

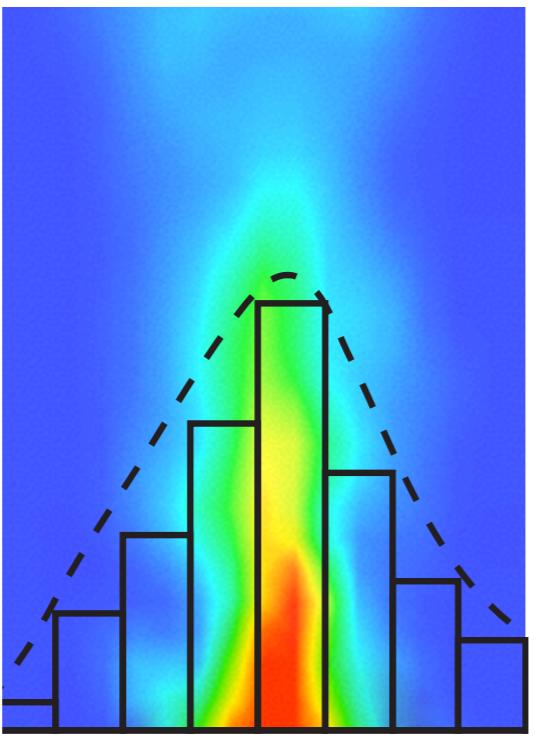


# A Parameter Uncertainty Framework for Fire Scenarios Using a Bayesian Inference Approach

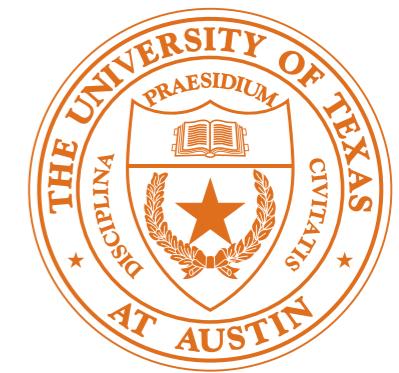
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Ofodike A. Ezekoye

October 28, 2013



NIST



# Outline

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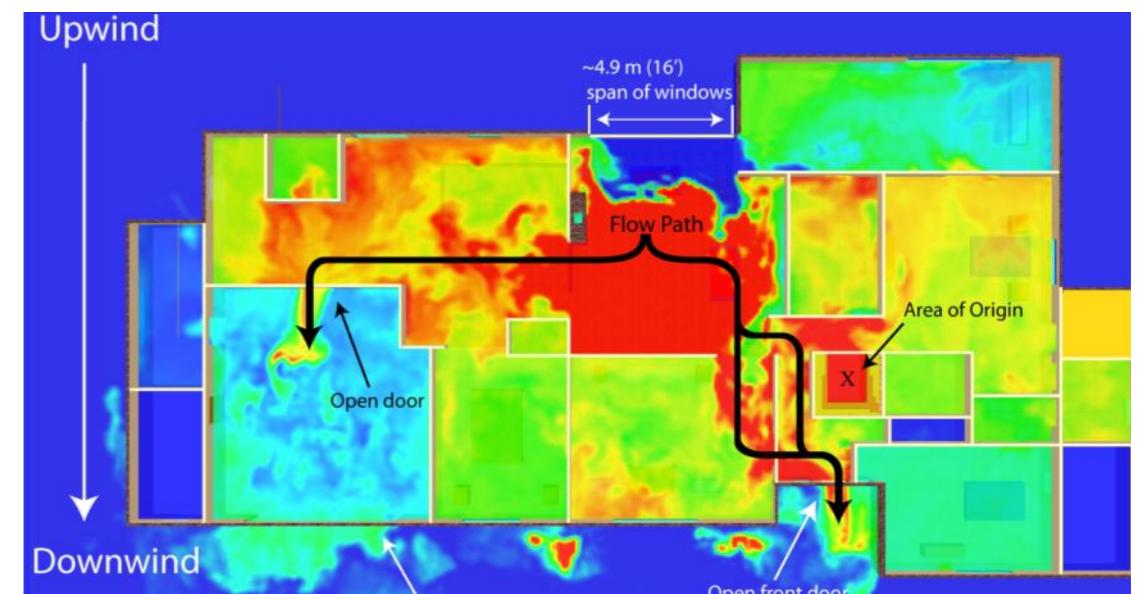
- Motivation
- Problem Statement
- Research Objectives
- Bayesian Inference Framework
- Examples Using Bayesian Inference in Fire Scenarios:
  - 1) Estimating Fire Size
  - 2) Estimating Material Properties
  - 3) Estimating Fire Location
- Conclusions

# Motivation

Fire modeling tools can be applied to model validation exercises, fire and arson investigations, and reconstructions of firefighter line-of-duty deaths (LODDs) and injuries.



Barowy and Madrzykowski, 2012



Barowy and Madrzykowski, 2012

The location and intensity (i.e., heat release rate) of a fire in a compartment are important model inputs that govern the evolution of thermal conditions in the fire compartment.

# Motivation

Compartment fires leave behind a record of fire activity and history (i.e., fire signatures).



NFPA 921, 2011 ed.



NFPA 921, 2011 ed.

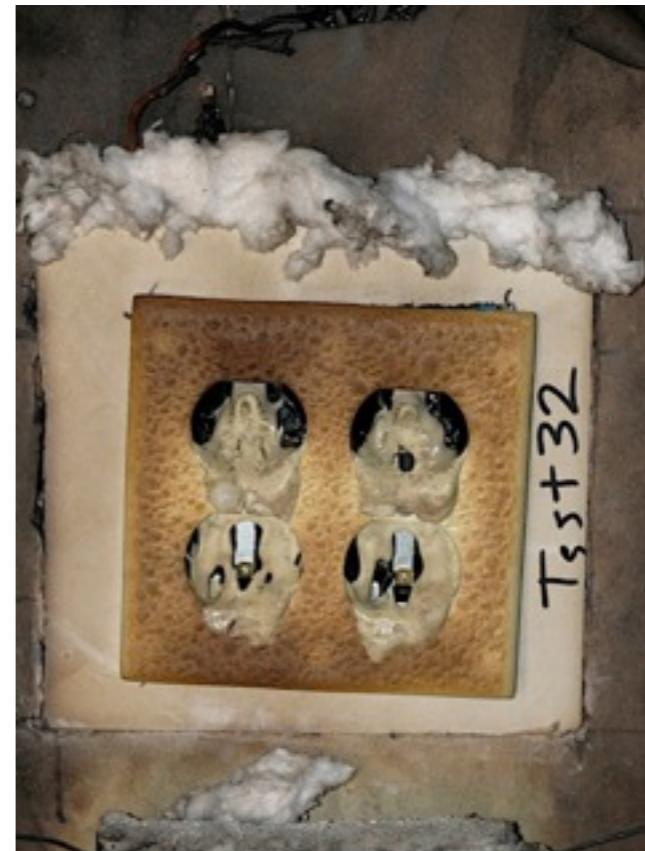
- Gypsum wallboard undergoes chemical reactions/calcination,
- Metal and plastic components melt and deform,
- Soot deposition to surfaces occurs.

# Motivation

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In fire scenarios, observations of fire damage can be a surrogate for measured data (e.g., degraded gypsum wallboard or melted switch plates and outlets).

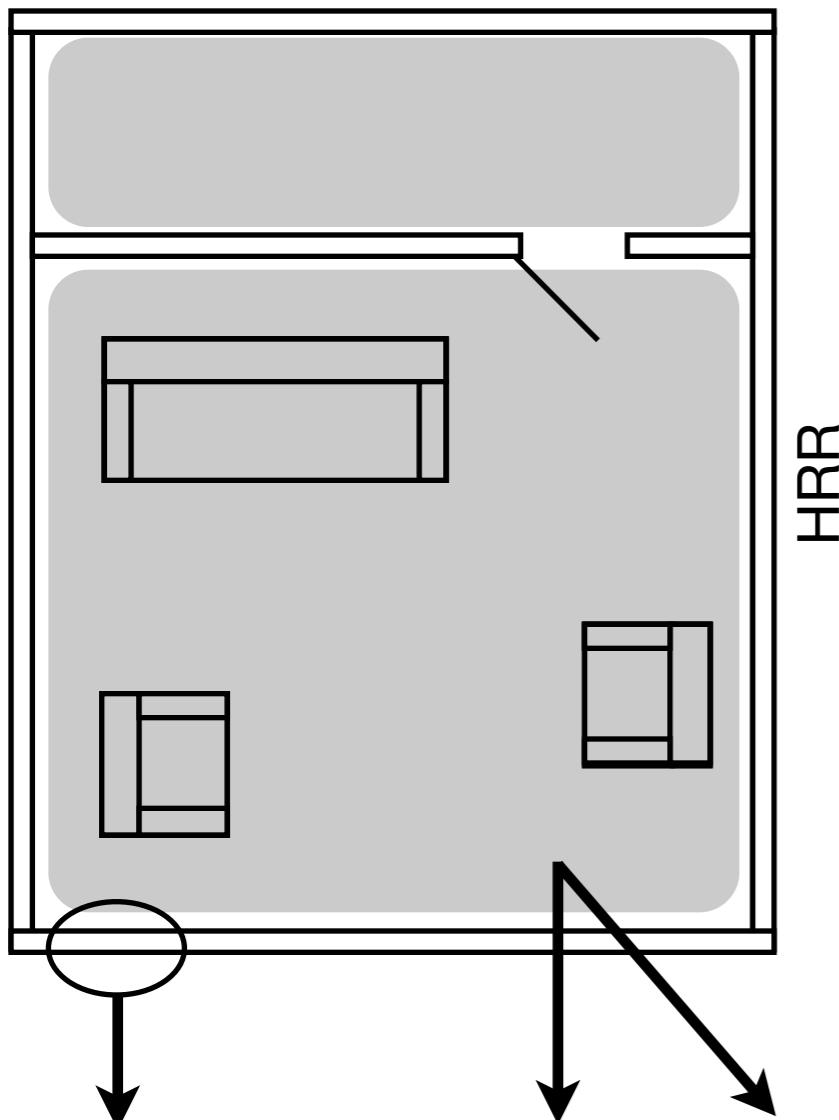
We can use various fire models and inversion techniques to estimate the size and location of a fire in a compartment.



$$Q = \int \dot{q}'' dt$$

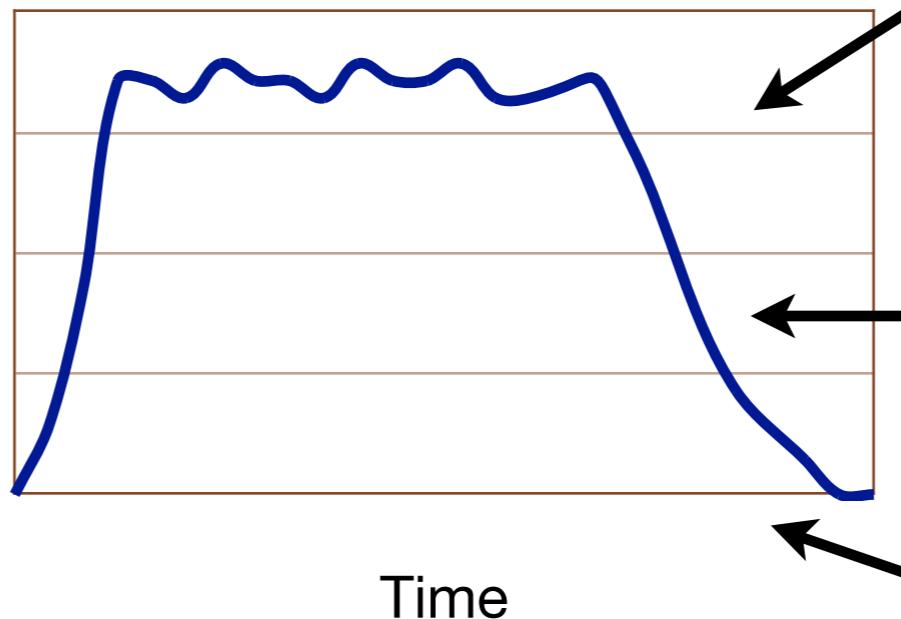
# Problem Statement

Compartment fire

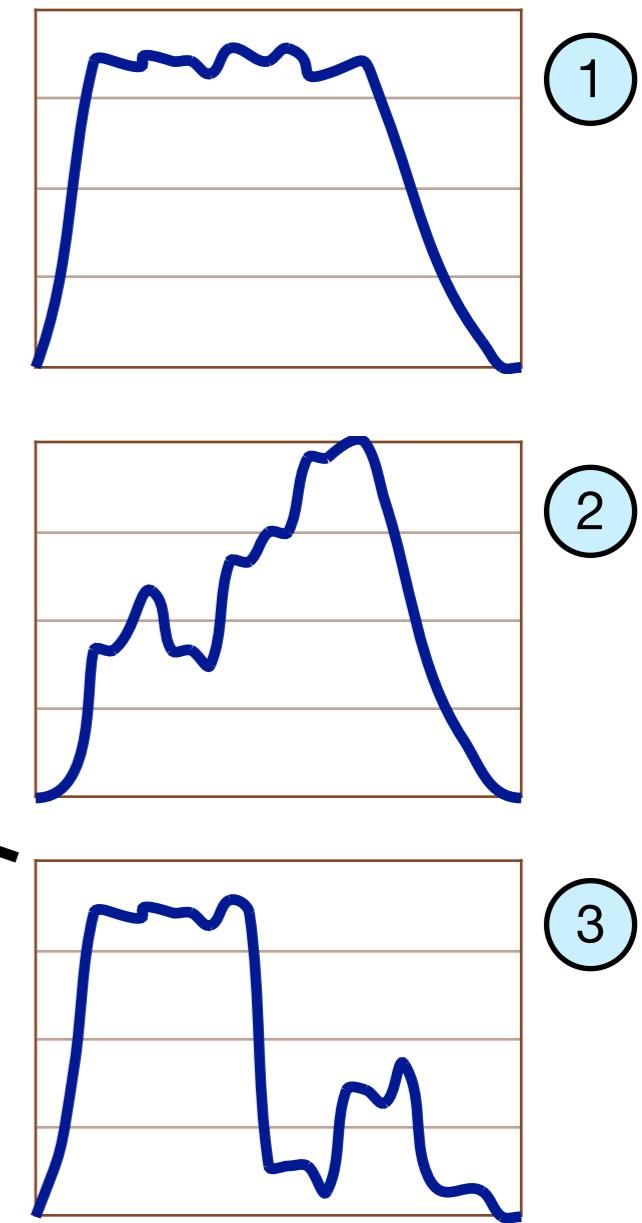


$$T_{gyp}(z) = f(T_u(t), L(t))$$

Actual Fire Scenario



Plausible Scenarios



# Institutional Decision Analysis

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In institutional settings (businesses, governments, or research organizations), **decisions need to be justified**, and **formal decision analysis** has a role to play in clarifying the relation between [...] a relevant probability model and the resulting estimates.

[...] forensic scientists use a particular quantitative approach to evaluating forensic laboratory results, the Bayesian approach, as a means of **quantifying uncertainty and communicating it accurately to judges, prosecutors, and defense lawyers** [...]

[...] using the Bayesian approach also brings about a particular type of intersubjectivity; [...] **quantifications must be consistent** across forensic specializations, which brings about a **transparency based on shared understandings and practices**.

# Institutional Decision Analysis

Numerical scale	Verbal scale	Likelihood ratio interval
+4	The results of the examination extremely strongly support that ...	$lr \geq 1,000,000$
+3	The results of the examination strongly support that ...	$6000 \leq lr < 1,000,000$
+2	The results of the examination support that ...	$100 \leq lr < 6000$
+1	The results of the examination support to some extent that ...	$6 \leq lr < 100$
0	The results of the examination support neither ... nor ...	$1/6 < lr < 6$
-1	The results of the examination support to some extent that ... was not ...	$1/6 \geq lr > 1/100$
-2	The results of the examination support that ... was not ...	$1/100 \geq lr > 1/6000$
-3	The results of the examination strongly support that ... was not ...	$1/6000 \geq lr > 1/1,000,000$
-4	The results of the examination extremely strongly support that ... was not ...	$lr \leq 1/1,000,000$

# Research Objectives

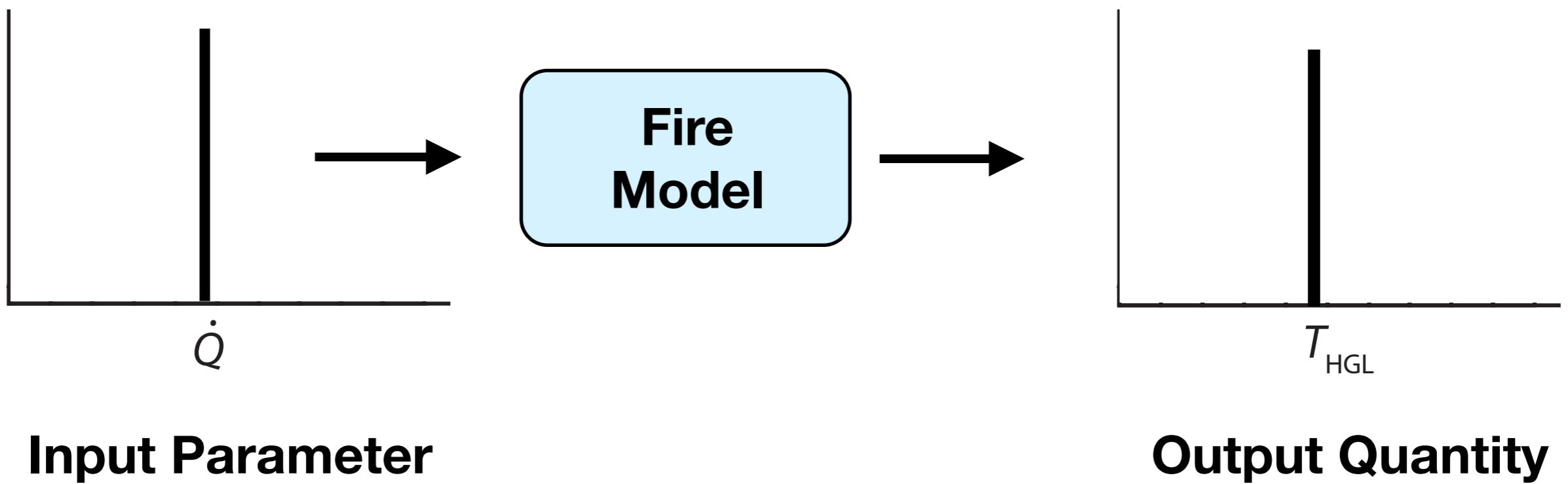
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To describe probability distributions that indicate the **amount of uncertainty in model inputs and outputs**.

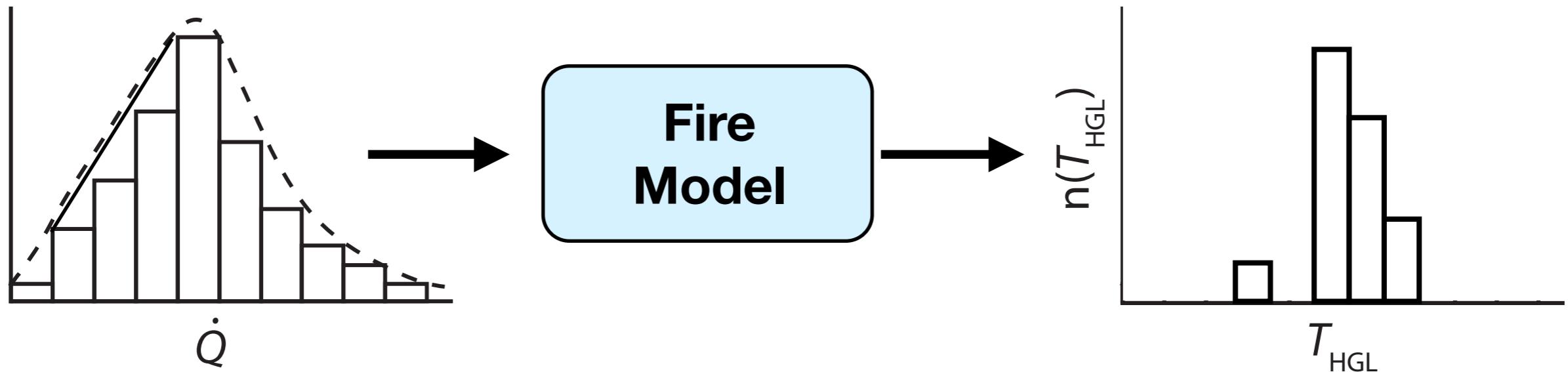
To quantify our **degree of certainty (or degree of belief)** in unknown input parameters for fire scenarios based on:  
1) a predictive model and 2) measured (or observed) data.

To apply a **statistical parameter inversion framework** to various fire scenarios to determine: 1) fire size, 2) fire location, and 3) material property parameters.

# Single Model Inputs and Outputs



# Uncertainty and Distributions in Models



## Input Parameter

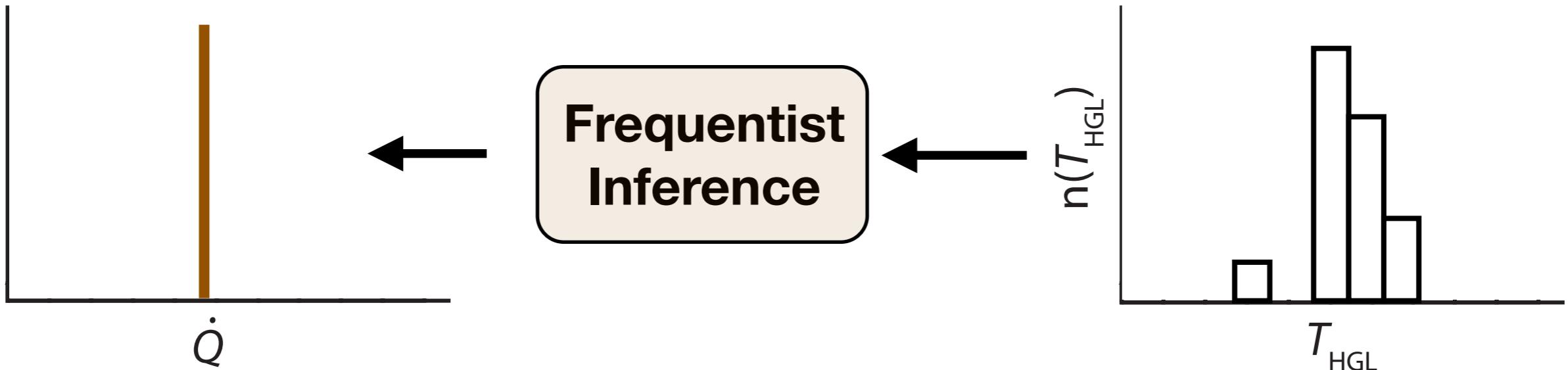
Consider the different use cases:

- Propagation of uncertainty (output distribution)
- FDS verification & validation process (model bias)
- Calculate distribution of input parameters given measured data

## Output Quantity

# Frequentist Inference Method

## Frequentist Approach



### Input Parameter

Inputs are fixed but unknown constants that do not depend on the data.

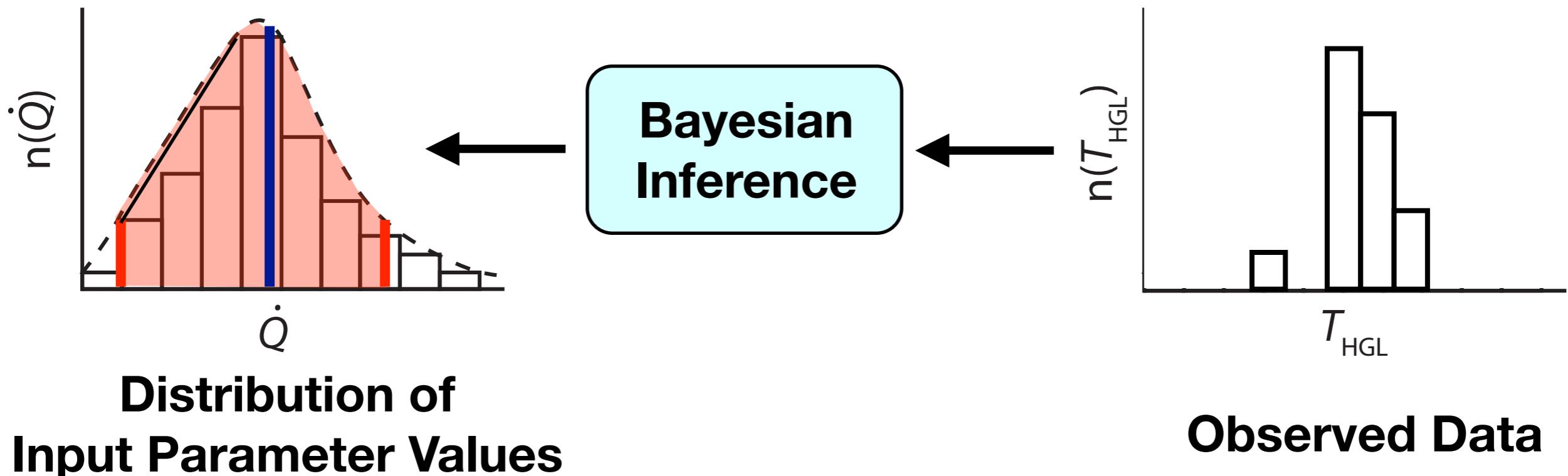
Uncertainty is expressed in terms of repeatability.

### Observed Data

Data are repeated random samples (with some frequency).

# Bayesian Inference Framework

## Bayesian Approach



Inputs are unknown random variables that we are uncertain about and depend on the data.

We model the data-generating process.

Data are fixed observations from a true distribution.

# Bayes' Theorem

## Definition of Bayes' Theorem

$$\widehat{P(A|B)} = \frac{\overbrace{P(B|A) \cdot P(A)}^{\text{Likelihood} \quad \text{Prior}}}{\underbrace{P(B)}_{\text{Normalizing constant}}}$$

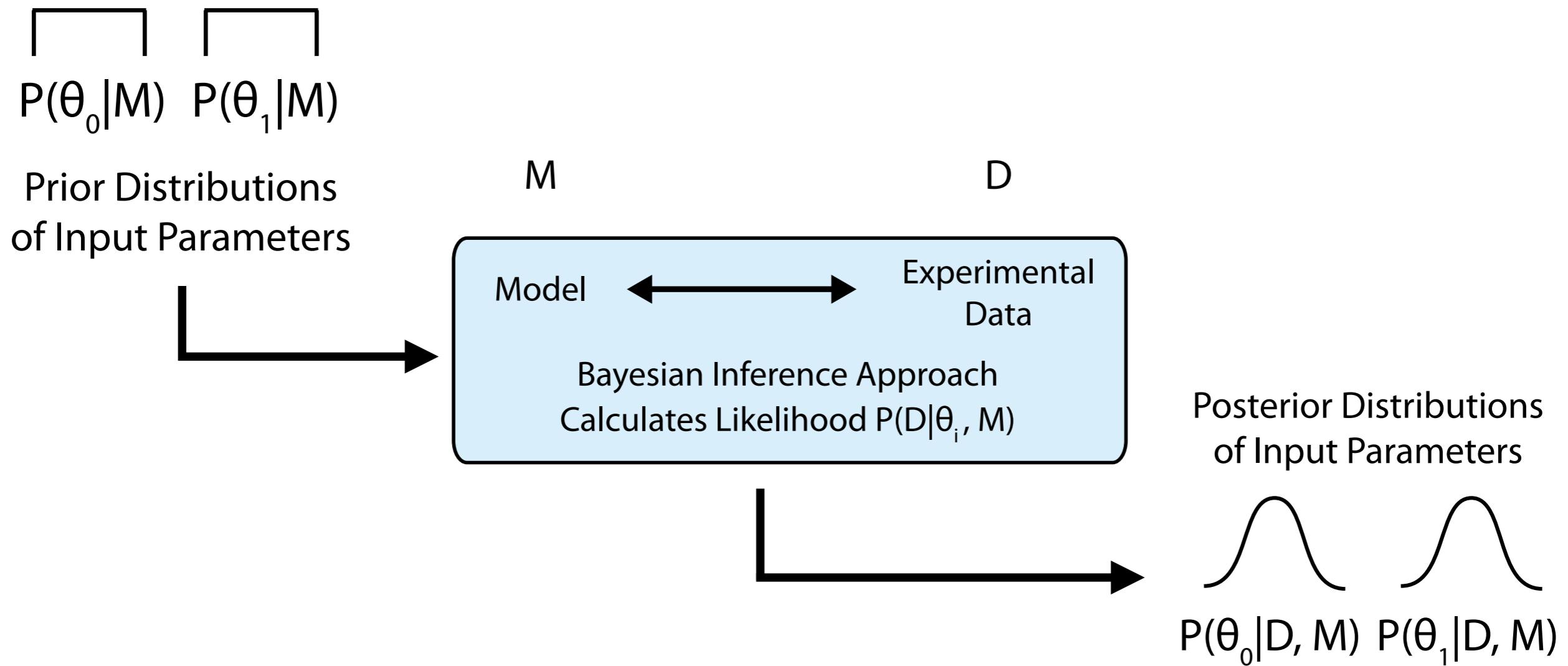
## Bayes' Theorem for Model Applications

$$P(\theta|D, \mathcal{M}) \propto P(D|\theta, \mathcal{M}) \cdot P(\theta|\mathcal{M})$$

Unknown parameter    Model  
Data  
Posterior              Likelihood              Prior

# Bayesian Inference Framework

## The Bayesian inference process



# Applications of Bayesian Inference

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## Examples using Bayesian inference in fire scenarios

1. Estimate fire size using measured heat flux data.
2. Use the FDS fire model to estimate material properties using measured mass loss data.
3. Estimate fire location using heat flux data.

# Computational Framework

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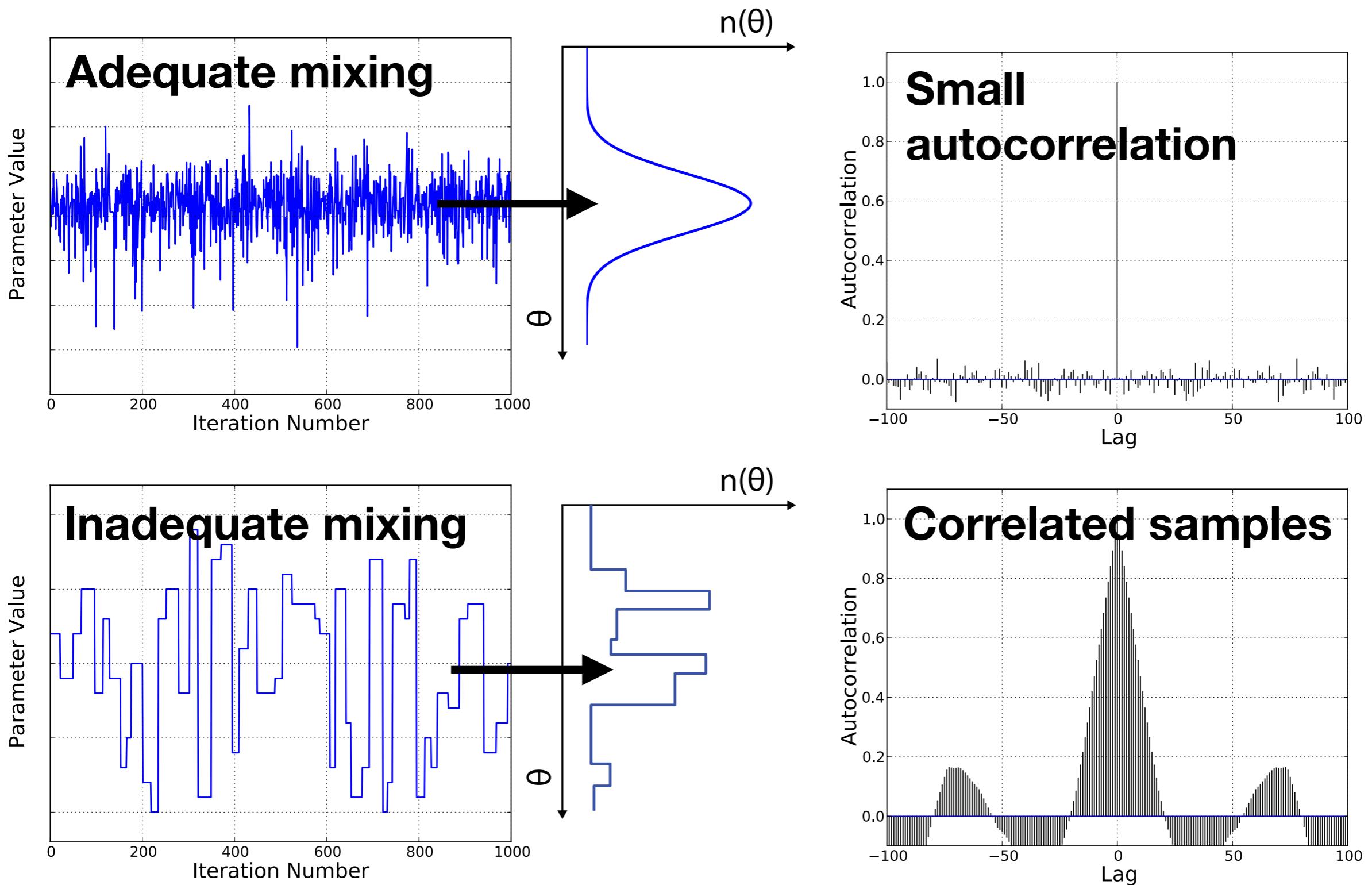
## **Fire modeling and visualization tools:**

- Empirical correlations
- Consolidated Model of Fire and Smoke Transport (CFAST)
- Fire Dynamics Simulator (FDS)
- Smokeview (SMV)

## **Computational, analysis, and visualization tools:**

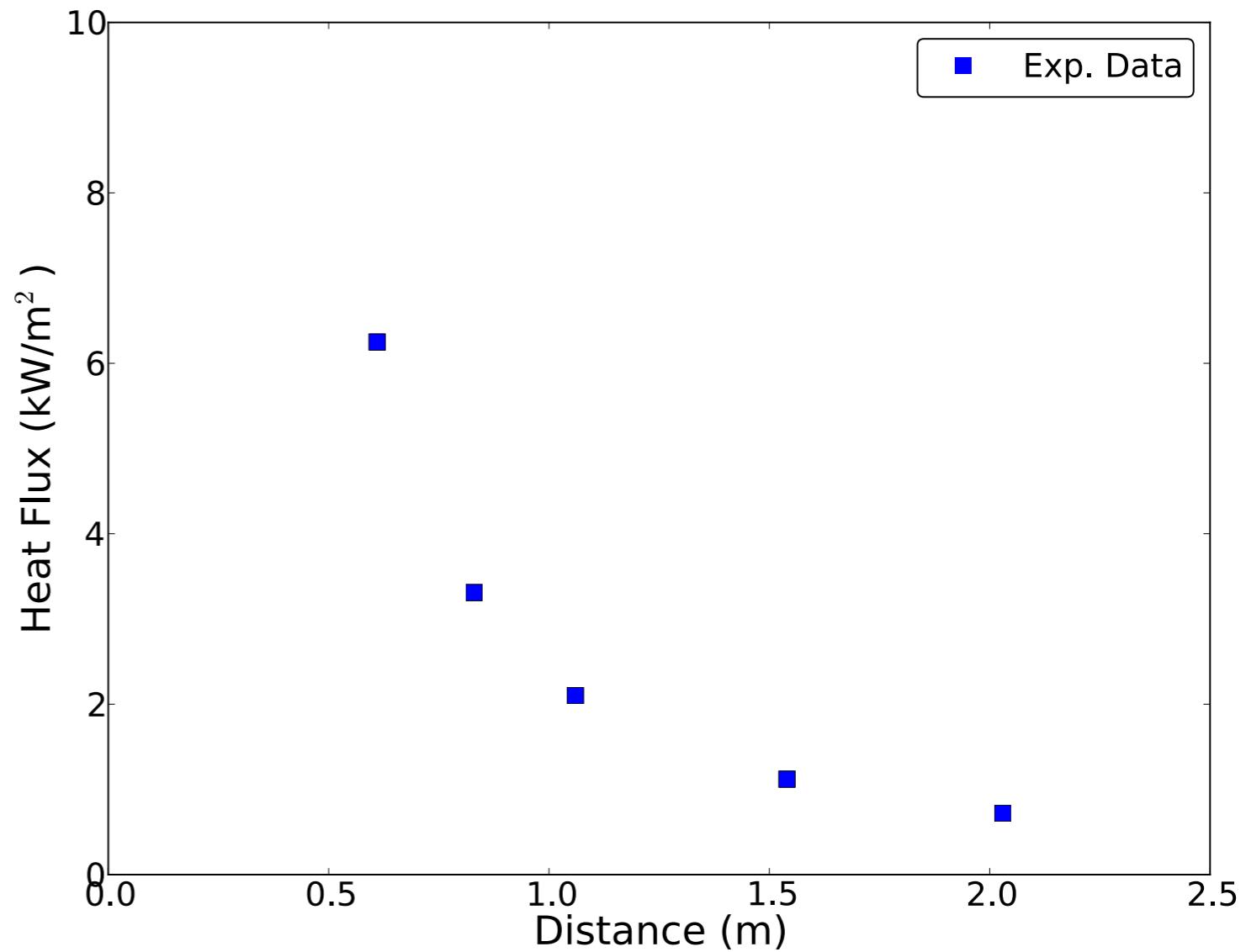
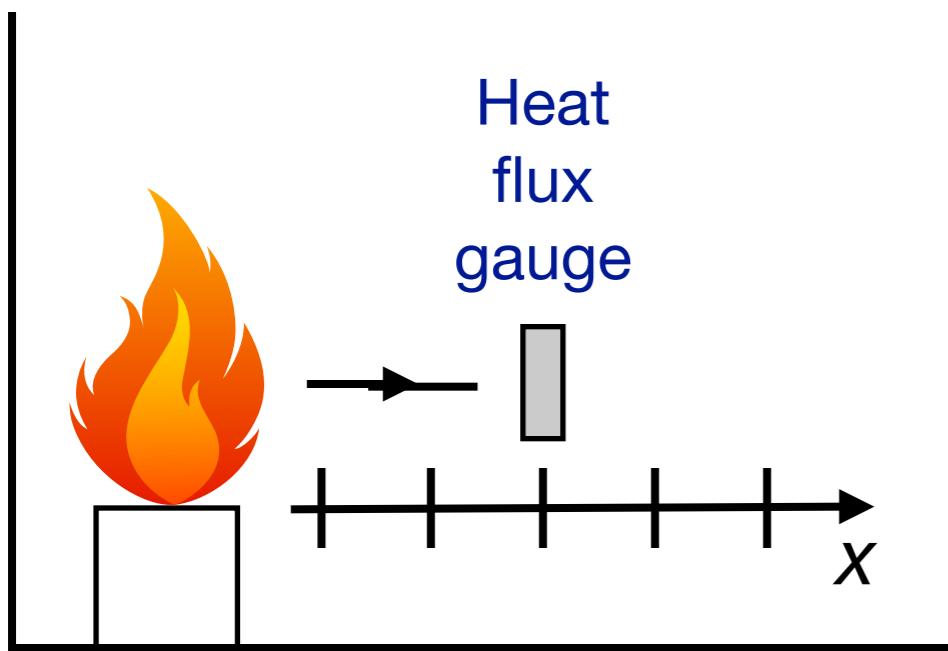
- Python
- Numeric Python (NumPy)
- Scientific Python (SciPy)
- Math plotting library (matplotlib)
- Bayesian Inference in Python (PyMC)

# Results of Bayesian Inference



# Example 1 - Estimating Fire Size

Fleury heat flux experiments; Measured heat flux vs. distance data;  
100 kW propane burner



R. Fleury, "Evaluation of Thermal Radiation Models for Fire Spread Between Objects," Master's thesis, University of Canterbury, Christchurch, New Zealand, 2010.

# Example 1 - Estimating Fire Size

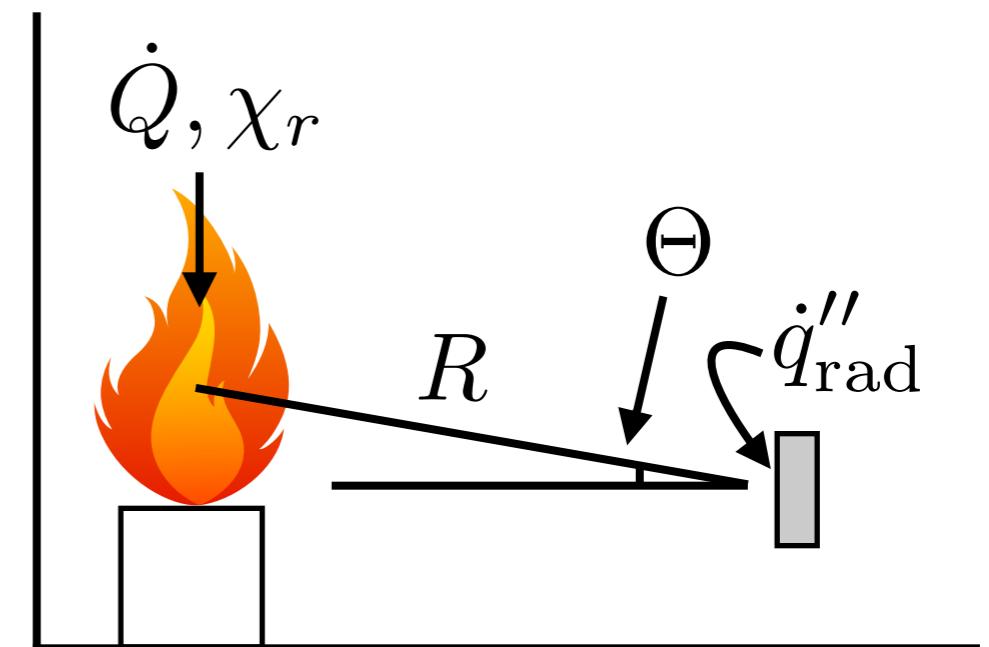
Model: Point source radiation equation

$$\dot{q}_{\text{rad}}'' = \cos(\Theta) \frac{\chi_r \dot{Q}}{4\pi R^2}$$

Known radiative fraction      **Unknown fire size parameter**

$\dot{q}_{\text{rad}}''$        $\dot{Q}$

Measured heat flux data      Known distance



Unknown parameter:  $\dot{Q}$

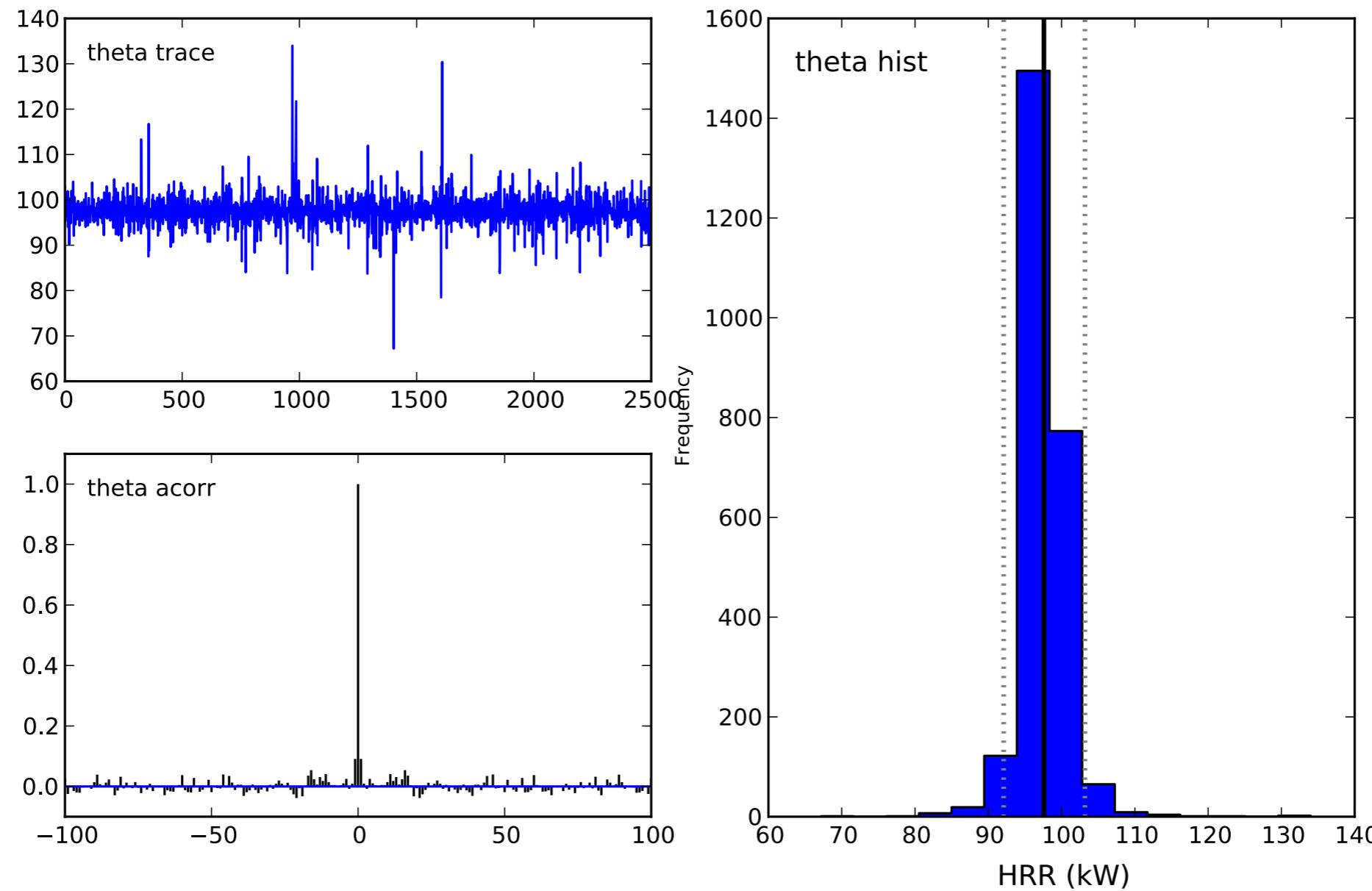
Prior: Uniform distribution:  $50 \text{ kW} < \dot{Q} < 300 \text{ kW}$

$$\dot{Q}(i=0) = 200 \text{ kW}$$

# Example 1 - Estimating Fire Size

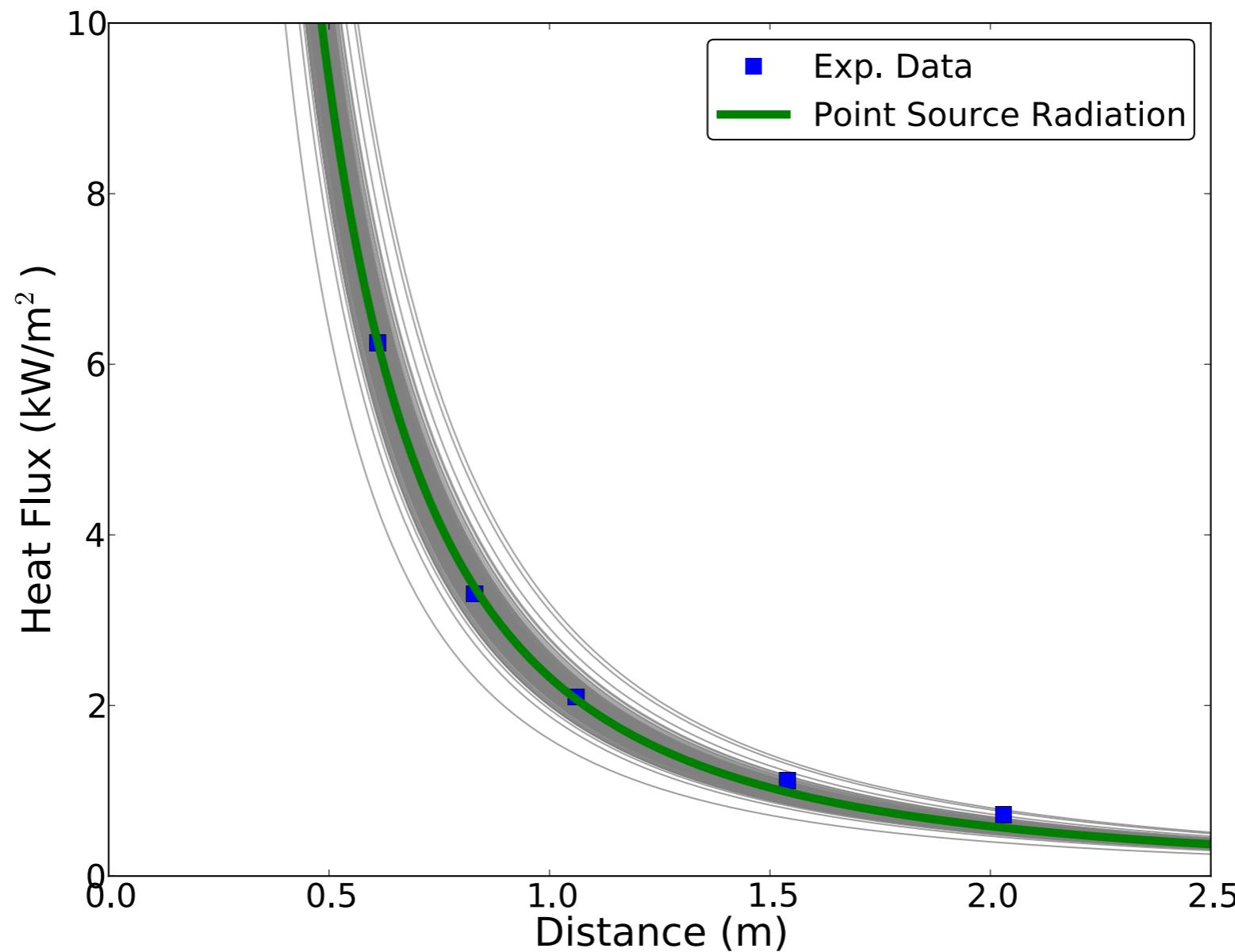
PyMC results for HRR parameter  $\dot{Q}$ :

Mean: 97.6 kW; Standard Deviation: 3.1 kW;  
95 % credible interval = [92 kW, 103 kW]



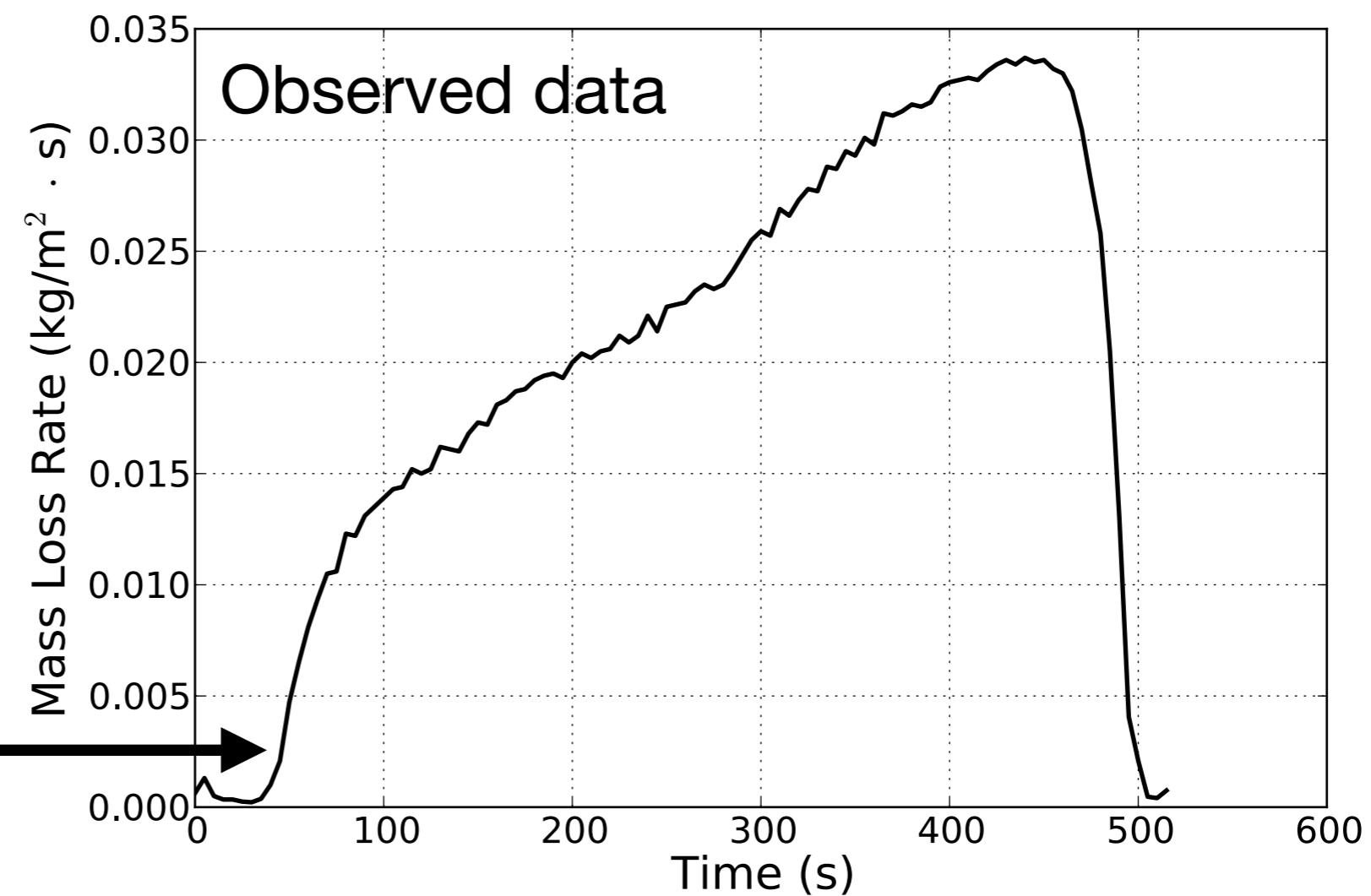
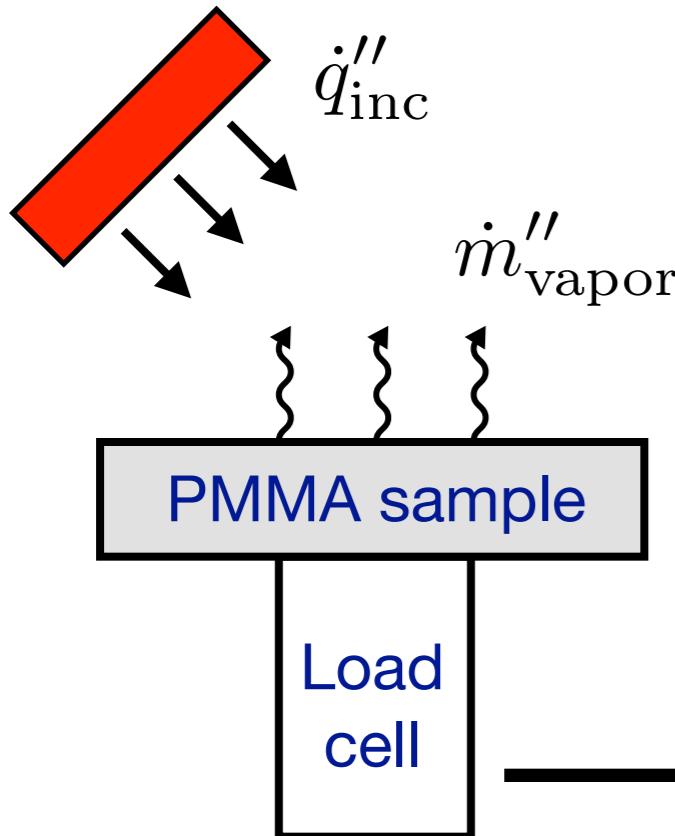
# Example 1 - Estimating Fire Size

Results of point source radiation model at posterior mean value (solid green line) and for all values from the posterior distribution (shaded gray area)



## Example 2 - Material Property Estimation

Transient mass loss rate of sample in the NIST gasification apparatus: 8.5 mm thick PMMA sample; incident heat flux was 52 kW/m<sup>2</sup>; 1 cm layer of insulation under the PMMA sample.



## Example 2 - Material Property Estimation

To predict the mass loss rate of the PMMA sample exposed to an external heat flux, FDS was run in “solid-phase only” mode in which no gas-phase combustion occurs.

$$\rho_s c_s \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} k_s \frac{\partial T}{\partial x} + \dot{q}_s''' ; \quad \dot{q}_s''' = \frac{\partial \rho_s}{\partial t} \Delta H_r - \dot{q}_r'''$$

↓                            ↓                                    ↓

Specific Heat      Thermal Conductivity      Heat of reaction

↑                            ↑                                    ↑

Density                      Function of pre-exponential factor, and activation energy      Function of absorption coefficient, emissivity

The pyrolysis model, external heat flux, and 1D heat conduction solver determine the reaction rate of the solid material.

## Example 2 - Material Property Estimation

Material properties for PMMA (from literature) and their associated uncertainty values.

Parameter	Literature Value	Uncertainty (%)	Measurement Technique	Source
Absorption Coefficient	2700 1/m	50	FTIR	[119]
Pre-Exponential Factor	$8.5 \times 10^{12}$ 1/s	50	TGA	[120]
Activation Energy	188 000 kJ/kmol	3	TGA	[120]
Emissivity	0.85	20	IS	[121]
Heat of Reaction	870 kJ/kg	15	DSC	[122]
Thermal Conductivity	0.20 W/m · K	15	TLC	[120]
Density	1100 kg/m <sup>3</sup>	5	Direct	[120]
Specific Heat	2.2 kJ/kg · K	15	DSC	[122]

Model: FDS

Unknown parameters: Eight material properties

Priors: Uniform distribution around literature values

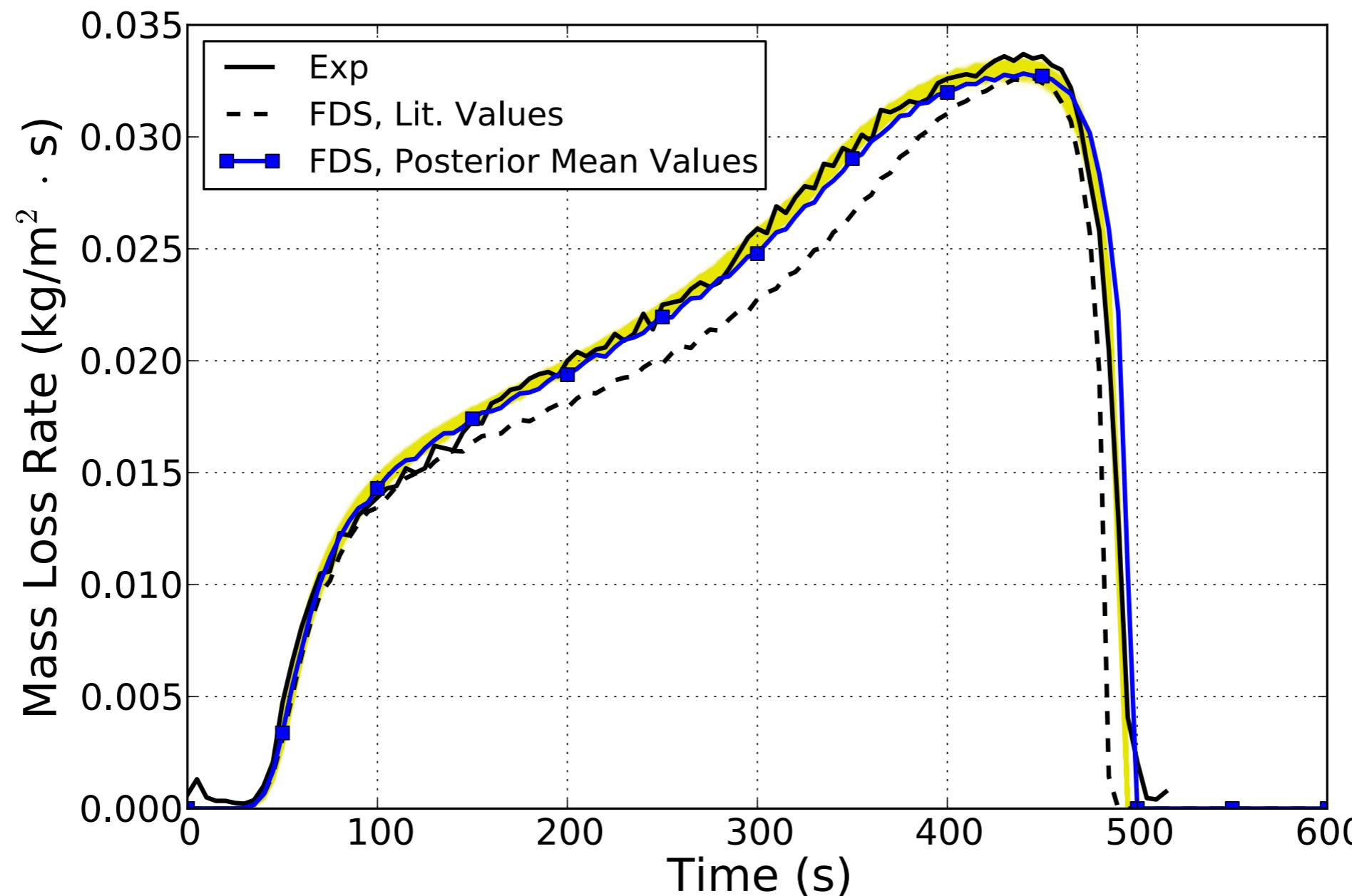
## Example 2 - Material Property Estimation

Resulting posterior mean values for the input parameters compared to literature values

Parameter	Units	Posterior Mean Value	Literature Value	Relative Difference
Heat of Reaction	kJ/kg	958	870	10%
Thermal Conductivity	W/m · K	0.22	0.20	10%
Density	kg/m <sup>3</sup>	1208	1100	9.8%
Specific Heat	kJ/kg · K	2.0	2.2	9.1%

## Example 2 - Material Property Estimation

Results from experiment (black line), literature values (dashed line), posterior mean values (blue line with boxes), and individual realizations over all posterior values (yellow region)



## Example 3 - Inverse Fire Localization

A fire is located in a compartment measuring  $10 \text{ m} \times 10 \text{ m} \times 2.4 \text{ m}$  with an open door measuring  $0.9 \text{ m} \times 2.4 \text{ m}$ . A 300 kW propane fire at  $(x, y) = (2, 2)$  was used in FDS to generate synthetic heat flux data. Six heat flux gauges are located near the fire at a height of 1.2 m.

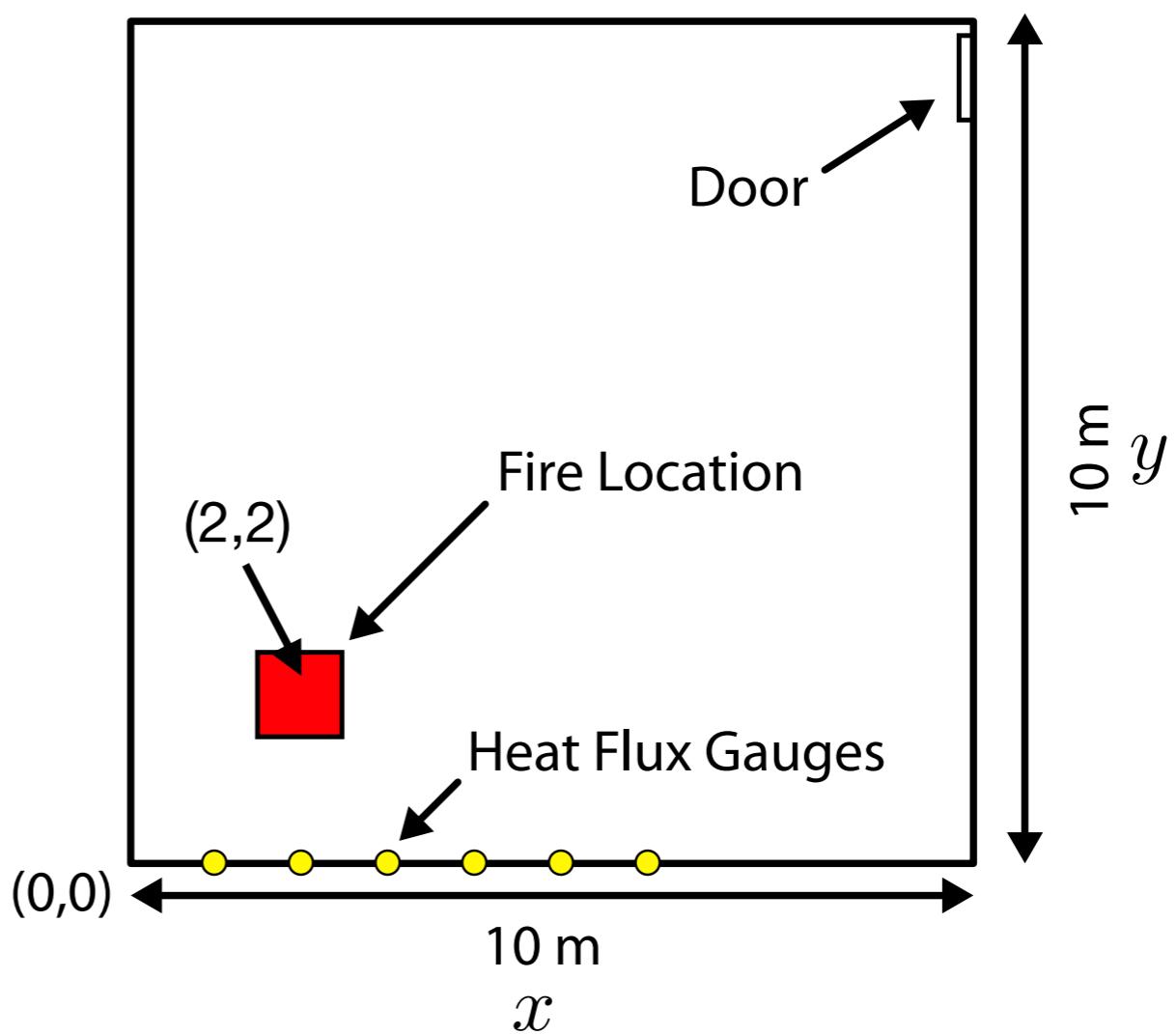
Model: Point source radiation equation

Unknown parameters:  $x, y$

Priors: Uniform distributions

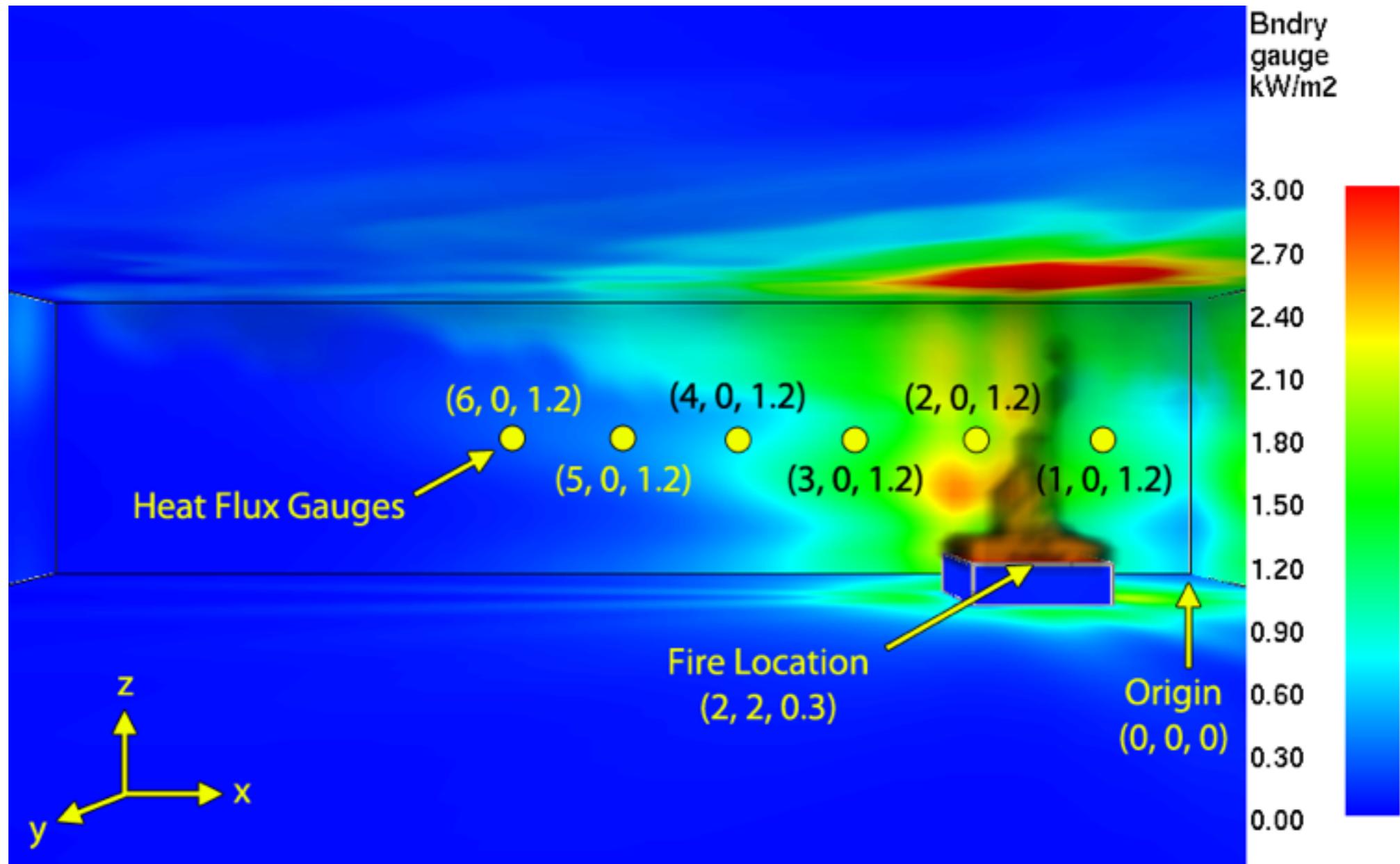
$$0 \text{ m} > x, y > 10 \text{ m}$$

$$x(i=0) = y(i=0) = 5 \text{ m}$$



## Example 3 - Inverse Fire Localization

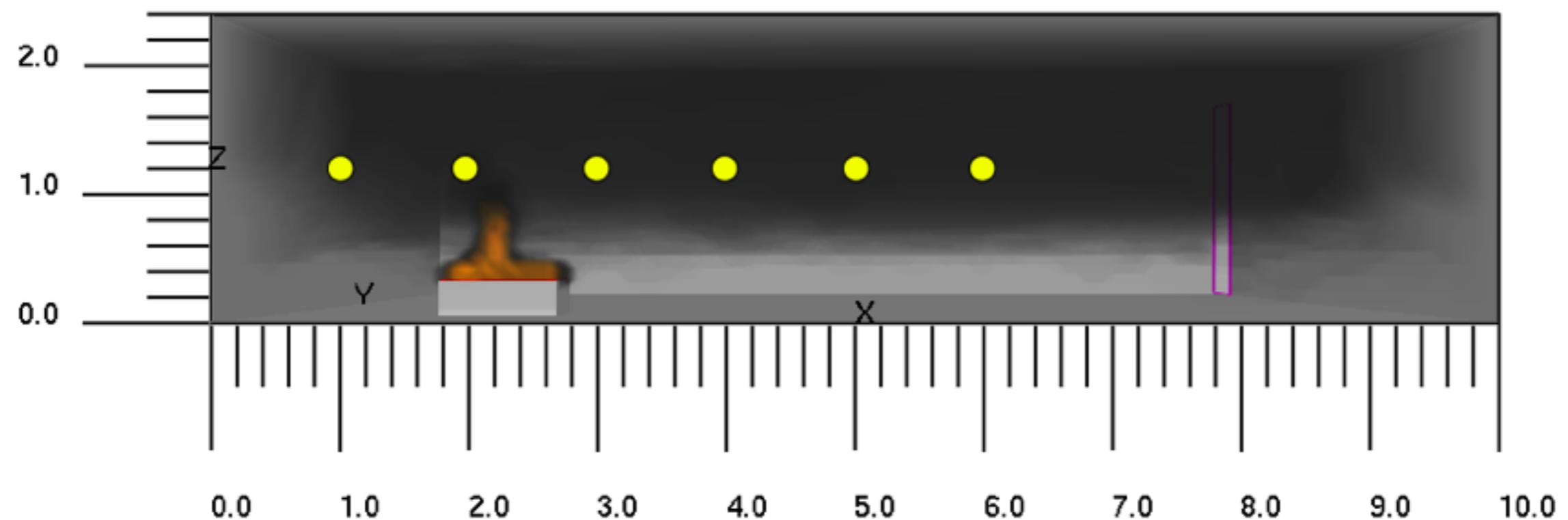
Visualization of gauge heat flux at walls ( $T_w = 20^\circ\text{C}$ ) for 300 kW case



$$\dot{q}_{\text{gauge}}'' = \dot{q}_{\text{r}}''/\varepsilon + \dot{q}_{\text{c}}'' + h(T_w - T_G) + \sigma(T_w^4 - T_G^4)$$

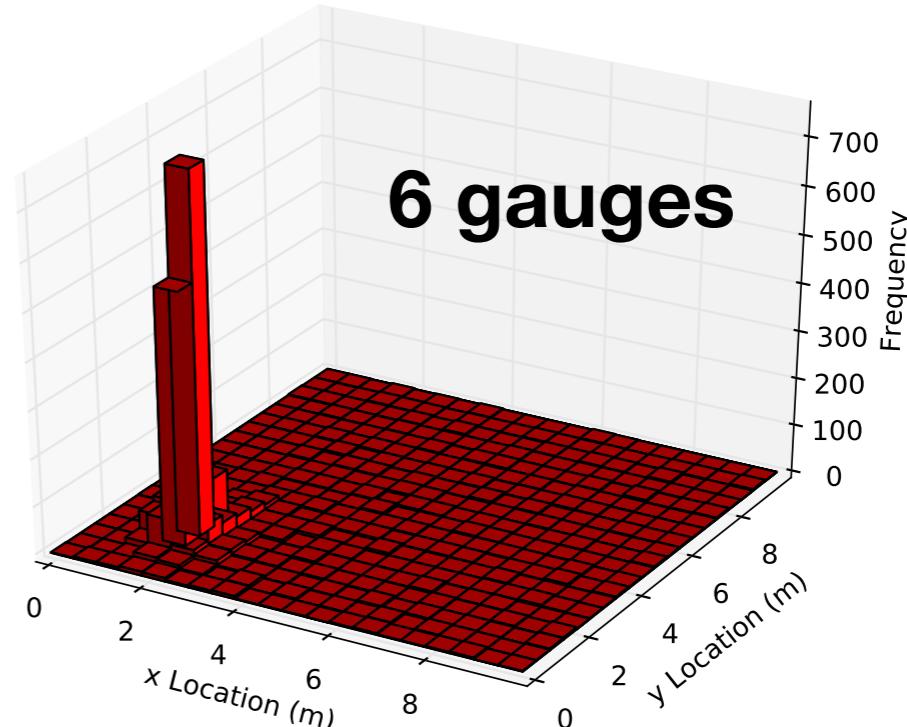
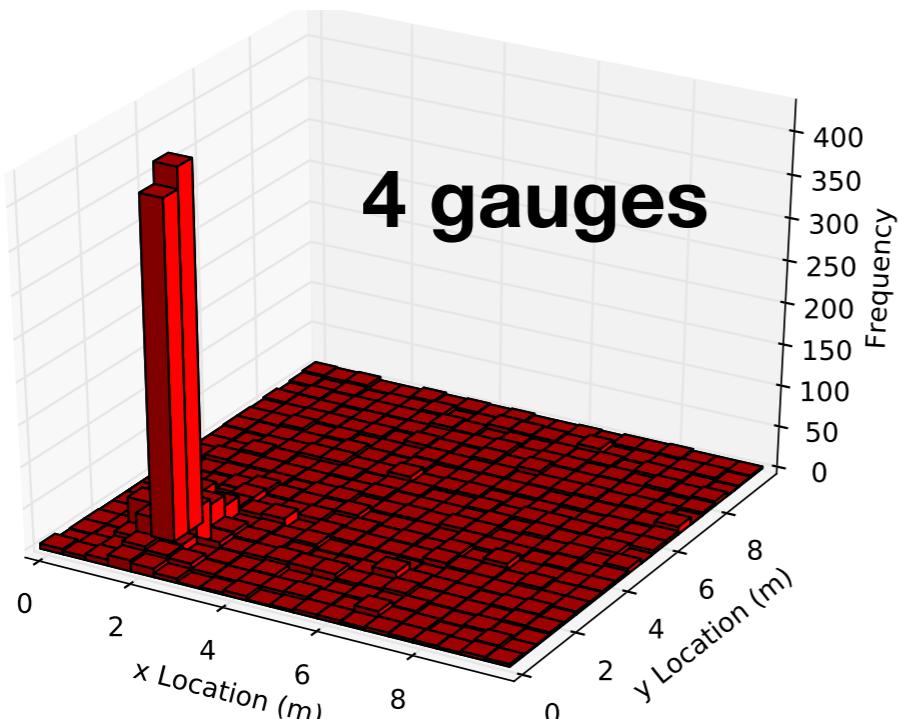
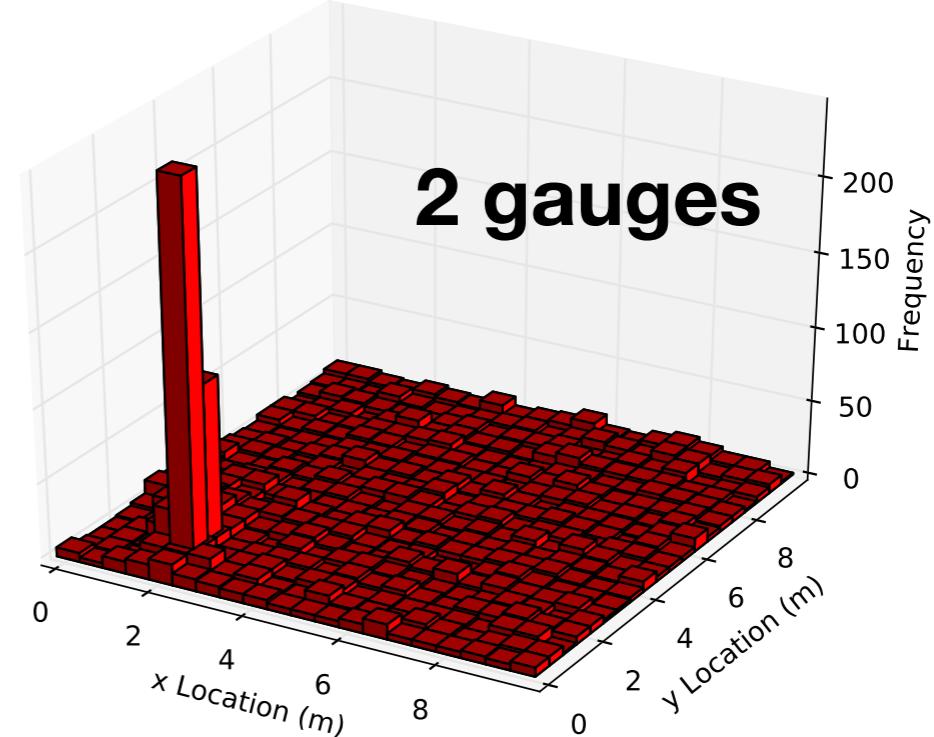
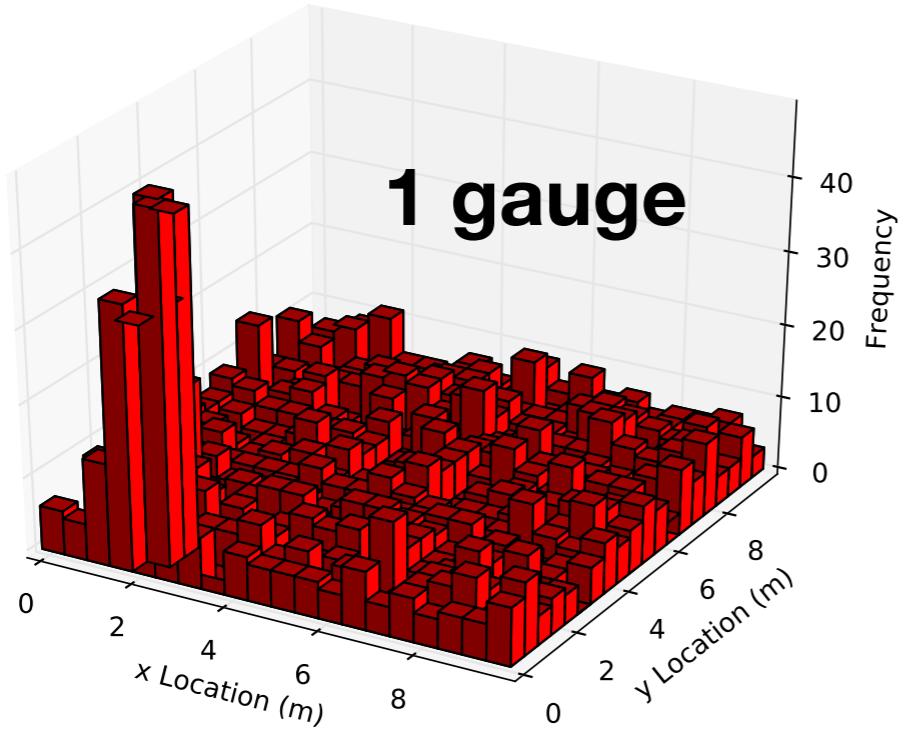
## Example 3 - Inverse Fire Localization

Visualization of fire and smoke layer for 300 kW case at 300 s



# Example 3 - Inverse Fire Localization

300 kW case using gauge heat flux value at 300 s



# Conclusions

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A Bayesian inference framework was applied to various fire scenarios (in both univariate and multivariate cases) to determine fire size, fire location, and material properties. This approach can be used to quantify our degree of certainty (or degree of belief) in input parameters or scenarios.

These inversion techniques have applications towards: model validation exercises, risk analyses, probabilistic risk assessments, fire and arson investigations, and reconstructions of firefighter line-of-duty deaths (LODDs) and injuries.

# Acknowledgements

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Funding for this research was provided by the  
NIST Department of Commerce  
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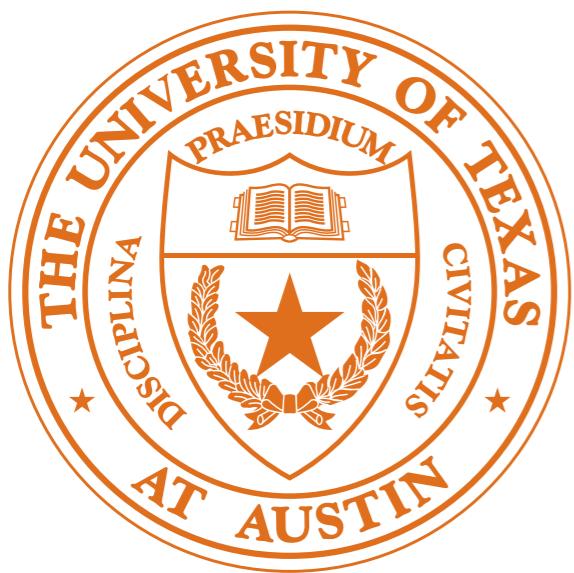
# Questions?

- Questions and discussion

NIST

[koverholt.com](http://koverholt.com)

[code.google.com/p/bayes-fire](http://code.google.com/p/bayes-fire)



Fire Research Group

[utfireresearch.com](http://utfireresearch.com)

# Inverse HRR Methodology

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Previous studies have demonstrated methods for:

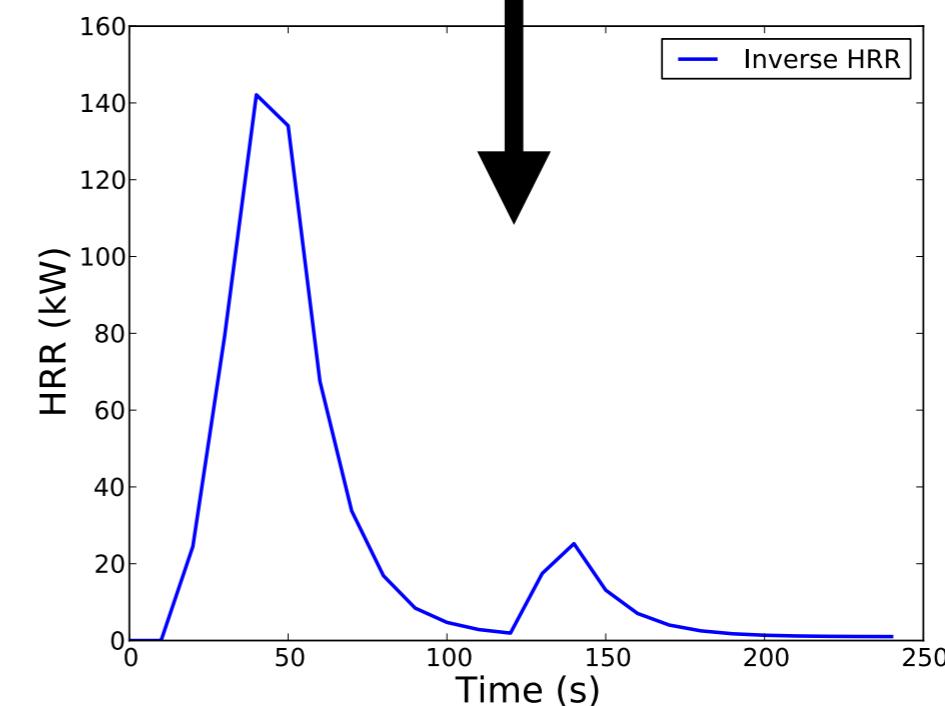
- Forecasting fire size using sensor signals (Jahn et al., 2011; Davis and Forney, 2001; Koo et al., 2010; Richards et al., 1997)
- Running precomputed fire scenarios based on sensors (Cowlard et al., 2010)
- Using a genetic algorithm to search for an inverse HRR solution (Neviackas, 2007; Neviackas and Trouv , 2007; Leblanc and Trouv , 2009)
- A sequential inverse method to determine the size/location of a compartment fire (Lee and Lee, 2005)

This work developed a low-order method for calculating a time-varying HRR solution.

# Inverse HRR Methodology

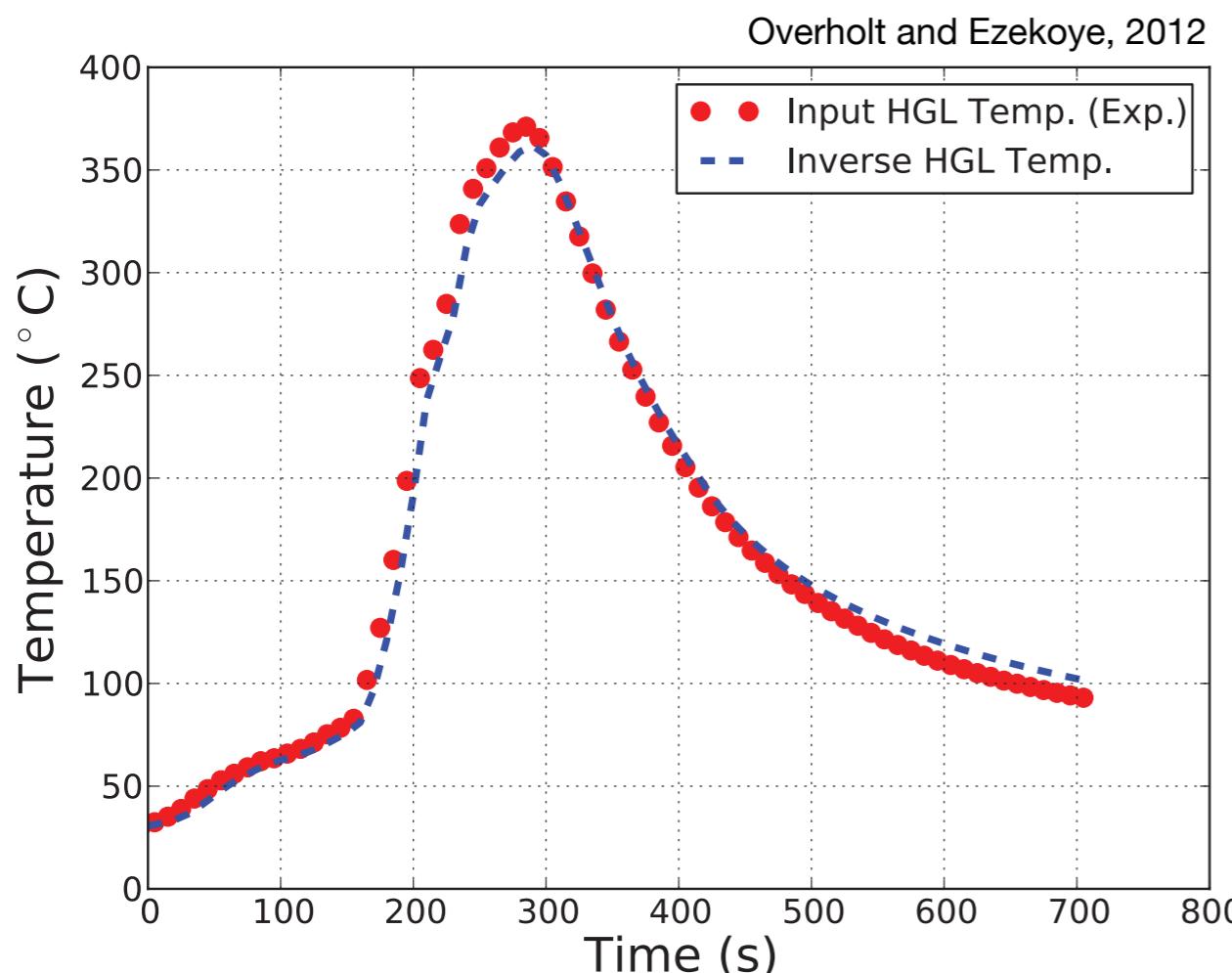
An inverse recovery methodology was developed that uses a fire model to search for a HRR and reconstruct a time-varying inverse HRR solution that uses temperatures as an input.

K.J. Overholt and O.A. Ezekoye,  
“Characterizing Heat Release Rates Using an Inverse Fire Modeling Technique”, Fire Technology, 2012

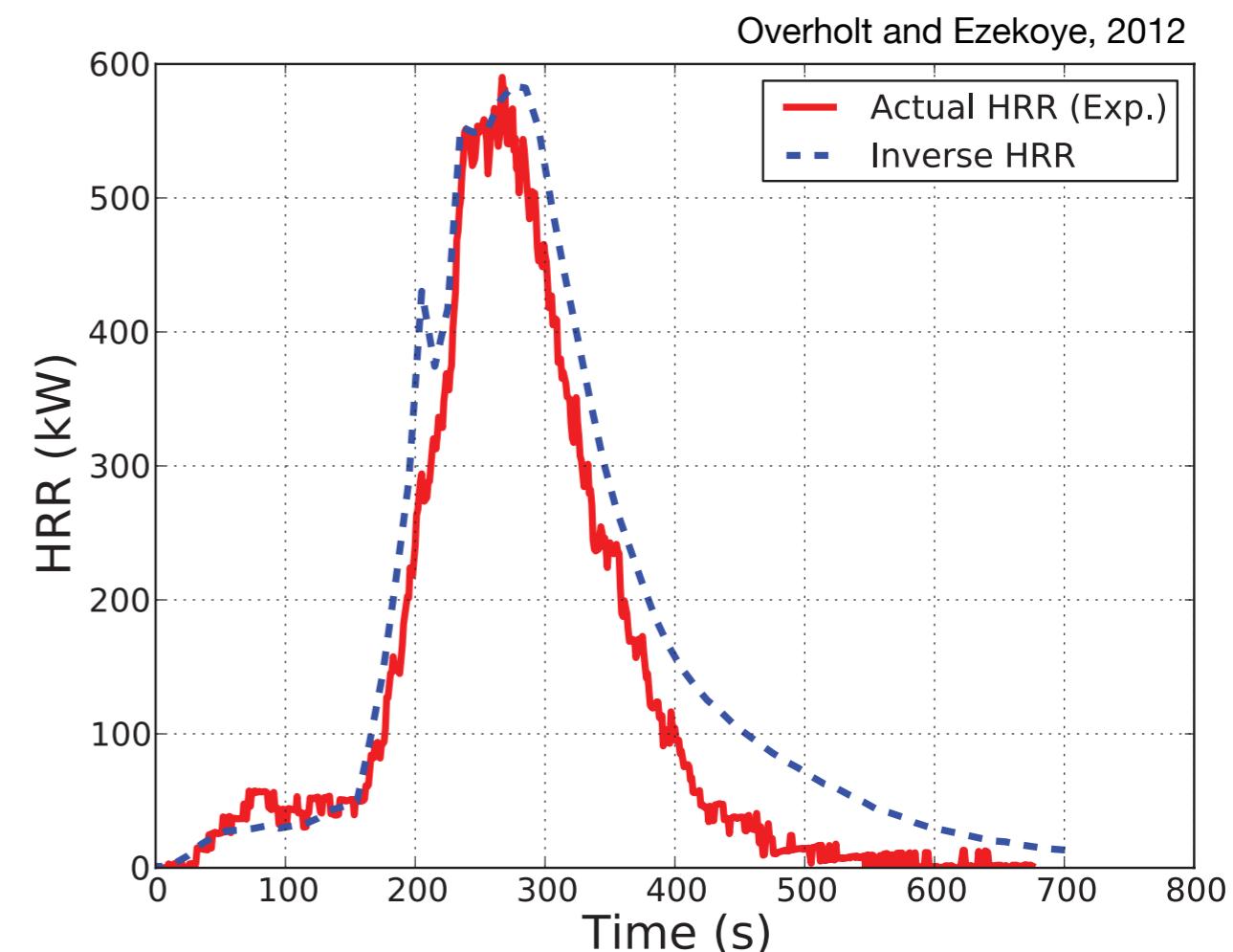


# Inverse HRR Methodology

## Measured and predicted temperatures



## Inverse HRR from three-seat sofa fire test compared to measured HRR



This slide summarizes partial results from SwRI Project No. 15998. This project was supported by Award No. 2010DN-UX-K221, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this study are those of the author and do not necessarily reflect those of the Department of Justice.

# Sampling Methods

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## Sampling Methods for Distributions

- Monte Carlo Methods
  - An approach that uses random sampling techniques to obtain numerical results.
- Latin Hypercube Sampling
  - Similar to Monte Carlo with stratified sampling, which ensures that all areas of the distribution are sampled equally; challenging for high dimensional problems.
- Markov Chain Monte Carlo (MCMC)

# Markov Chain Monte Carlo Procedure

## 1. Initialize parameter

Choose an initial value for  $\theta$  from the prior distribution.

## 2. Propose new value

At time step  $t$ , randomly sample a proposed value  $\theta^*$  from a proposal distribution.

$$q_t(\theta|\theta^*)$$

## 3. Calculate acceptance ratio

$$\alpha(\theta, \theta^*) = \frac{P(\theta^*|D, \mathcal{M})}{P(\theta|D, \mathcal{M})}$$

## 4. Accept or reject

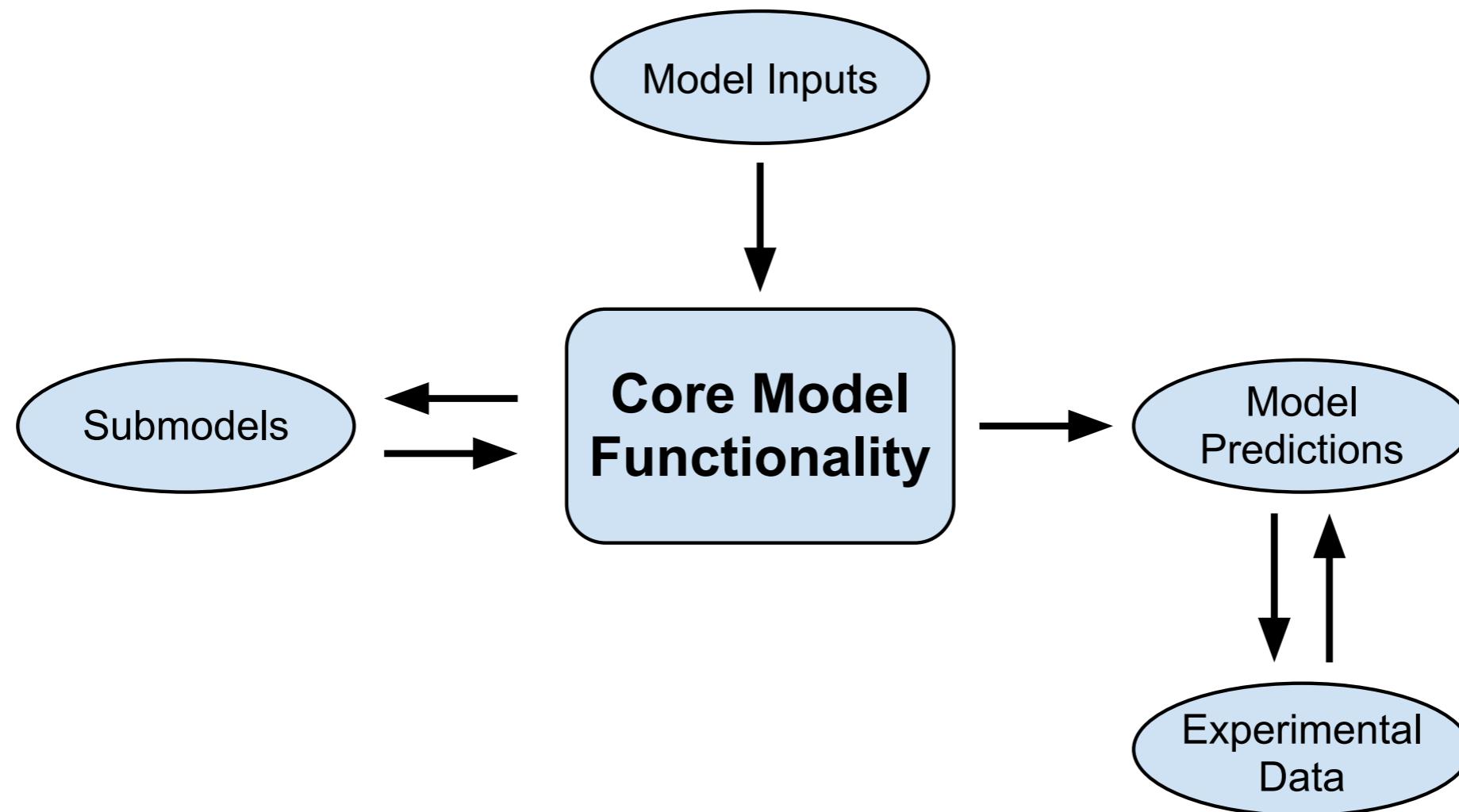
Generate a random value for  $u$  from

$$0 < u < 1$$

$$\theta^{(t+1)} = \begin{cases} \theta^* & \text{if } \alpha(\theta, \theta^*) > u & (\text{accept}) \\ \theta & \text{otherwise} & (\text{reject}) \end{cases}$$

# Introduction

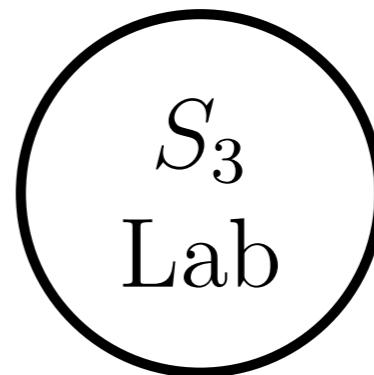
Flowchart of computational model workflow, from model inputs to comparison of model predictions to experimental data.



# Markov Chains

## Introduction to Markov chains

Consider a state space  $\mathbf{S} = [S_1, S_2, S_3]$



Define a random variable  $X(t) = S_i$

An example time history of  $X(t)$ :

$$X(t) = [X(0), X(1), X(2)] = [S_2, S_1, S_3]$$

# Markov Chains

## Introduction to Markov chains

Define a transition matrix  $\mathbf{T}$

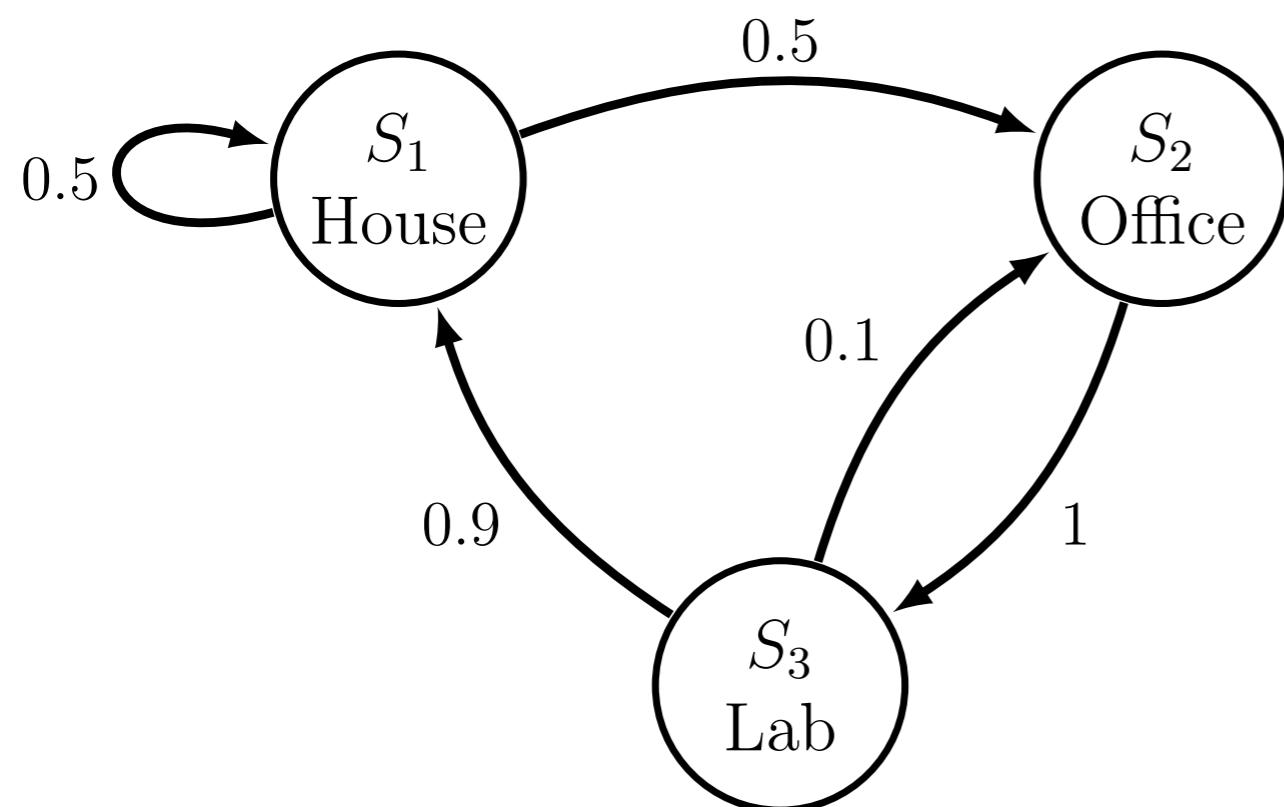
$$\mathbf{T} = \begin{bmatrix} P_{11} & P_{12} & \dots & P_{1k} \\ P_{21} & P_{22} & \dots & P_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ P_{j1} & P_{j2} & \dots & P_{jk} \end{bmatrix}$$

Each entry contains the probabilities of transitioning from one state to another.

# Markov Chains

## Introduction to Markov chains

We can construct a transition matrix  $\mathbf{T}$  from a state transition diagram



$$\mathbf{T} = \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0 & 1 \\ 0.9 & 0.1 & 0 \end{bmatrix}$$

# Markov Chains

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## Introduction to Markov chains

For a stochastic variable  $X(t)$ , the probability of occupying a given state  $S_i$  (i.e., the **occupation probability**) at time step  $t$

$$s_i(t) = P[X(t) = S_i]$$

We can then define a state vector  $\mathbf{s}(t)$  that gives the occupation probability for each state  $S_i$  at time step  $t$

$$\mathbf{s}(t) = [s_1(t), s_2(t), \dots, s_i(t)]$$

An initial state vector  $\mathbf{s}(0)$  defines the occupation probability for each state  $S_i$  at time step 0

$$\mathbf{s}(t) = [s_1(t), s_2(t), \dots, s_i(t)]$$

# Markov Chains

## Simulating a Markov Process

Choose an arbitrary initial state vector:  $s(0) = [0.2, 0.7, 0.1]$

To calculate the occupation probability distribution at the next time step  $t + 1$ , a state vector can be multiplied by a transition probability matrix as  $s(t + 1) = s(t)\mathbf{T}$ .

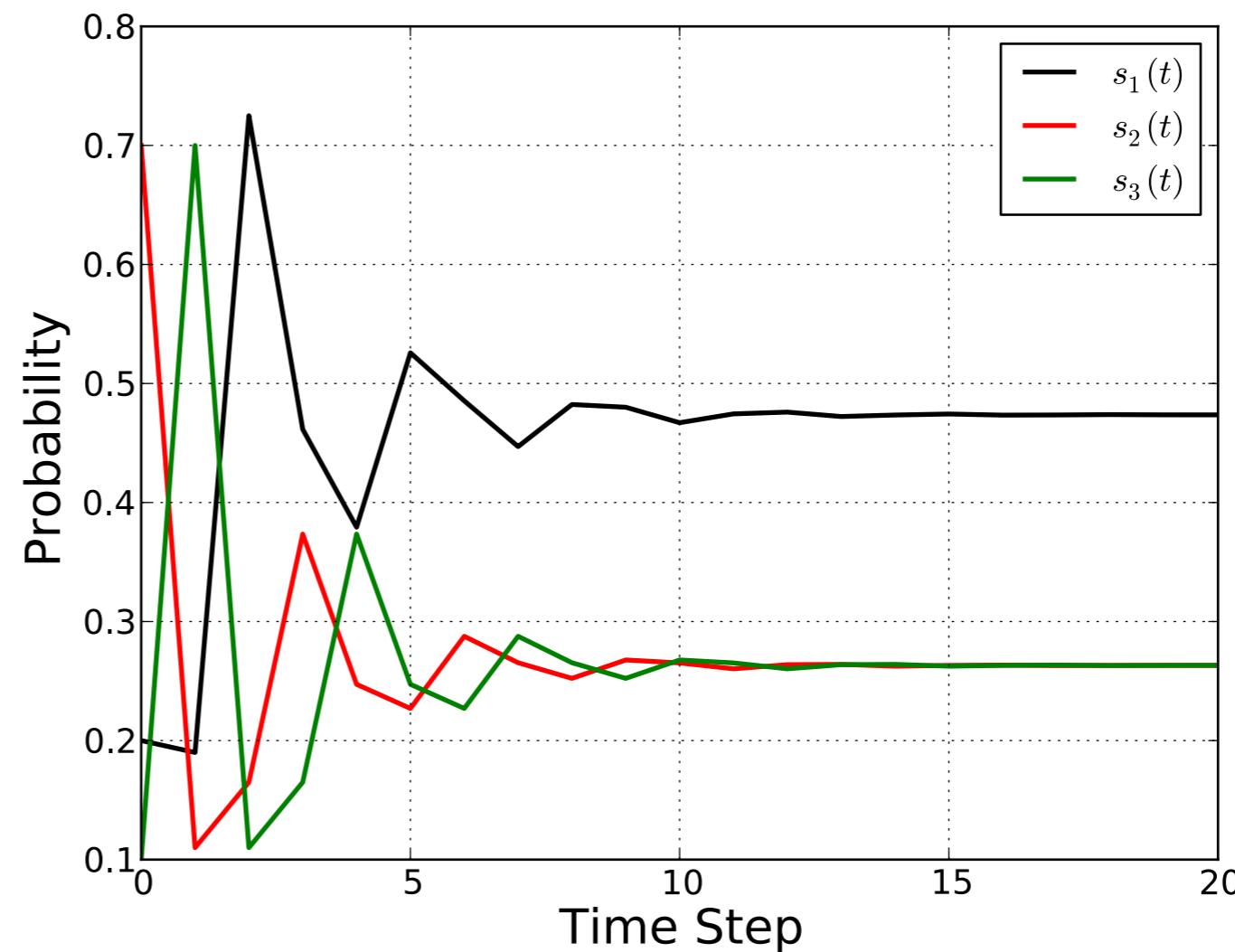
$s(0)$	$\approx$	$[0.200, 0.700, 0.100]$	$\vdots$	
$s(1)$	$\approx$	$[0.190, 0.110, 0.700]$		$s(48) \approx [0.474, 0.263, 0.263]$
$s(2)$	$\approx$	$[0.725, 0.165, 0.110]$		$s(49) \approx [0.474, 0.263, 0.263]$
$s(3)$	$\approx$	$[0.462, 0.374, 0.165]$		$s(50) \approx [0.474, 0.263, 0.263]$

# Markov Chains

## Simulating a Markov Process

At long times, the distribution becomes time-invariant, and is called the **stationary distribution**  $\mathbf{s}|_{t \rightarrow \infty} \approx [0.474, 0.263, 0.263]$

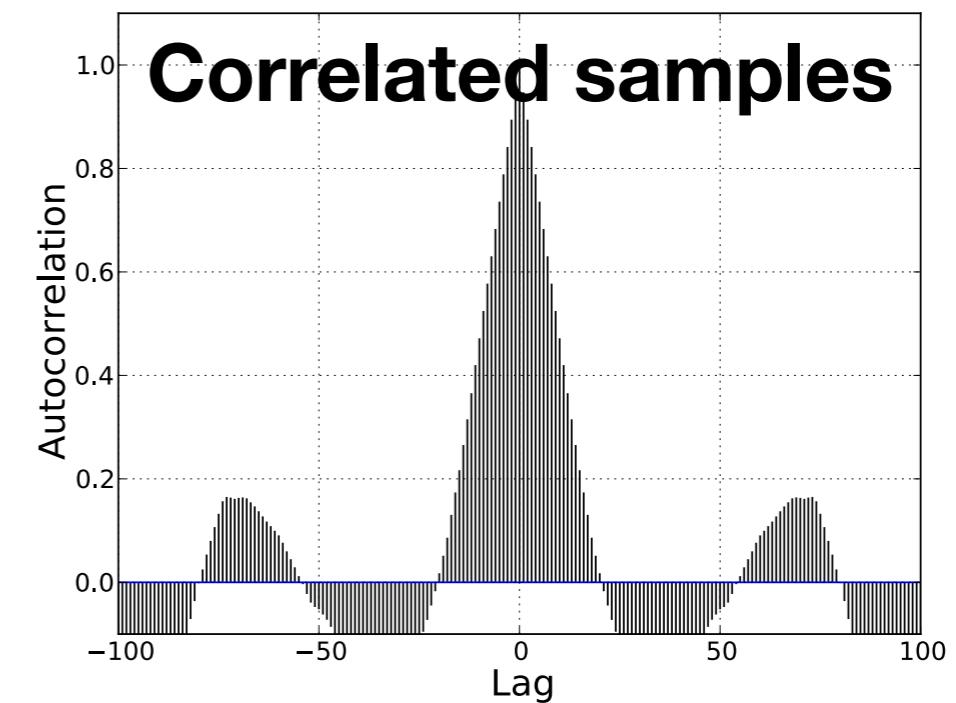
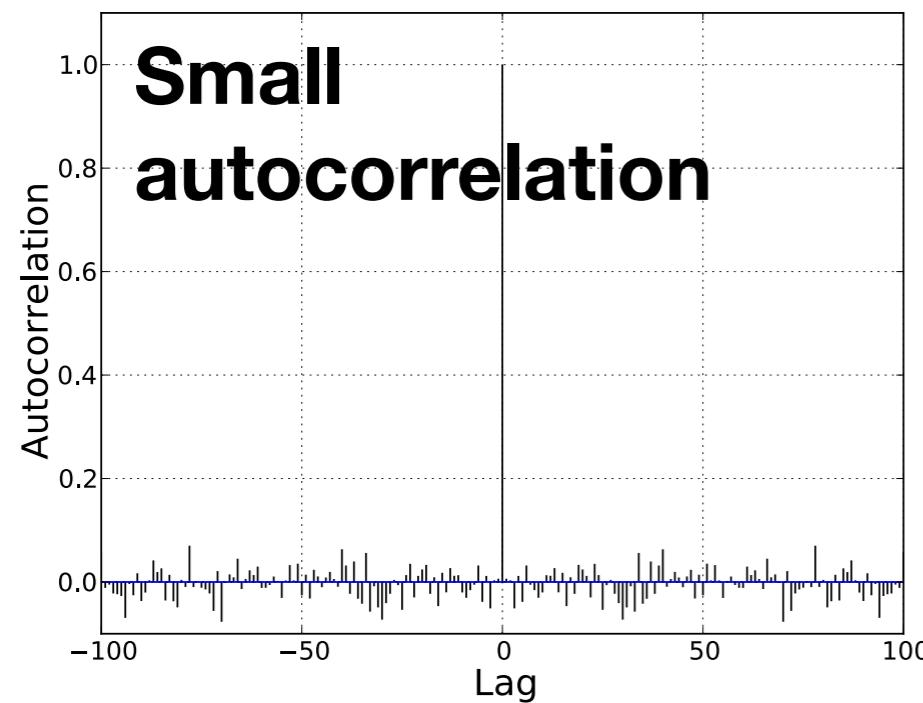
A **parameter trace** shows a history of the occupation probability for each state over the time steps (i.e., the Markov chain).



# Markov Chain Monte Carlo

## Correlation between samples

Autocorrelation indicates poor mixing of the region of high probability, which means that the posterior distribution might not be representative of the true posterior distribution.



## Example 2 - Material Property Estimation

Resulting posterior mean values for the input parameters compared to literature values

Parameter	Units	Posterior Mean Value	Literature Value	Relative Difference
Absorption Coefficient	1/m	1924	2700	29%
Pre-Exponential Factor	1/s	$8.5 \times 10^{12}$	$8.5 \times 10^{12}$	0.0%
Activation Energy	kJ/kmol	188 369	188 000	0.2%
Emissivity	(-)	0.91	0.85	7.1%

# Example - Estimating Steady-State HRR

Layout of Steckler fire testing enclosure; 63 kW methane fire

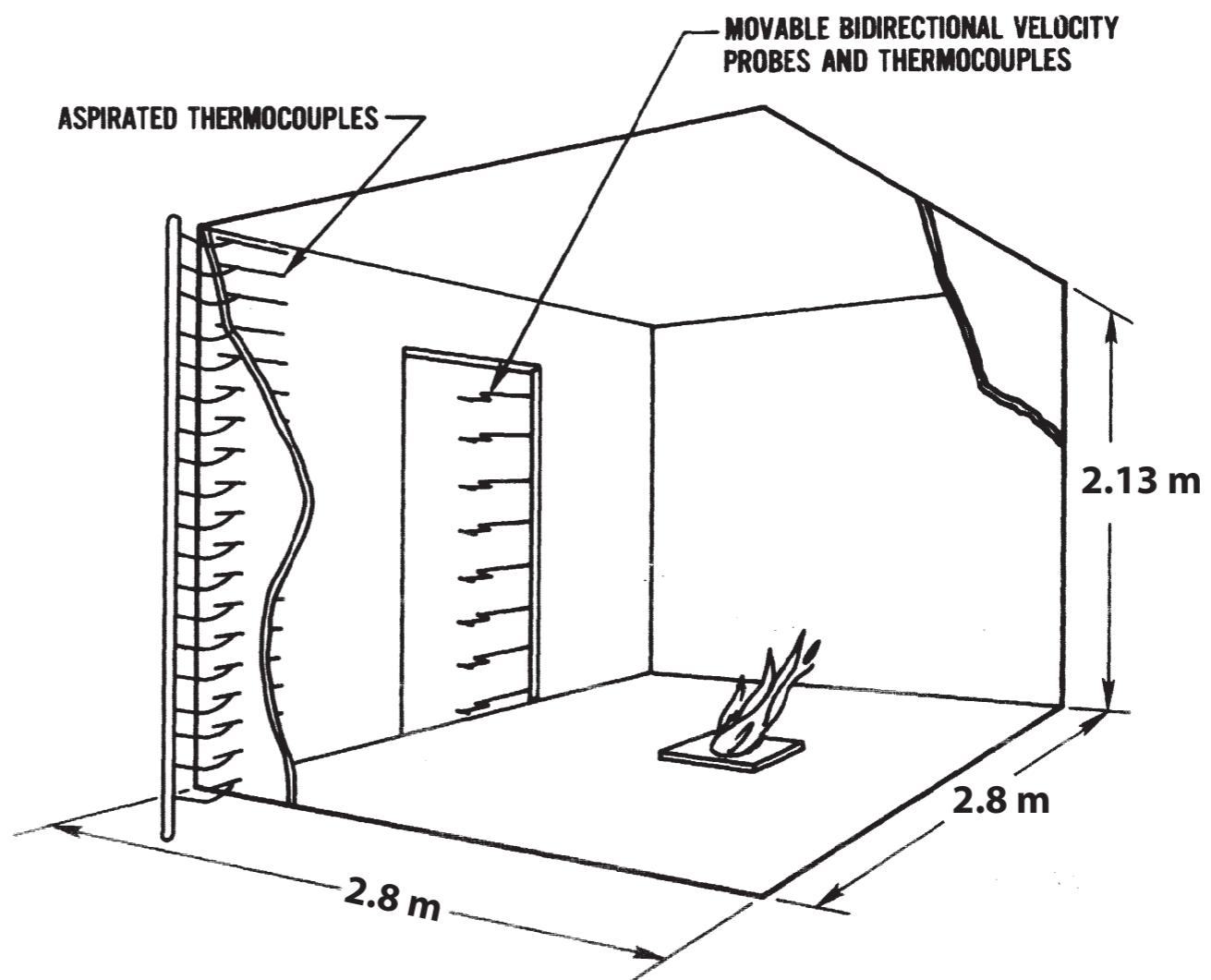
Model: CFAST

Unknown parameter:  $\dot{Q}$

Prior: Uniform distribution

$$1 \text{ kW} > \dot{Q} > 100 \text{ kW}$$

$$\dot{Q}(i = 0) = 50 \text{ kW}$$



K. Steckler, J. Quintiere, and W. Rinkinen, "Flow Induced By Fire in A Compartment," NBSIR 82-2520, National Bureau of Standards, Gaithersburg, Maryland, September 1982.

# Example - Estimating Steady-State HRR

Summary of experimental parameters and measured HGL temperature data for Steckler compartment fire tests

Opening Configuration	Door Width (m)	Door Height (m)	$\dot{Q}_{\text{exp}}$ (kW)	$T_{\text{HGL}}$ (°C)	$T_{\infty}$ (°C)
2/6 Door	0.24	1.83	62.9	190	26
3/6 Door	0.36	1.83	62.9	164	28
4/6 Door	0.49	1.83	62.9	141	22
4/6 Door	0.49	1.83	62.9	135	13
5/6 Door	0.62	1.83	62.9	129	23
6/6 Door	0.74	1.83	62.9	129	29
6/6 Door	0.74	1.83	62.9	130	31
6/6 Door	0.74	1.83	62.9	109	12
6/6 Door	0.74	1.83	62.9	116	13
7/6 Door	0.86	1.83	62.9	120	26
8/6 Door	0.99	1.83	62.9	109	22

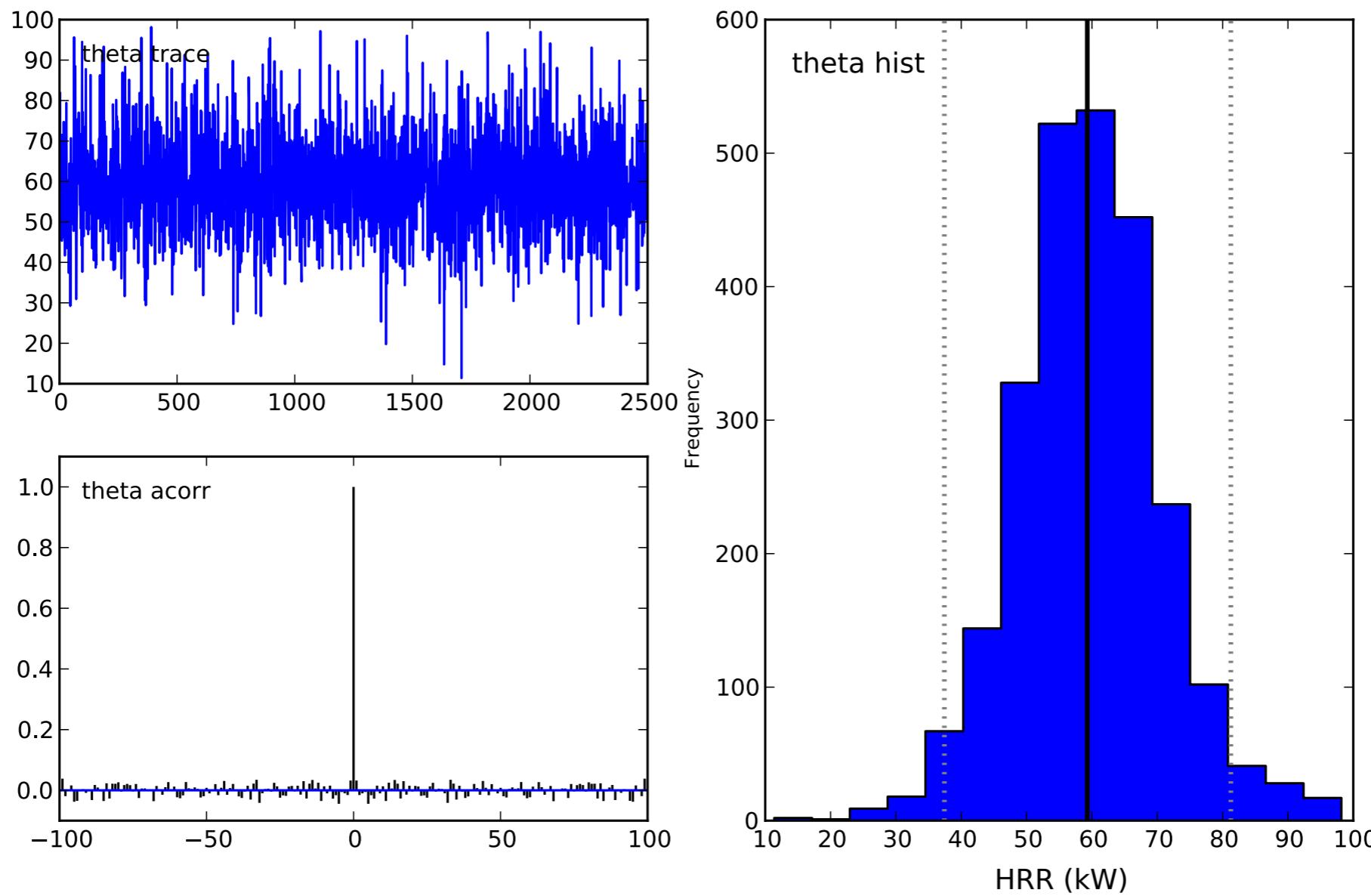
Observed data

50

# Example - Estimating Steady-State HRR

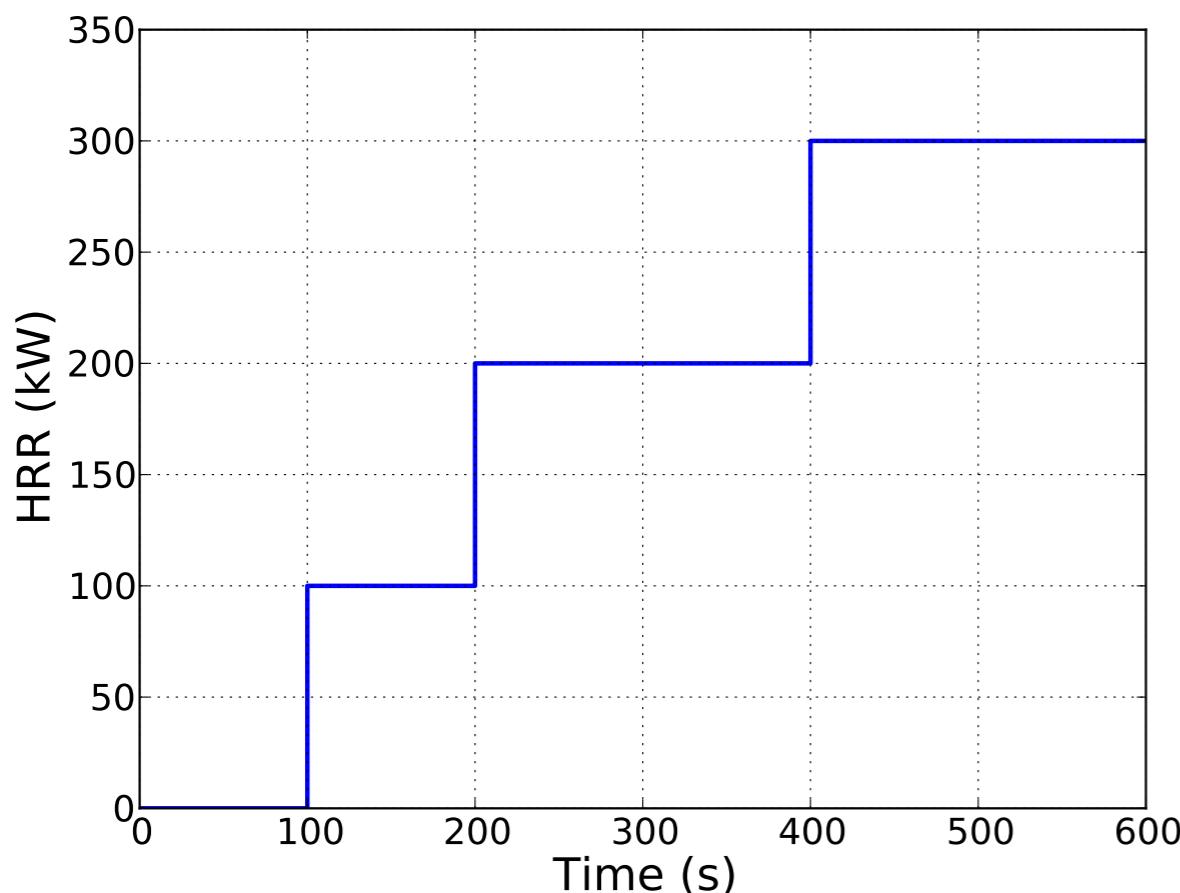
PyMC results for HRR parameter  $\dot{Q}$ :

Mean: 59.7 kW; Standard Deviation: 11.1 kW;  
95 % credible interval = [37 kW, 81 kW]

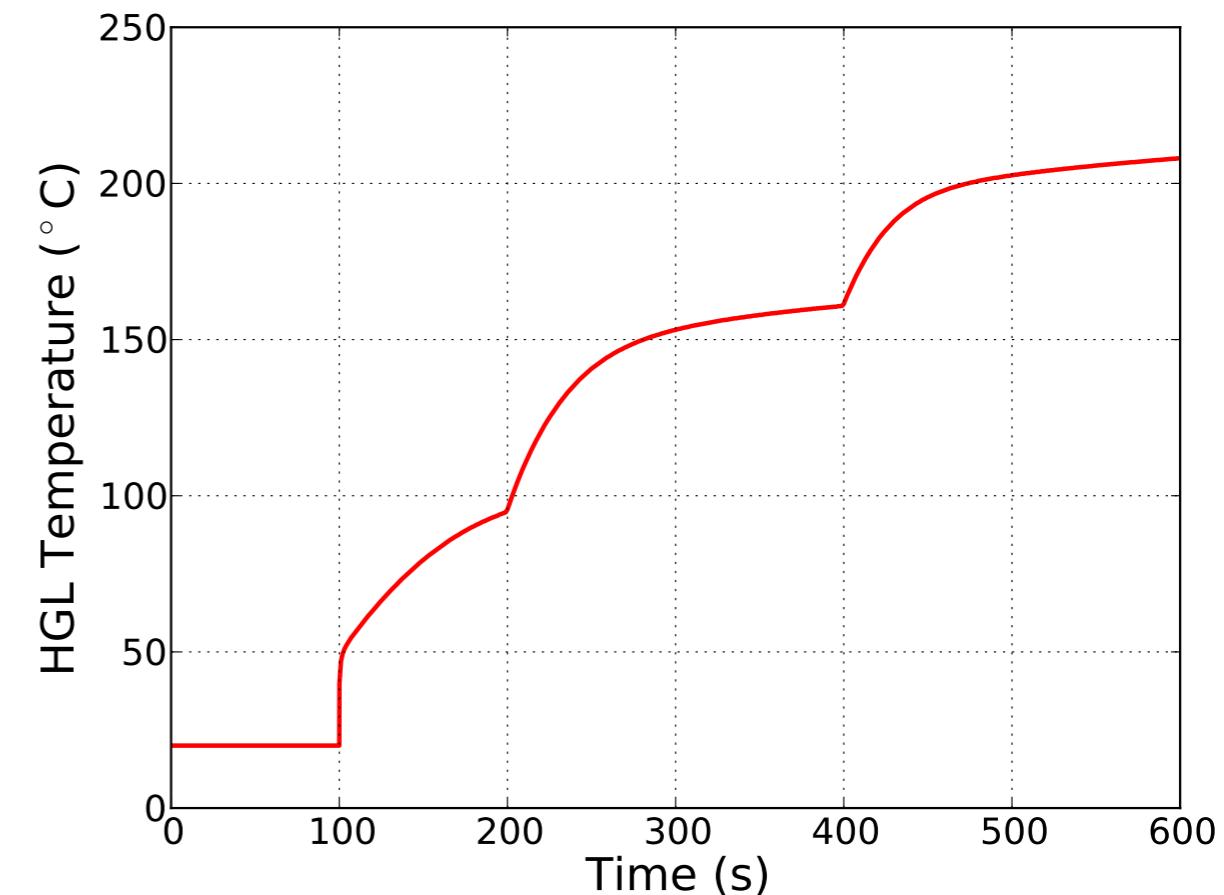


# Example - Estimating Transient HRR

Multiple step function HRR curve



**Input HRR  
(Actual HRR)**



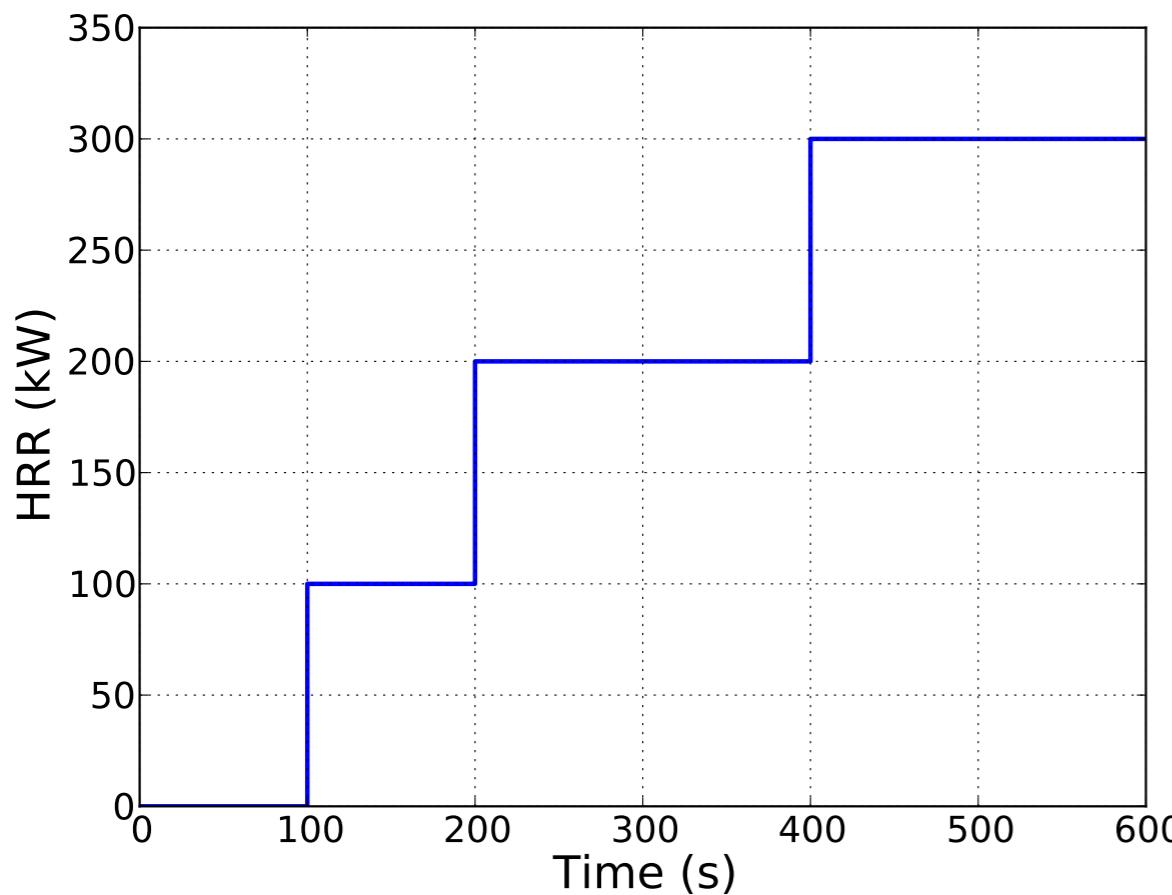
**HGL Temperature  
(Observed Data)**

# Example - Estimating Transient HRR

The transient HRR is parameterized as a piecewise linear function

$$\dot{Q}(t) = \dot{Q}_i \left( \frac{t - t_{i+1}}{t_i - t_{i+1}} \right) + \dot{Q}_{i+1} \left( \frac{t - t_i}{t_{i+1} - t_i} \right)$$

↑  
Unknown fire  
size parameters



Model: CFAST

61 unknown parameters:  $\dot{Q}_i$

Priors: Uniform distribution

$$0 \text{ kW} > \dot{Q}_i > 500 \text{ kW}$$

$$\dot{Q}_i(i=0) = 50 \text{ kW}$$

# Example - Estimating Transient HRR

Results of CFAST model at posterior mean value (dashed blue line) and for all values from the posterior distribution (shaded gray area)

