

A Probabilistic Framework for Model Uncertainty in Fire Simulation Codes

Mohammad Modarres

University of Maryland

Presented at the American Nuclear Society
Risk Management
Embedded Meeting, Nov. 2009



Other Contributors/ Acknowledgements

Other University of Maryland Team Members:

- ☒ Victor Ontiveros
- ☒ Adrien Cartillier¹
- ☒ Charlotte le Gac¹

Technical Contributors:

- ☒ Rick Peacock (NIST)
- ☒ Reza Azarkhail² (UMD)



Objectives

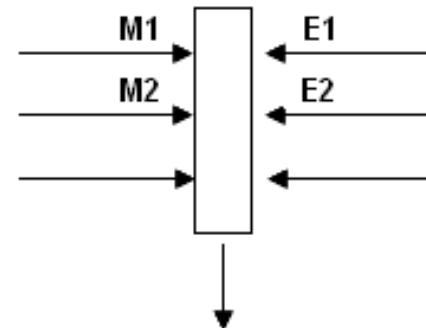
- # Assess model prediction uncertainty in light of experimental results
- # Experimental data involve uncertainties
- # In this example the “Model” is referred to a computer code with multiple outputs and multiple Sub-models (e.g., Physical Correlations)
- # The sub-models are developed based on other experiments and data not used in the output updating process

Black-Box Representation

Deterministic
Input



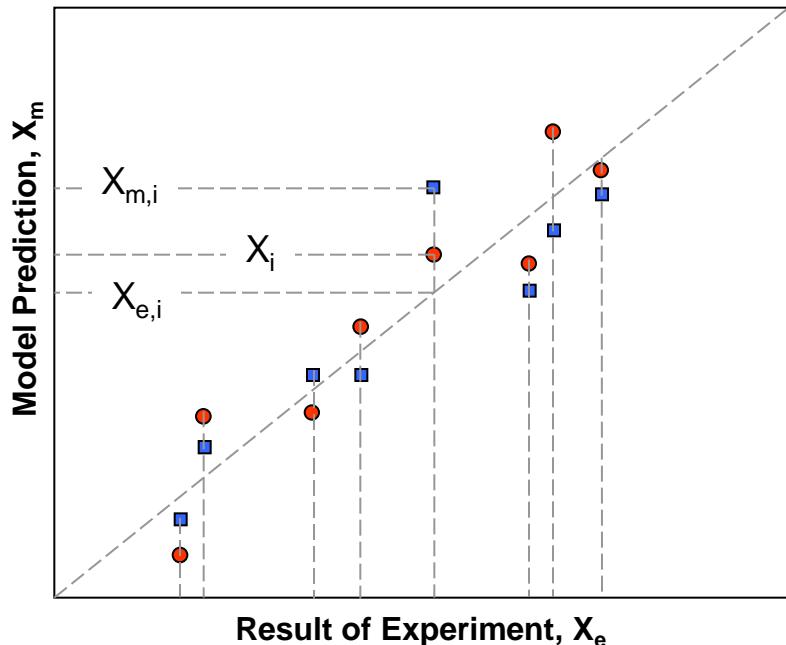
Deterministic
Output



Deterministic
Experimental Values

Bayesian
Inference

Multiplicative Error: Bayesian Posterior



Substituting (1) in (2) :

$$\left. \begin{aligned} F_{e,i} X_{e,i} &= F_{m,i} X_{m,i} \\ \frac{X_{e,i}}{X_{m,i}} &= \frac{F_{m,i}}{F_{e,i}} = F_{t,i} \\ \text{Independency of } F_m, F_e \end{aligned} \right\} \Rightarrow F_t \sim LN(b_m - b_e, \sqrt{\sigma_m^2 + \sigma_e^2})$$

$$\frac{X_i}{X_{e,i}} = F_{e,i} \quad ; \quad F_e \sim LN(b_e, \sigma_e) \quad (1)$$

$$\frac{X_i}{X_{m,i}} = F_{m,i} \quad ; \quad F_m \sim LN(b_m, \sigma_m) \quad (2)$$

where :

X : Real Quantity

X_e : Result of experiment

X_m : Model prediction

F_e : The error factor for experimental data

F_m : The error factor for model predictions

b_e, σ_e : Mean and SD of experimental error factor

b_m, σ_m : Mean and SD of model error factor

Multiplicative Error: Bayesian Posterior

$$f(b_m, \sigma_m | X_{e,i}, X_{m,i}, b_e, \sigma_e) = \frac{f_0(b_m, \sigma_m) \times L(X_{e,i}, X_{m,i}, b_e, \sigma_e | b_m, \sigma_m)}{\int \int f_0(b_m, \sigma_m) \times L(X_{e,i}, X_{m,i}, b_e, \sigma_e | b_m, \sigma_m) db_m d\sigma_m} \quad (3)$$

where:

$$L(X_{e,i}, X_{m,i}, b_e, \sigma_e | b_m, \sigma_m) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi} \left(\frac{X_{e,i}}{X_{m,i}} \right) \sqrt{\sigma_m^2 + \sigma_e^2}} e^{-\frac{1}{2} \times \left[\ln \left(\frac{X_{e,i}}{X_{m,i}} \right) - (b_m - b_e) \right]^2}$$

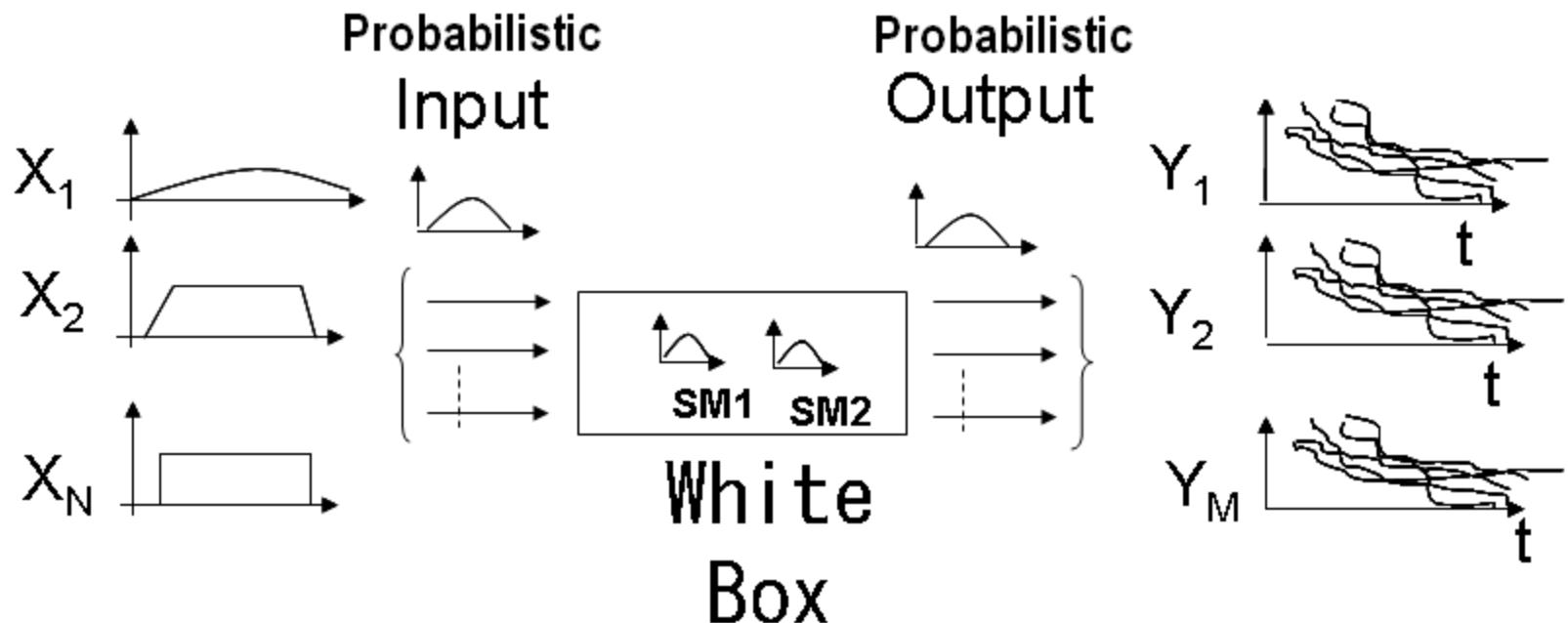
$f_0(b_m, \sigma_m)$: Prior Joint Distribution of Parameters

$f(b_m, \sigma_m | X_{e,i}, X_{m,i}, b_e, \sigma_e)$: Posterior Joint Distribution of Parameters

Given a model prediction such as X_m the distribution of X will be estimated as following:

$$\left. \begin{array}{l} X_m \text{ given as model prediction} \\ F_m \sim LN(b_m, \sigma_m) \\ X = F_m X_m \end{array} \right\} \Rightarrow X \sim LN(\ln(X_m) + b_m, \sigma_m)$$

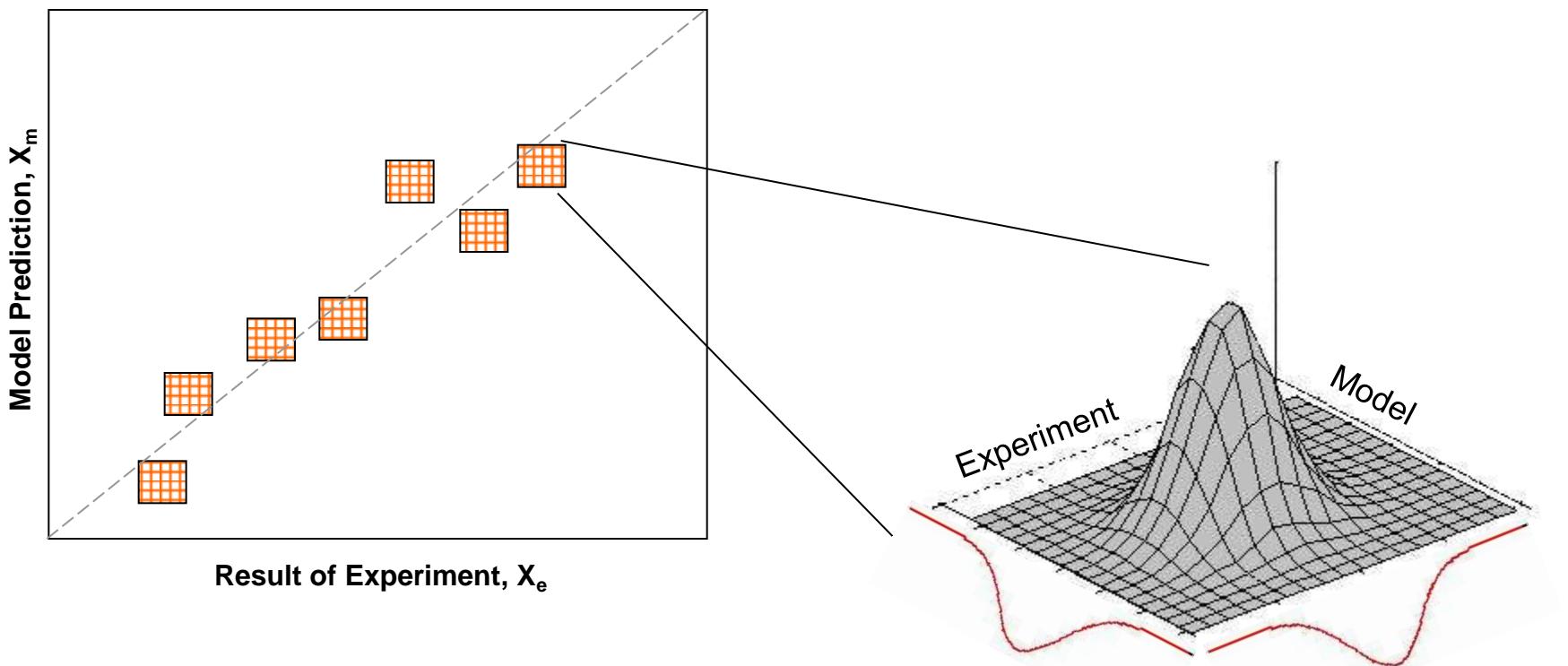
White-Box Representation



White-Box Representation (cont.)



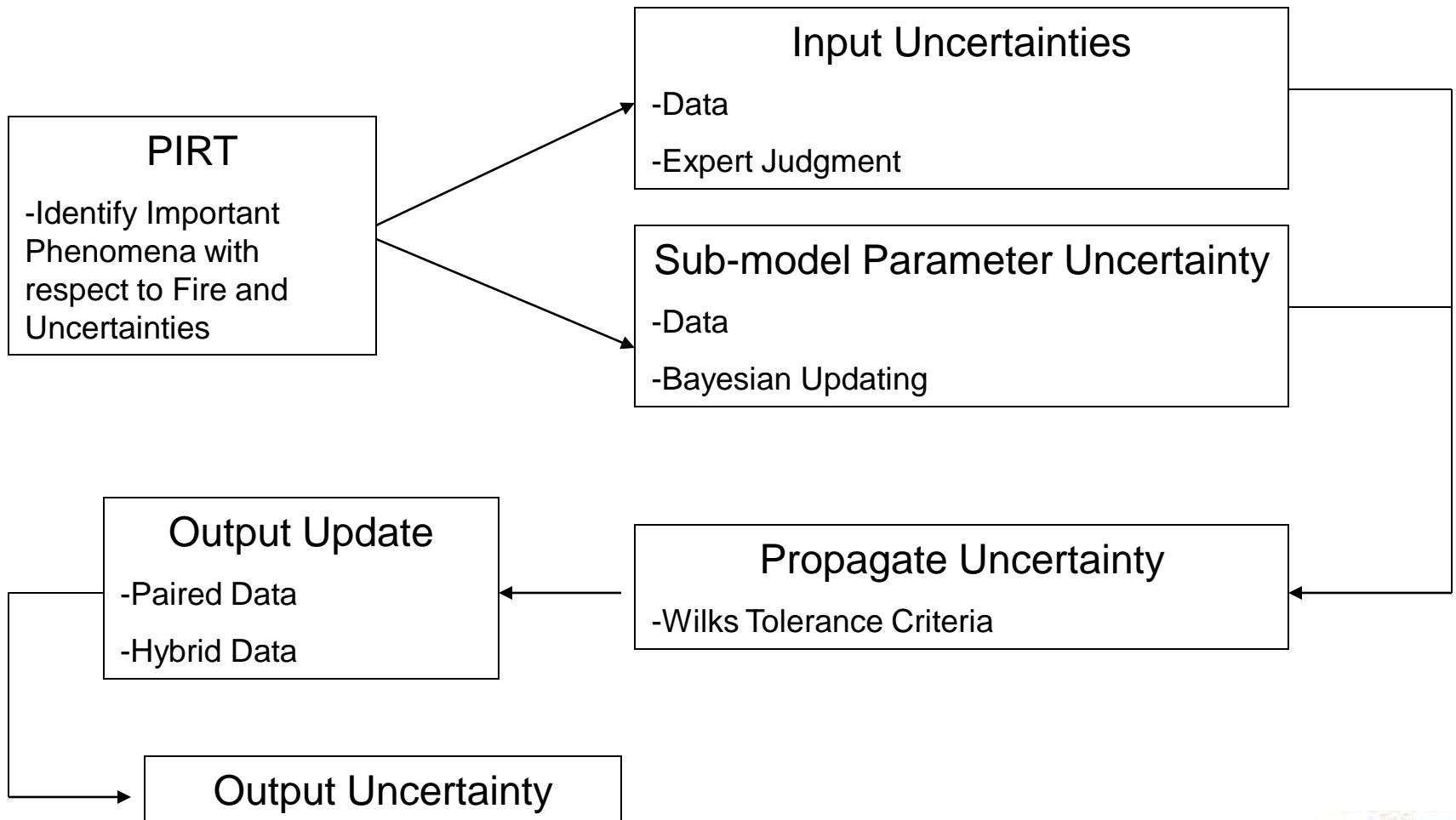
When Both Model Output and Experimental Data Are Uncertain:



Why use White-Box Approach?

- ⌘ Black-box approach does not take into account :
 - ⌘ Input uncertainties
 - ⌘ Model parameter uncertainties
- ⌘ White-box approach takes input and model parameter uncertainties into account while keeping the output updating step seen in the black-box analysis.

Methodology



CFAST: Flame Height: PIRT

- ⌘ CFAST [Jones] uses Heskestad's flame height equation [Heskestad]:

$$z_f = -1.02D + 0.235\dot{Q}^{2/5}$$

☒ PIRT – Identify sub-model that influence the flame height calculation

- ☒ heskestad.f90 – performs calculation of flame height
- ☒ PYROLS.f90 – changes HRR input to account for energy losses

☒ PIRT – Phenomena:

- ☒ Equation parameters -1.02, 0.235, 2/5
- ☒ Model inputs Q and D
- ☒ $g, p, T_{\infty}, c_p, \Delta H_c, r$



CFAST: Flame Height: Sub-model Parameter Uncertainties

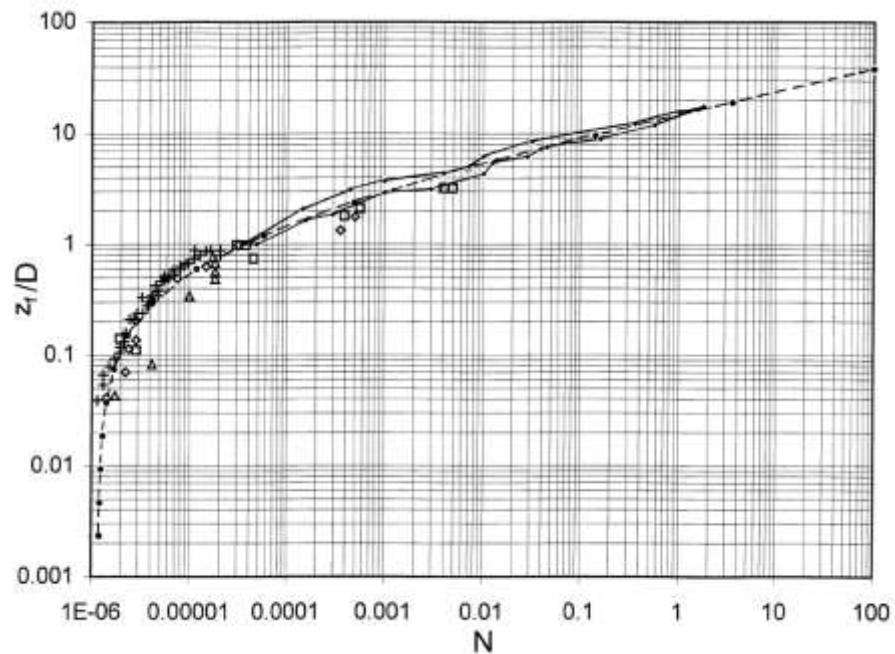
⌘ CFAST

$$z_f = -1.02D + 0.235\dot{Q}^{2/5}$$

⌘ Data [Heskestad]

$$\frac{z_f}{D} = -1.02 + 15.6N^{1/5}$$

$$N = \left[\frac{c_p T_\infty}{g \rho_\infty^2 \left(\frac{\Delta H_c}{r} \right)^3} \right] \left(\frac{\dot{Q}^2}{D^5} \right)$$



where :

z_f : Flame Height

D : Source Diameter

\dot{Q} : Heat Release Rate

c_p : Specific Heat

T_∞ : Ambient Temperature

ρ_∞ : Ambient Density

H_c : Actual Lower Heat of Combustion

r : Actual Mass Stoichiometric ratio, air to fuel volatiles

CFAST: Flame Height: Sub-model Parameter Uncertainties (cont.)

- ☒ Bayesian regression estimation of parameters.
- ☒ Results in distribution over model parameters in an empirical form

$$\frac{z_f}{D} = -\alpha + \beta N^\gamma$$

$$f(\alpha, \beta, \gamma | z_f / D, N) = \frac{f_0(\alpha, \beta, \gamma) \times L(z_f / D, N | \alpha, \beta, \gamma)}{\int_{\theta} f_0(\alpha, \beta, \gamma) \times L(z_f / D, N | \alpha, \beta, \gamma) d\alpha d\beta d\gamma}$$

where :

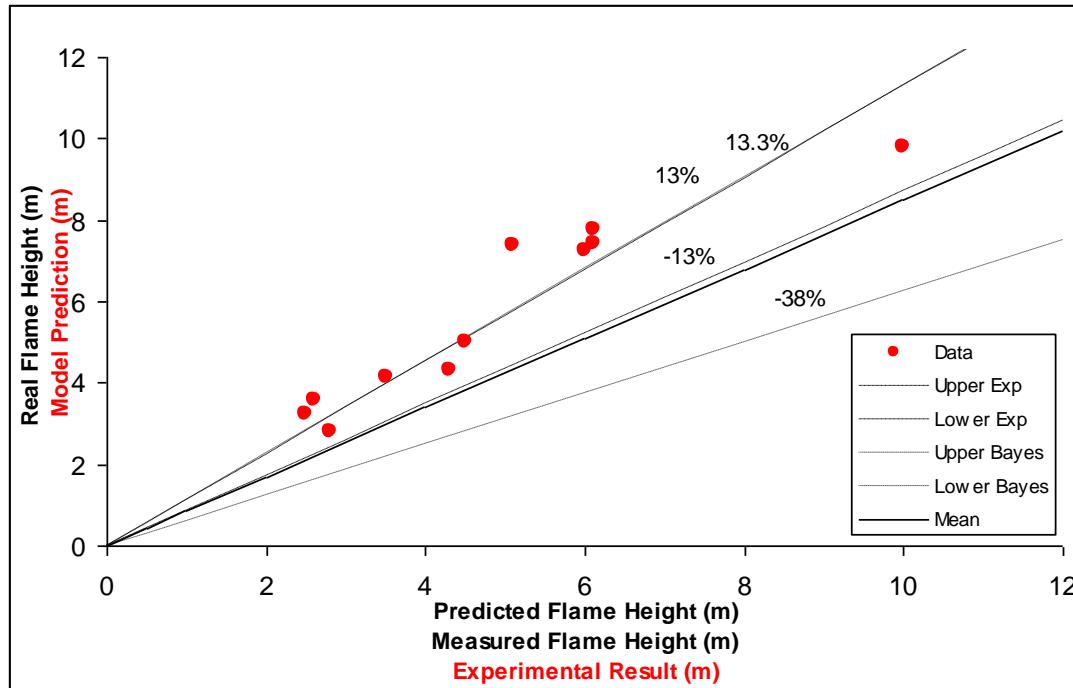
$$L(z_f / D, N | \alpha, \beta, \gamma) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2} \times \frac{(z_f / D - \alpha - \beta N^\gamma)^2}{\sigma}}$$

$f_0(\alpha, \beta, \gamma)$: Prior Joint Distribution of Parameters

$f(\alpha, \beta, \gamma | z_f / D, N)$: Posterior Joint Distribution of Parameters

CFAST: Flame Height: Results – Black-Box

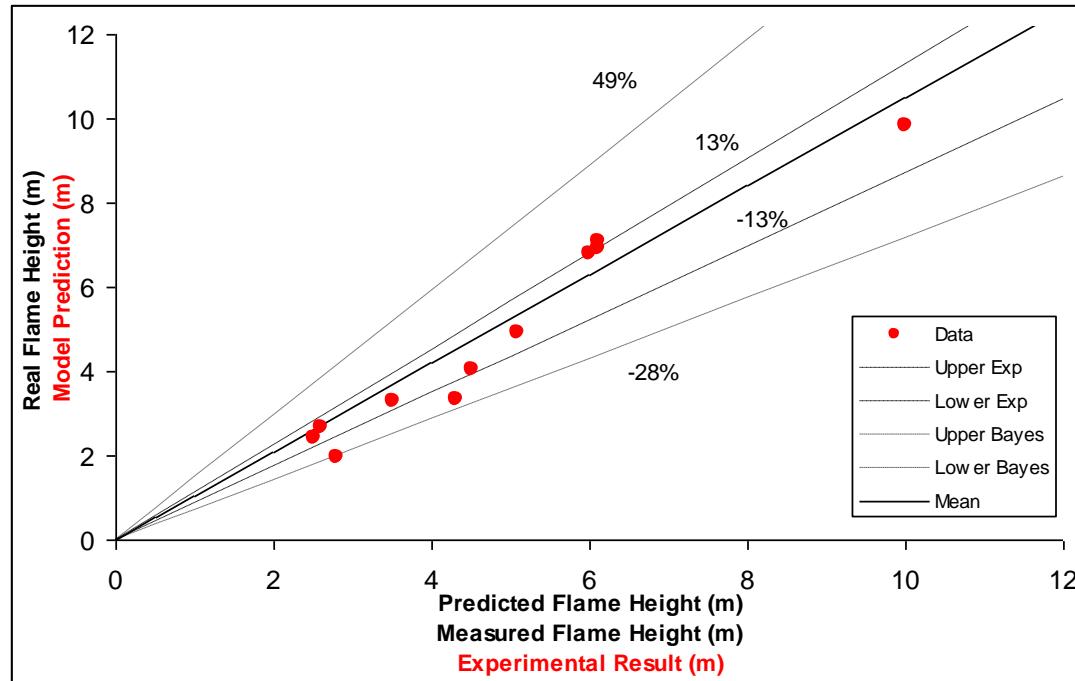
Test	X_m	X_e
BE3	2.8	2.81
BE2	4.3	4.3
NIST 5	3.6	2.6
NIST 6	3.2	2.5
NIST 7	4.2	3.5
NIST 14	7.4	5.1
NIST 15	7.8	6.1
NIST 17	7.3	6
NIST 18	5.0	4.5
NIST 20	7.4	6.1
NIST 21	9.8	10



Parameter	Mean	SD	2.50%	Median	97.50%
b_m	-0.176	0.047	-0.268	-0.176	-0.084
s_m	0.134	0.045	0.067	0.127	0.243
F_m	0.848	0.127	0.625	0.839	1.133

CFAST: Flame Height: Results – White-Box

Test	X_m	X_e
BE3	2.0	2.81
BE2	3.3	4.3
NIST 5	2.7	2.6
NIST 6	2.4	2.5
NIST 7	3.3	3.5
NIST 14	4.9	5.1
NIST 15	7.1	6.1
NIST 17	6.8	6
NIST 18	4.0	4.5
NIST 20	6.9	6.1
NIST 21	9.8	10



Parameter	Mean	SD	2.50%	Median	97.50%
b_m	0.032	0.055	-0.077	0.032	0.142
s_m	0.164	0.052	0.090	0.155	0.292
F_m	1.049	0.195	0.718	1.030	1.492

Conclusions

⌘ Advantages:

- ◻ Method allows for propagation of all uncertainties
- ◻ In accounting for model uncertainties
 - ◻ Results can show appropriate use of the model
 - ◻ Results can show where more research is needed

⌘ Considerations:

- ◻ Application of methodology is computationally intensive
 - ◻ Intense knowledge of sub-models
 - ◻ To fully account for uncertainties multiple sub-models should run simultaneously