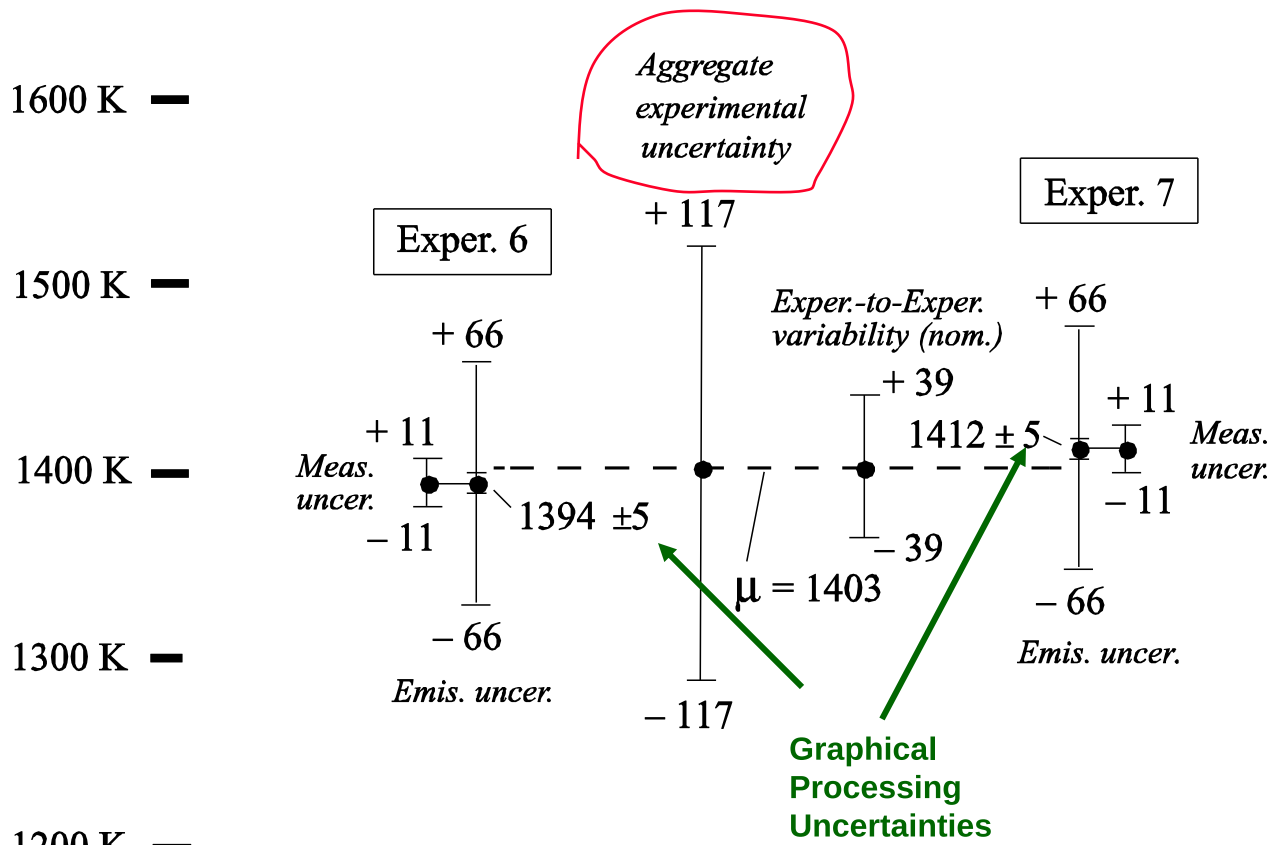
4 parallel planes

Details in conference paper:

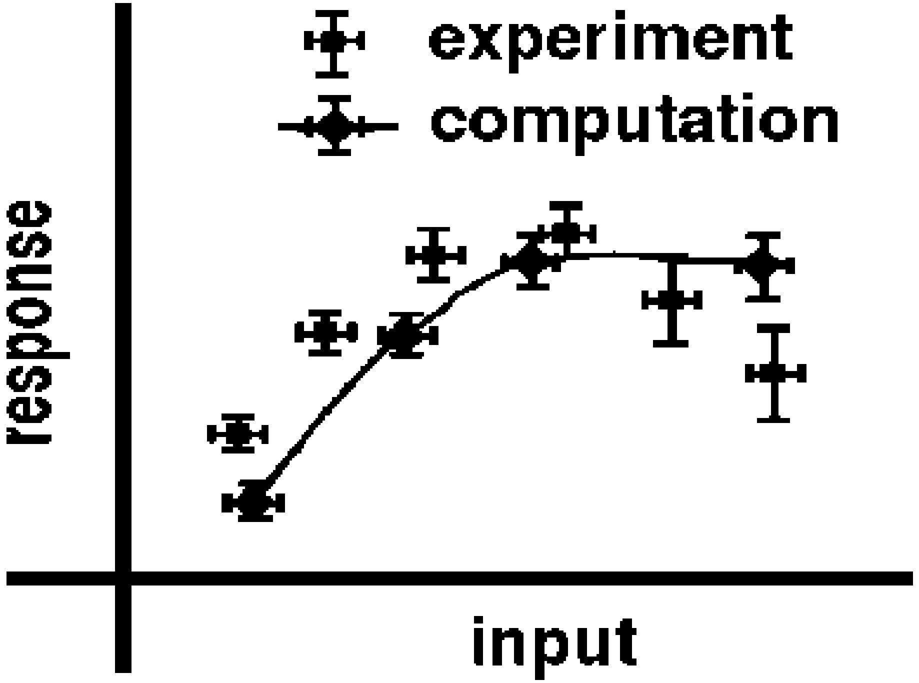
"*Data & Model Conditioning for Multivariate Systematic Uncertainty in Model Calibration, Validation, and Extrapolation*," V. Romero, paper AIAA-2010-2511, 12th AIAA Non-Deterministic Approaches Conference, 12-15 April 2010, Orlando, Fl.

Aggregate Experimental Uncertainty

Experimental uncer's. and rollup to aggregate experimental uncertainty in steady-state temp. at TC5



Construction of Uncertainty Bars on Simulation Results



"Traveling Uncertainties" intrinsic to Fire-Dynamics CFD Model

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Epistemic parameter and model-form uncertainties:

- **heat of combustion:** 44.66kJ/mol ± 10%
- **soot extinction coefficient:** 7 ± 10%
- **flame volume coefficient:** 2.13 ± 30%
- **flame loading coefficient:** 0.41 ± 30%
- **turbulence model form:** TFNS versus BVG
- **convection coefficient at object surface:** calculated value -50% to +100%

- **each simulation took ~ 6wks. on 256 CPUs**
- **could only afford 5, for 6-factor UQ**

Disgression next 4 slides:
Use of other application problems & code for Sensitivity info. on Fire Model Uncertainties

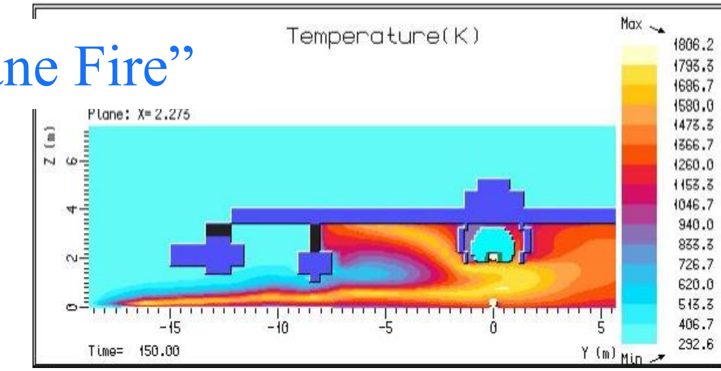
(sims. & analysis 2000-'02 by Victor Figueroa, Sam Yoon, J. Nelsen, V. Romero)

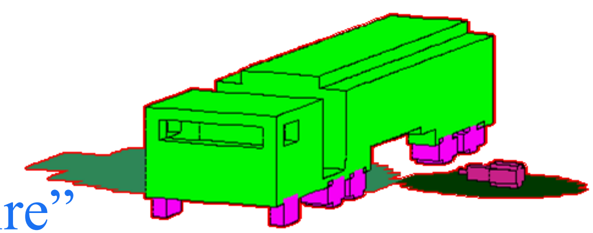
Block-structured grids with non-parallel code VULCAN

- **Each Accident Scenario:**
  - **16 simulations to investigate sensitivity to 8 sources of uncertainty (below)**
  - **parameter sets by structured Experimental Design**

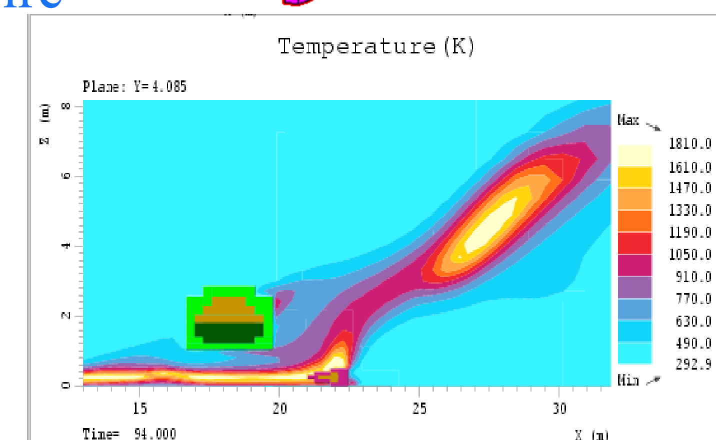
- **Modeling uncertainties:**
  - Calculation Resolution in Time, Space
  - Turbulent Kinetic Energy Model (2 alternate plausible models)
  - Heat of Combustion
  - Soot Extinction Coefficient
  - Flame Volume Coefficient
  - Flame Loading Coefficient
  - Convection Coefficient

"Airplane Fire"

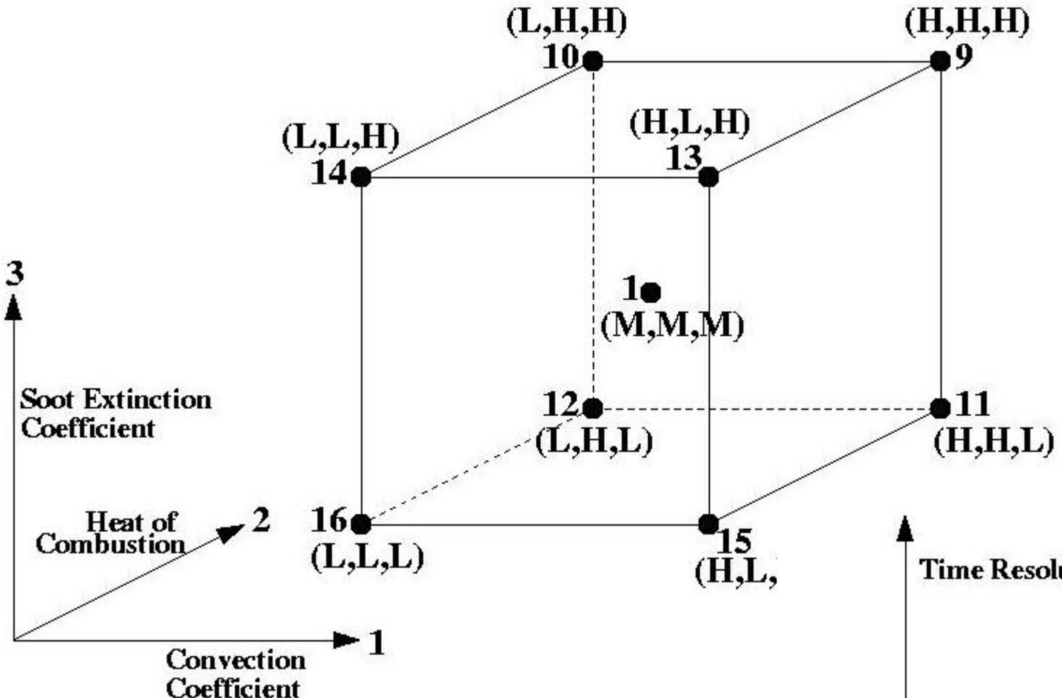


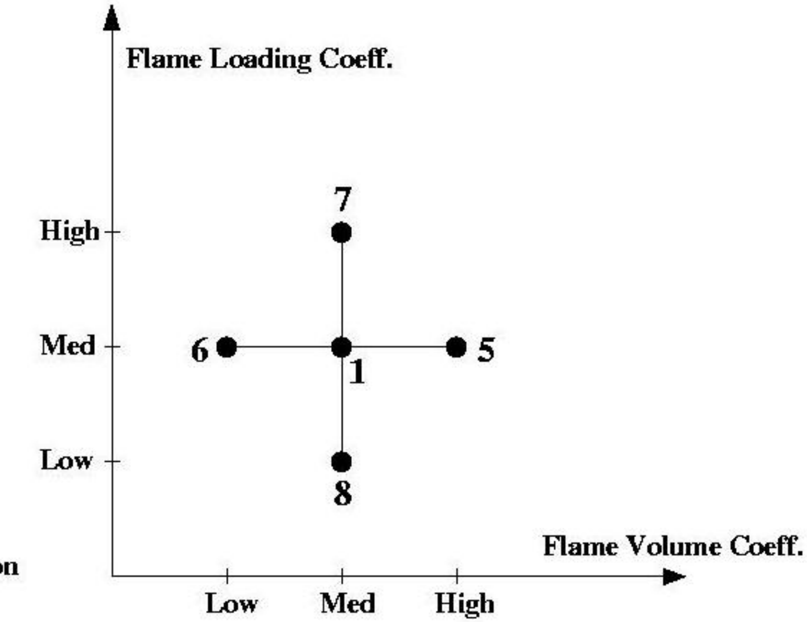


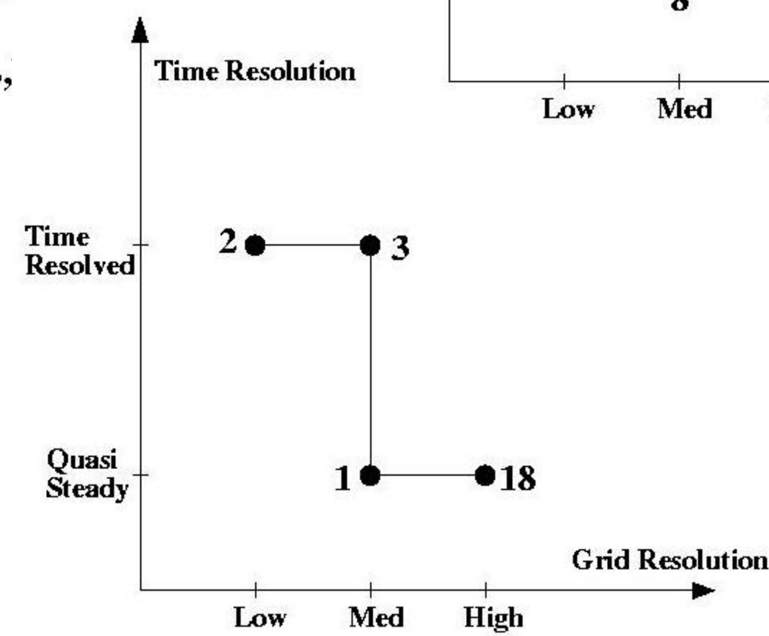
"Truck Fire"

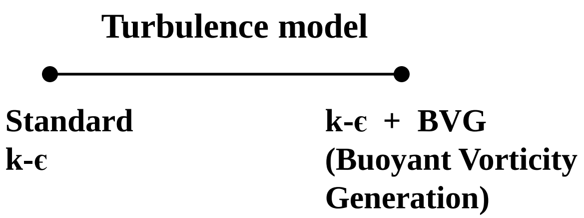


Block-Structured Experimental Designs





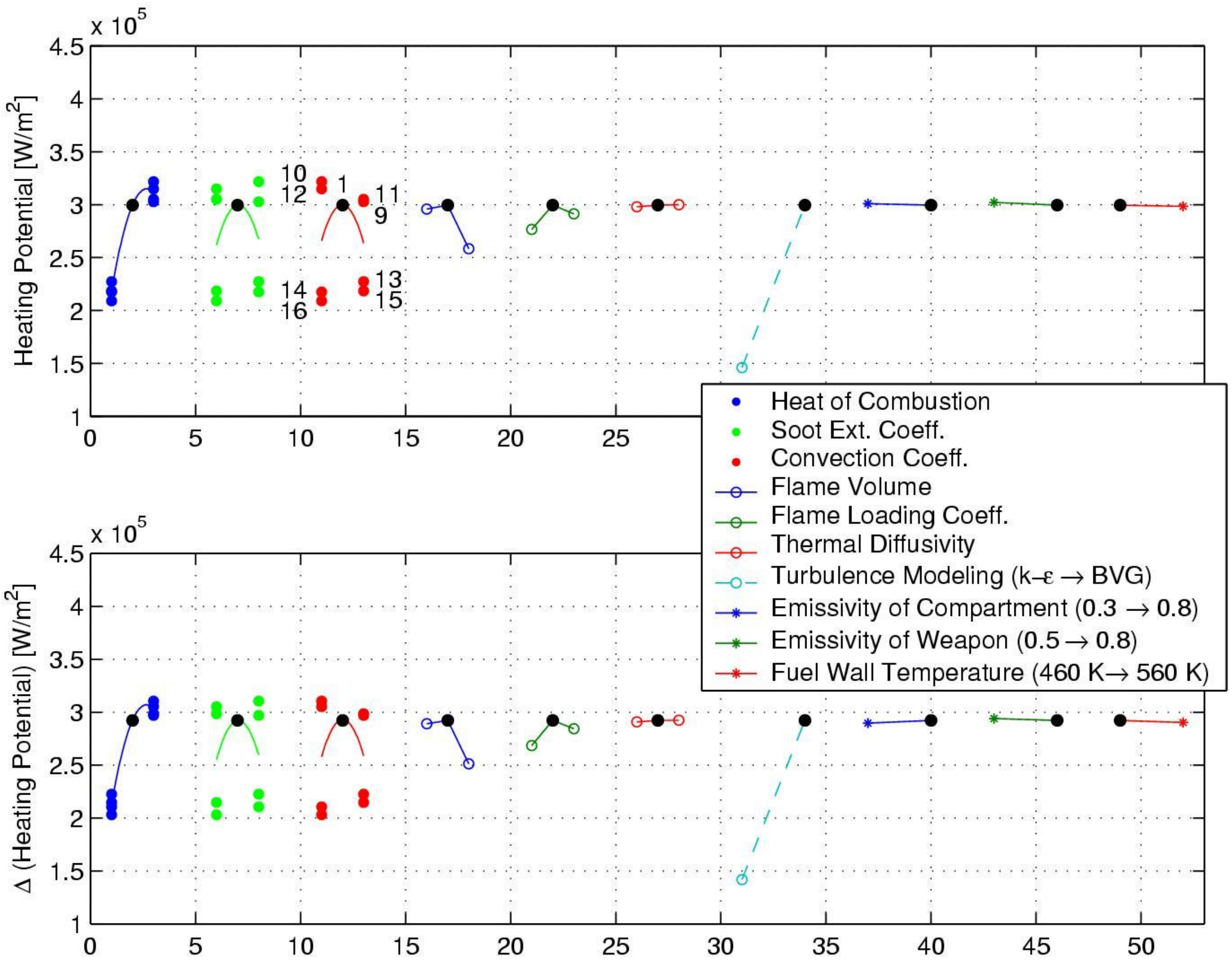




Sensitivity Results

➢ sensitivities consistent between Truck and Airplane fire simulations

Time = 170 sec., Metric is Heating Potential at object surface



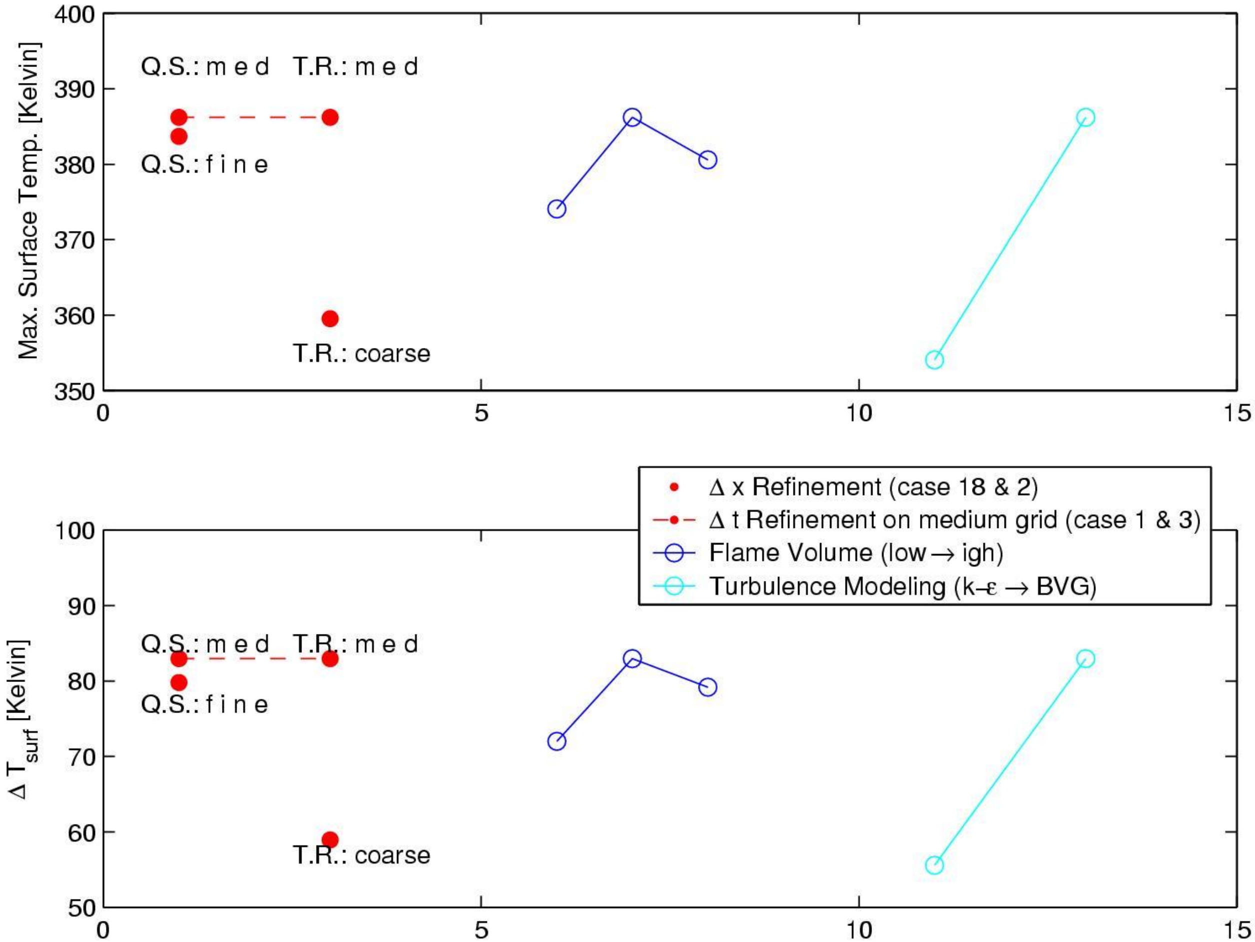
- Sensitivities used to determine the combinations of parameter values (over their ranges of uncertainty) that give enveloping high and low fire intensities
- Used to estimate bounds on calculated heat imparted to object in model validation study

Airplane-Fire Sensitivity Results

~ Relative Magnitude of Discretization Effects

Is important to assess discretization effects on calculated results

Time = 22 sec., Metric is Object Surface Temperature



- Difference between coarse-mesh and medium-mesh results is same scale of effect as dominant physical uncers.
- Comparisons at medium and fine discretizations indicate relatively insignificant diffs.

Extrapolation Uncertainty for computed steady-state temperatures at TC5 location

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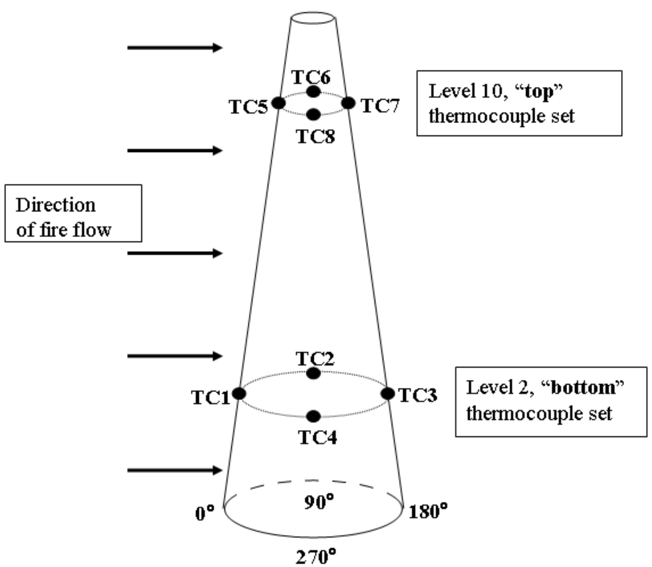
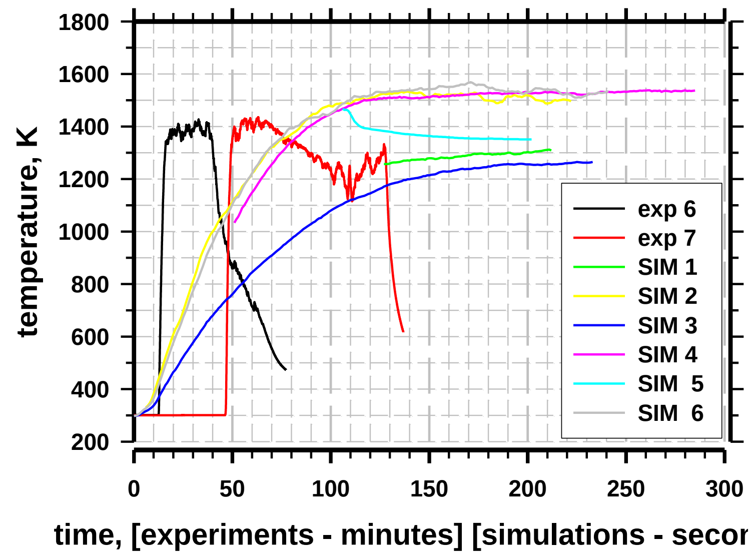
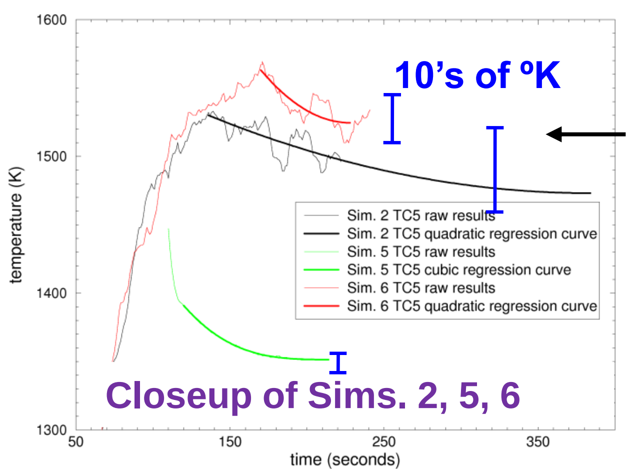
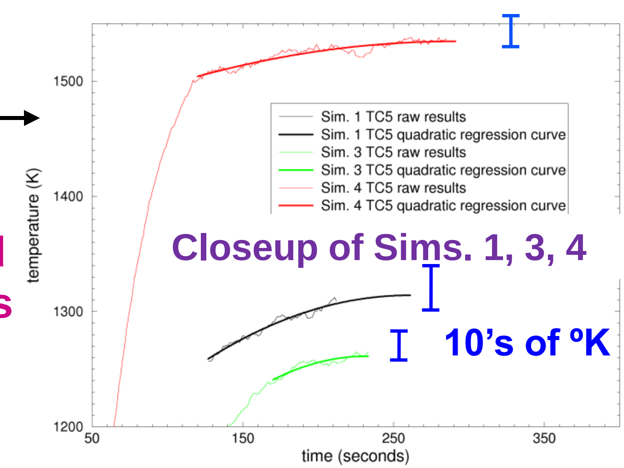


Experimental & simulation results at **TC #5** location

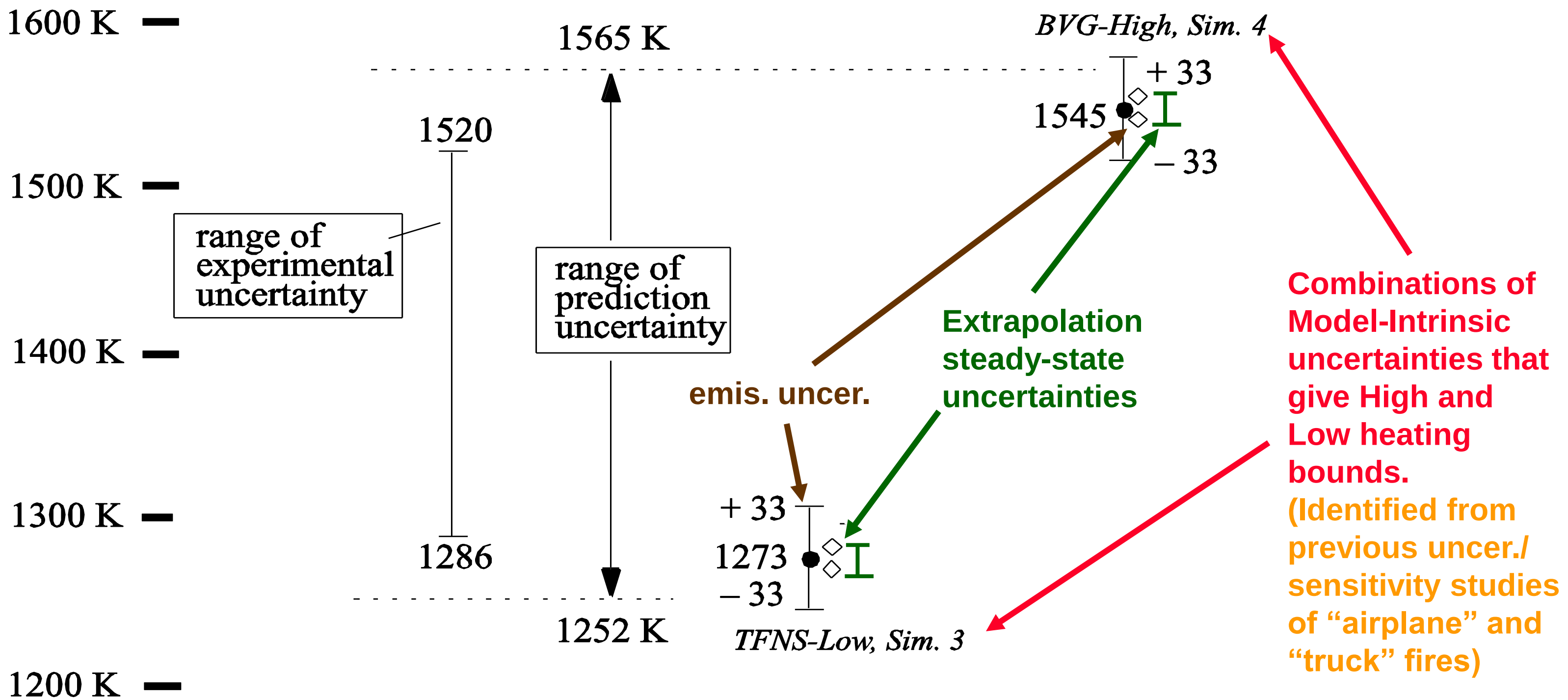




regression and extrapolation of simulation results to gauge estimated uncertainty bounds for steady-state temperatures



Uncertainty Rollup of Simulation Results, with Validation Comparisons to Experimental Uncertainty



✓ **Propagated uncertainty in the fire CFD model predictions provisionally* bounds the experimental temperatures w/uncer. — at TC5 <u>and the 7 other TCs on the calorimeter</u>**

*see next slide for caveats

Caveats and Conclusions

- simulations were terminated before steady-state results were established, and mesh-related calculation verification was not performed ⇨ steady-state solutions may lie outside the estimated uncertainty bars

- ±2σ bounds on experimental variability were calculated from only 2 repeat tests; actual variability could be much greater, large enough to extend well past the simulation bounds

- A substantial buffer of >35K exists at upper and lower ends against potential analysis errors from above two causes. Error buffer is much greater at the other 7 TCs analyzed.

Caveats and Conclusions (cont'd.)

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- A pragmatic Real Space approach to model validation has been demonstrated that is versatile, economical, and robust enough to handle the many real difficulties and types & sources of uncertainties encountered in this tough model validation problem—and other types of difficulties and uncertainties not encountered here.

- Some aspects of the uncertainty quantification in the fire CFD validation problem were admittedly "ugly" and crudely approximate, but associated with the problem itself and not the Real Space validation methodology.