A Description of a UQ-Predictive Validation Framework for Combustion Applications

$$C_{\mathcal{E}} = max\ \gamma \text{ subject to constraints:}$$

$$\begin{cases} \beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, \ldots, n \\ (1-\gamma)u_e \geq |y_m(\mathbf{x}) - y_e| \geq l_e(1-\gamma), \\ \qquad\qquad\qquad \text{for each } e \in \mathcal{E} \end{cases}$$

THE UNIVERSITY OF UTAH®

ICSE

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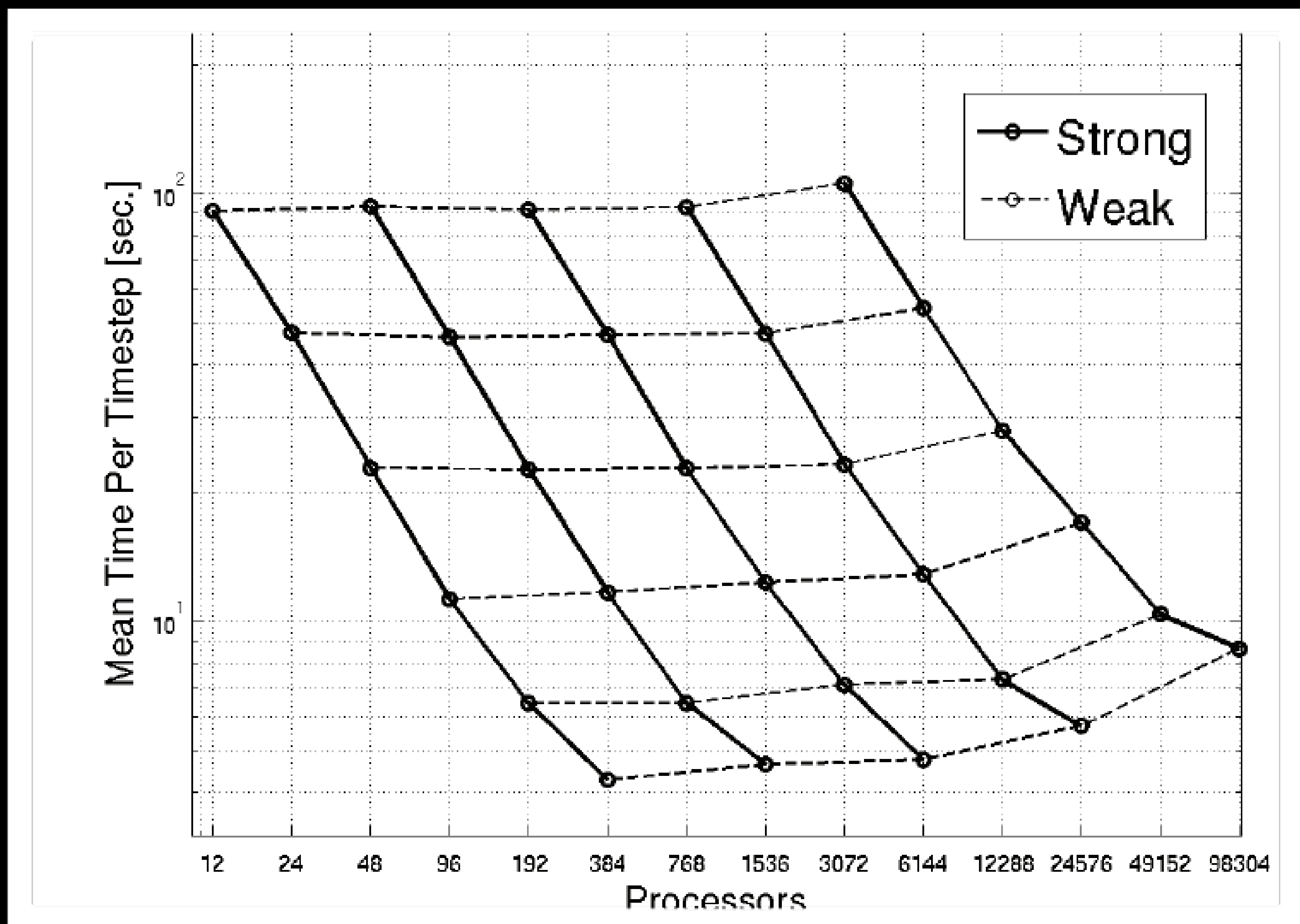
THE INSTITUTE FOR CLEAN AND SECURE ENERGY

collaborators: M.Frenklach, A.Packard - UC Berkeley

expensive data - simulation & experiment

- simulation
  - HPC scaling
  - 1600 cores - 3-5 days



- experiment
  - demonstration scale
  - $1M - 1 year / test

UQ - Predictive Validation (V/UQ)

$$\beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, \ldots, n$$

$$u \geq y_m(\mathbf{x}) \geq l,$$

Bayesian probability:

- *probability as "a measure of a state of knowledge"*
- *enables reasoning with uncertain statements*
- *specifies some prior probability which is updated in light of new data*

UQ - Predictive Validation (V/UQ)

"theories are instruments of prediction. From one set of observable data, theories form a bridge over which the investigator can pass to another set of observable data." (Ernst Mach)

what does new data infer about model predictivity?

- **Validation:** $$u \geq [y_m(\mathbf{x}) - y_e] \geq l$$

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- **Validation:** $u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$
- **Prediction:** $u \geq [y_m(\mathbf{x}) - y_e] \geq l$

?

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- **Validation:** $u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$
- **Prediction:** $u' \geq y'_m(\mathbf{x}) \geq l',$

?

Predictivity = Validation = Uncertainty Quantification = Error Budget

1. *"All scientifically relevant data have an uncertainty."*
2. *"Data without uncertainty cannot be relevant scientifically"*

Manfred Drosg

$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$$

- **Experimental Uncertainty (y_e +/- u_e)**
- **Verification Error - Numerics (y_v or x_v +/- u_v)**
- **Model Form / Model Parameters (x_m +/- u_m)**
- **Scenario Parameters (x_s +/- u_s)**

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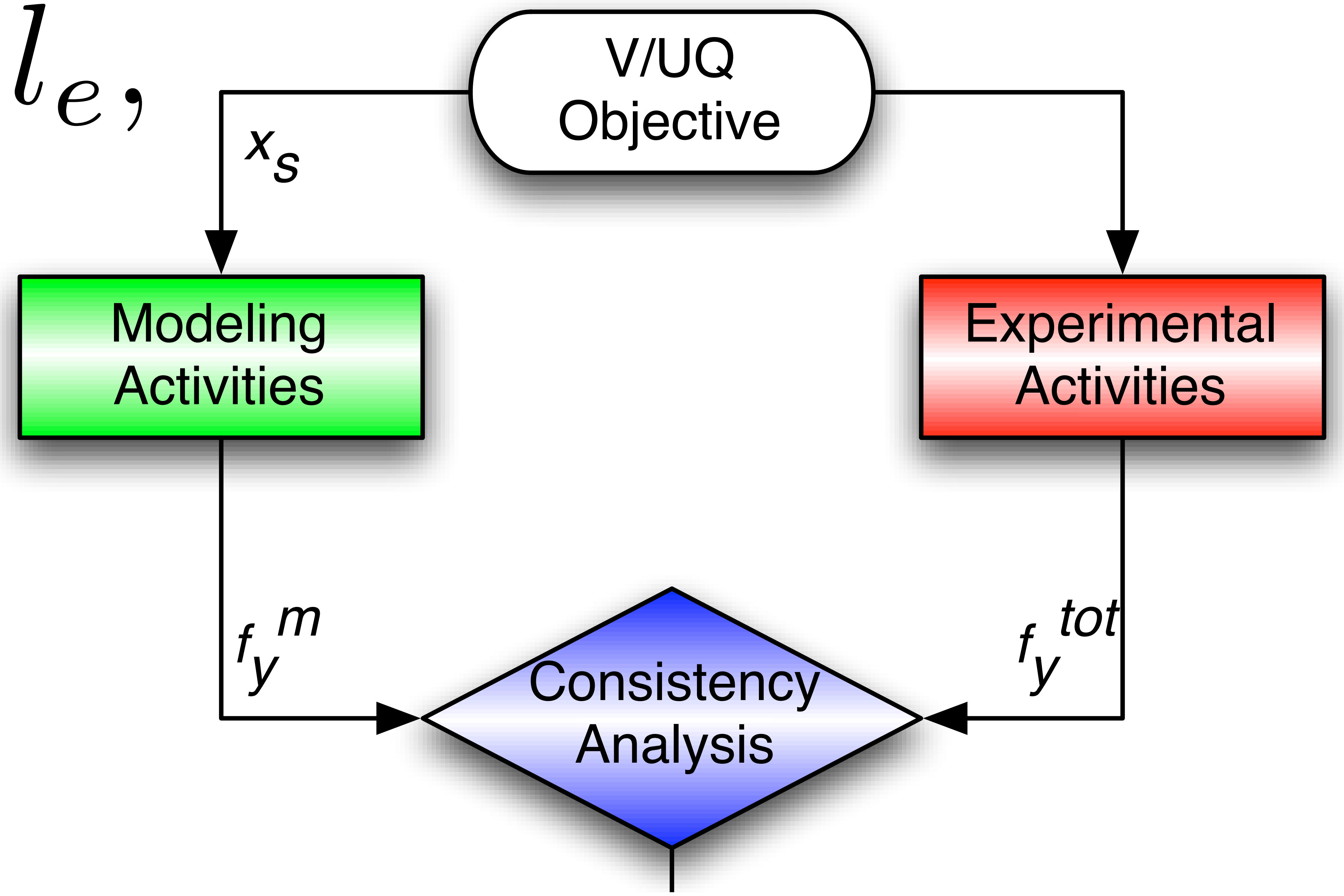

– Ryan Feeley, Pete Seiler, Andrew Packard, and Michael Frenklach, J. Phys. Chem. A 2004, 108, 9573-9583

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A Framework for Validation of Computer Models

M. J. Bayarri, J. O. Berger, R. Paulo, J. Sacks, J. A. Cafeo, J. Cavendish, C. H. Lin, J. Tu

Technical Report Number 162 April 2005

National Institute of Statistical Sciences 19 T. W. Alexander Drive
PO Box 14006 Research Triangle Park, NC 27709-4006

- **create I/U map**
- **define intended use**
- **develop DoE**
- **create surrogate model**
- **perform consistency analysis**
- **iterate & predict**

$C_{\mathcal{E}} = max\ \gamma$ subject to constraints:

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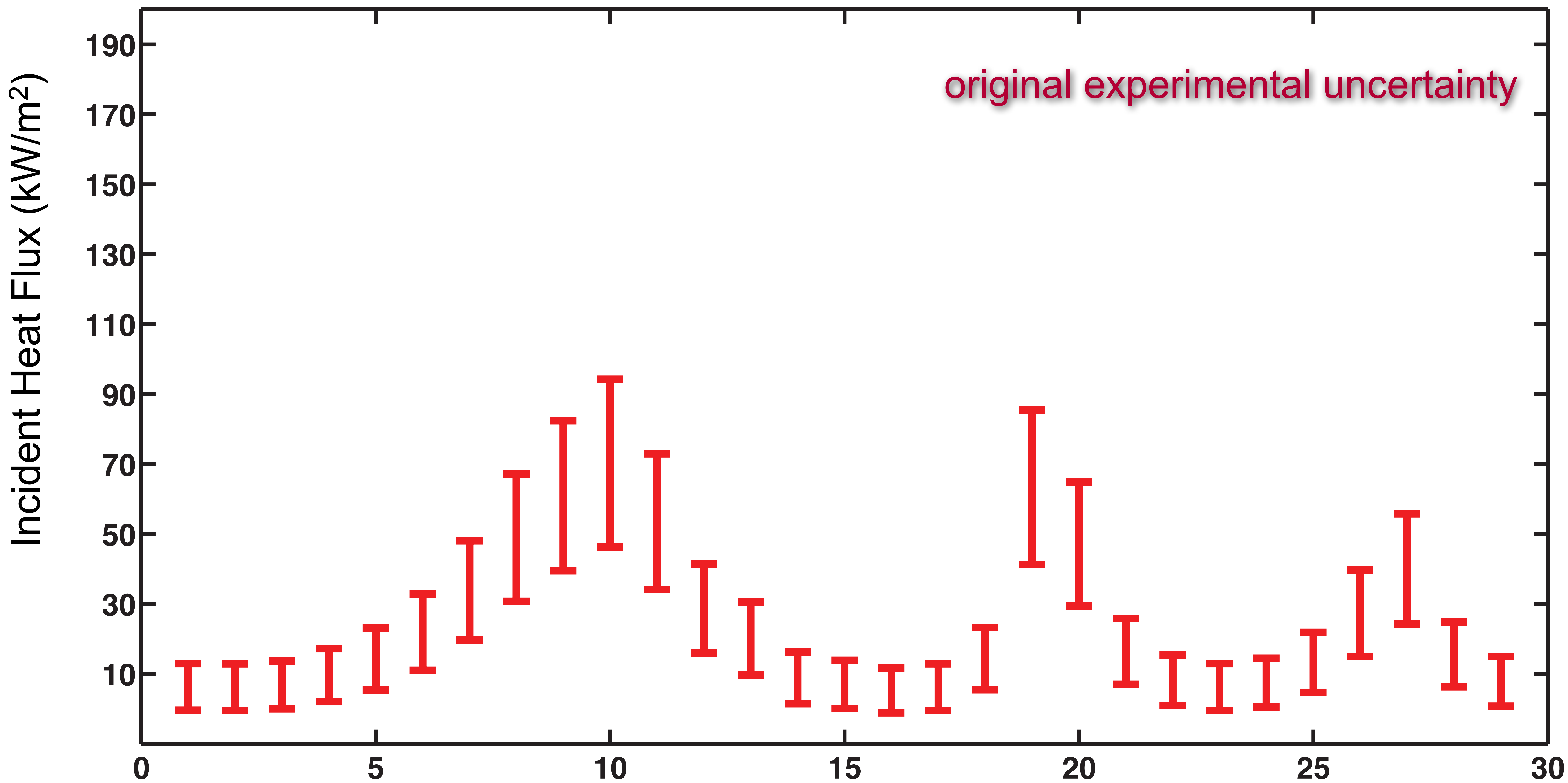
$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$$

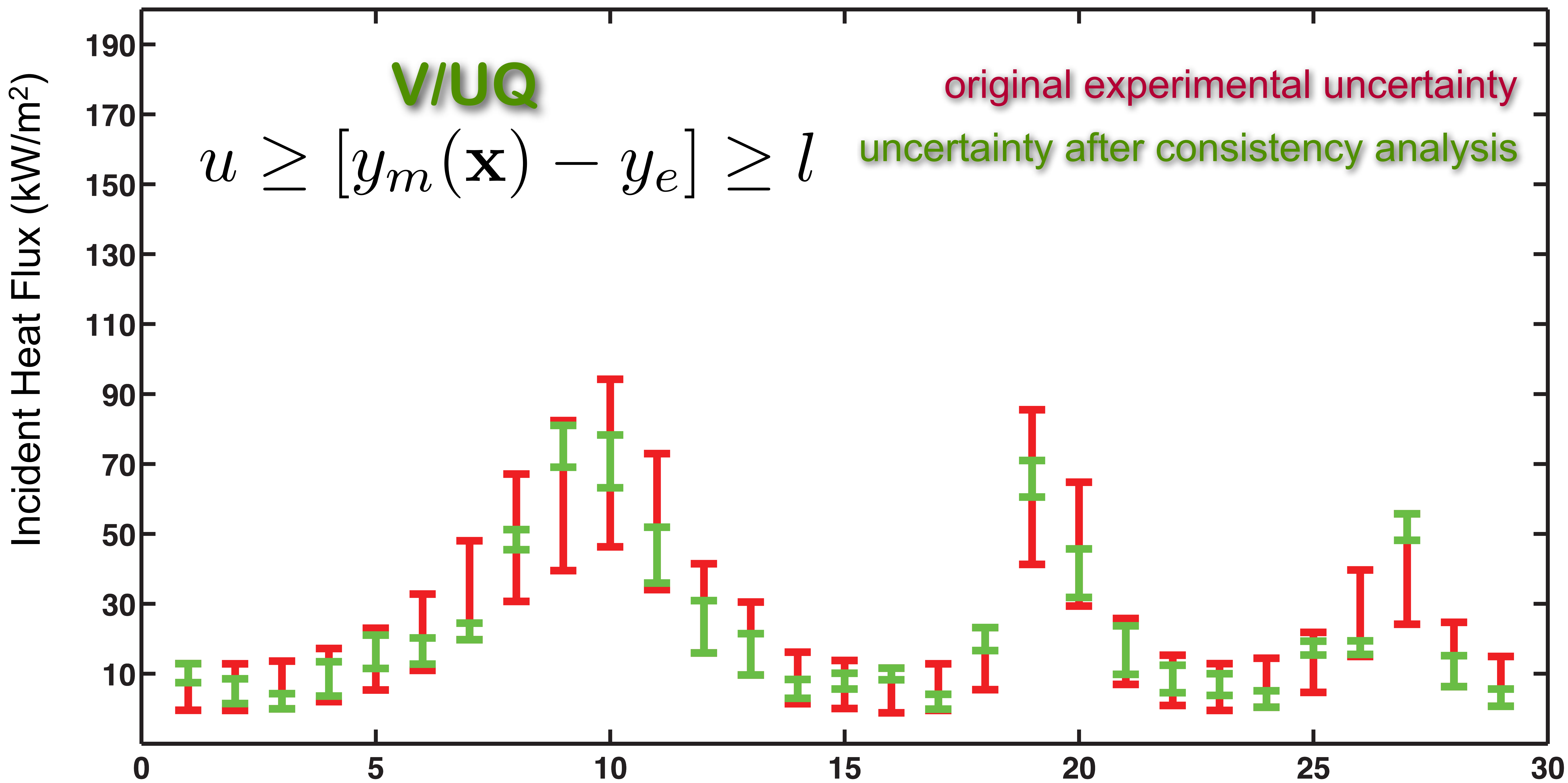
- **deterministic solution procedure**
- **Bayesian (w uniform distributions)**
- **Inferential (priors to posteriors)**
- **hierarchical**
- **iterative**
- **predictive**

$$C_{\mathcal{E}} = max\ \gamma \text{ subject to constraints:}$$
$$\begin{cases} \beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, ..., n \\ (1-\gamma)u_e \geq |y_m(\mathbf{x}) - y_e| \geq l_e(1-\gamma), \\ \qquad\qquad \text{for each } e \in \mathcal{E} \end{cases}$$

V/UQ: heat flux from large pool fires



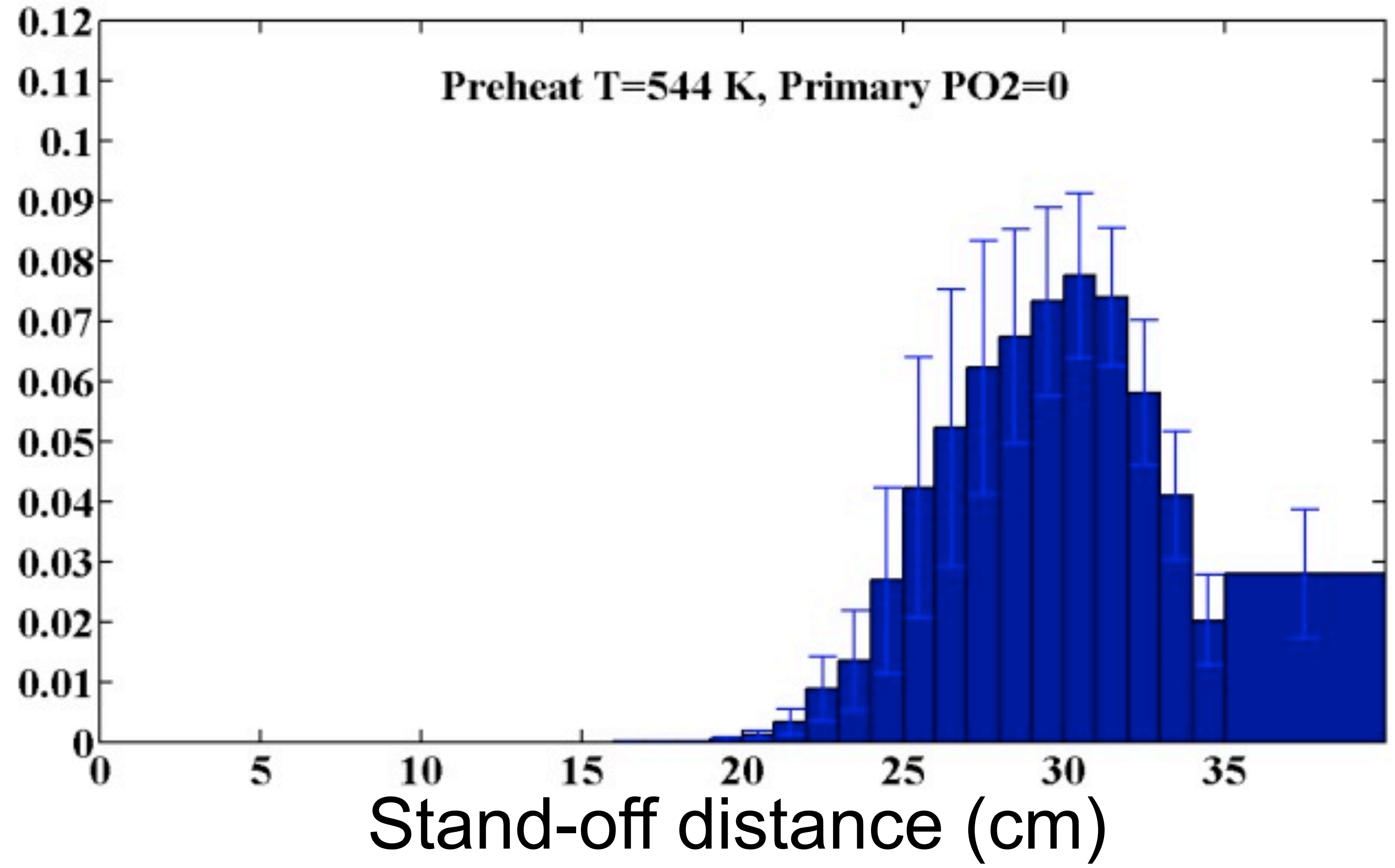
V/UQ: heat flux from large pool fires

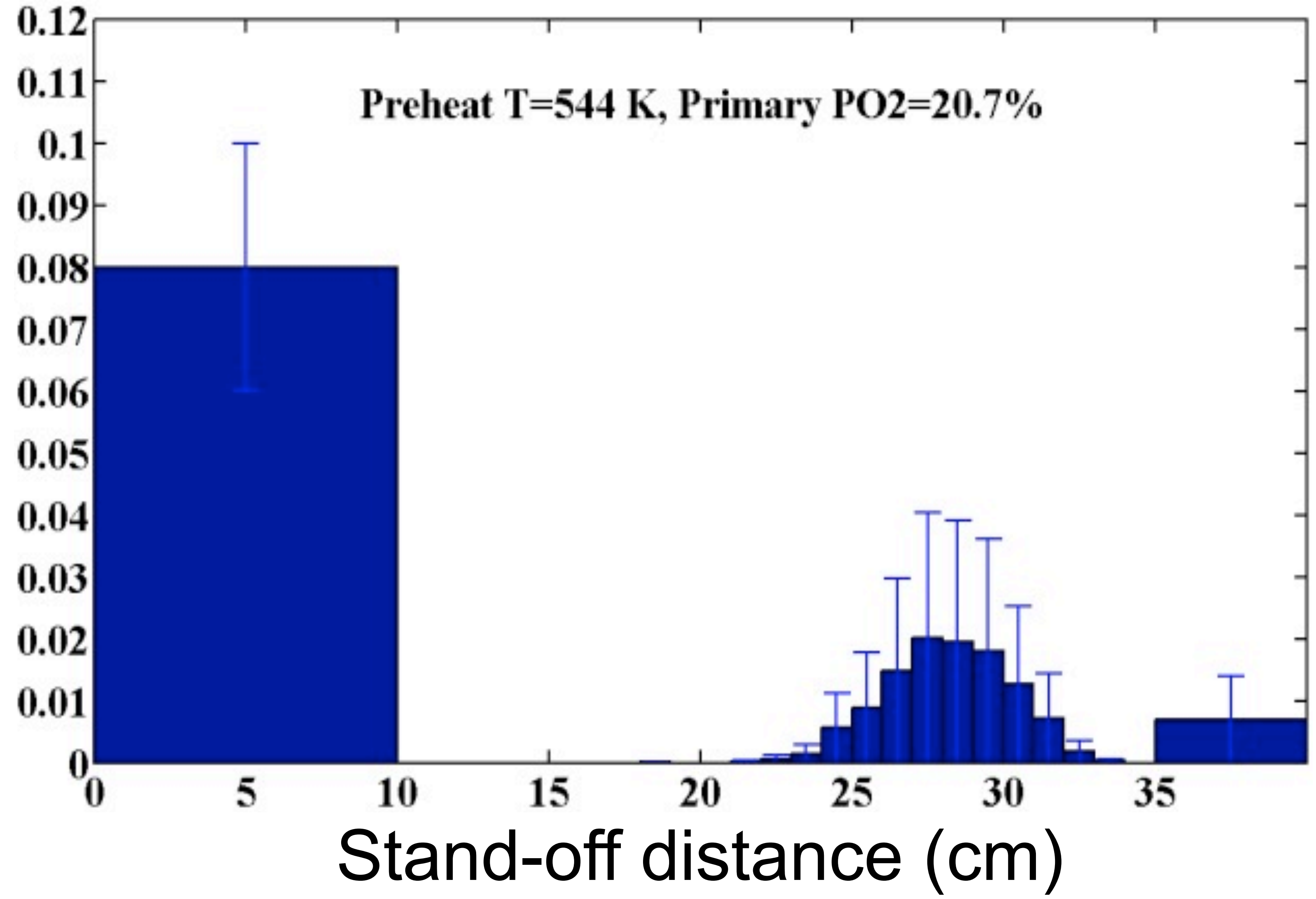


oxy-coal: effect of primary $[O_2]$ on burner stability

$P_{O2(primary)}$ = 0%

$P_{O2(primary)}$ = 21%

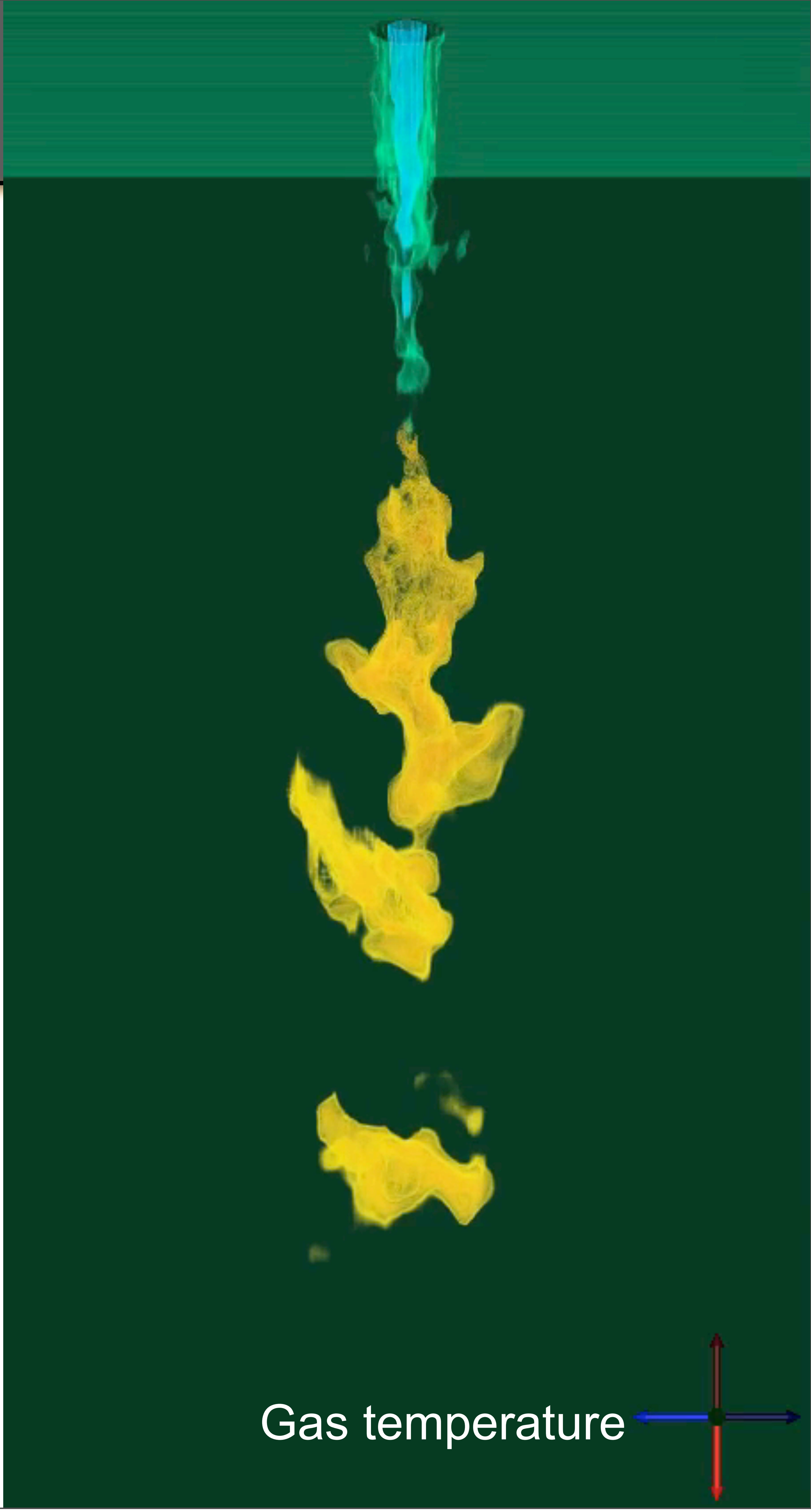




oxy-coal simulation: LES & DQMoM
(7 internal coordinates)

$P_{O2(primary)} = 0\%$

$P_{O2(primary)} = 21\%$



traditional validation:

P_{O_2} primary	Wall temperature (K)	Measured average stand-off distance	Predicted average stand-off distance
0%	1283K	30 cm	31 cm
20.9%	1283K	12 cm	31 cm

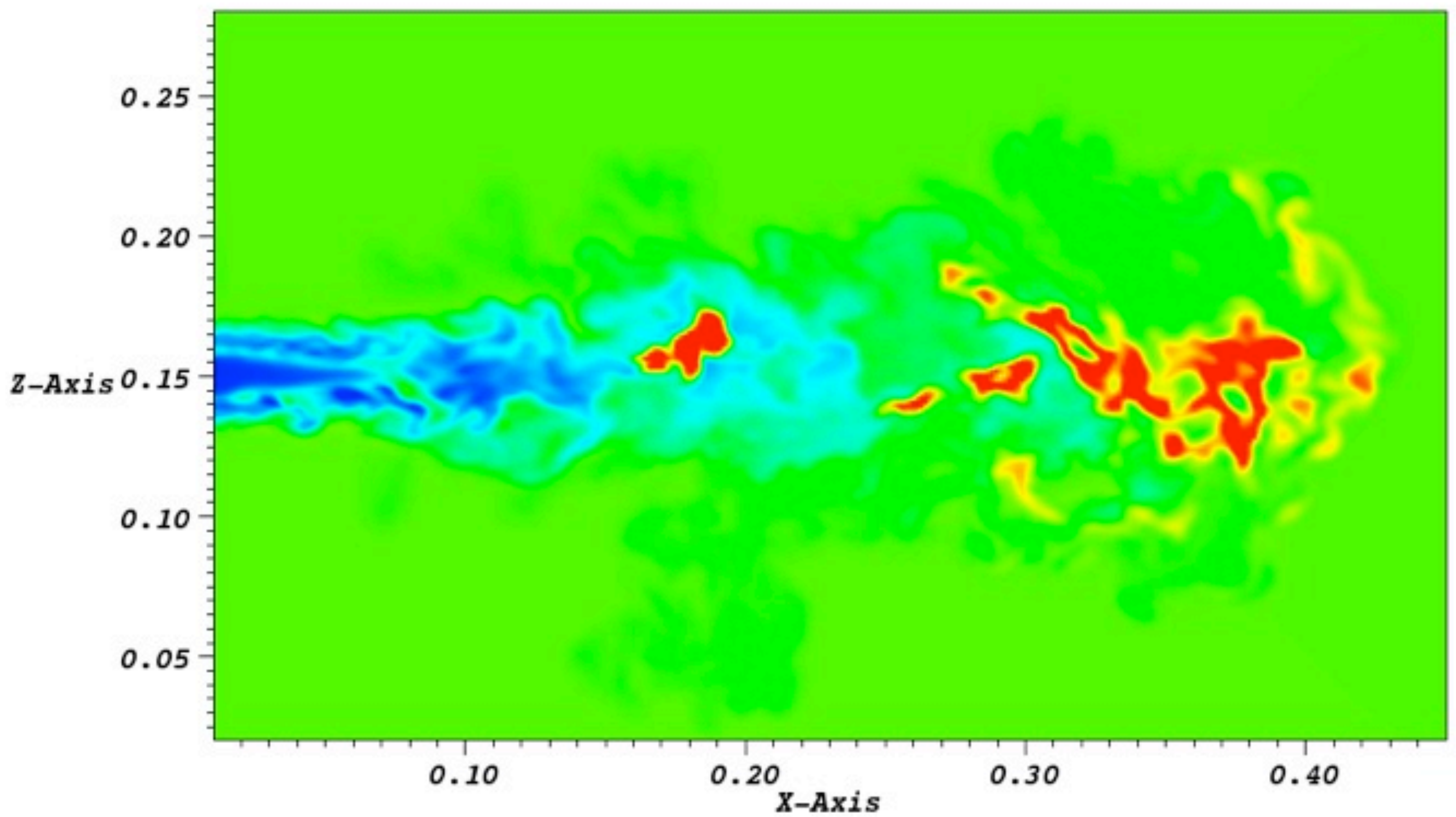
predicted flame stand-off distance shows no sensitivity to P_{O_2} in the primary

V/UQ observations

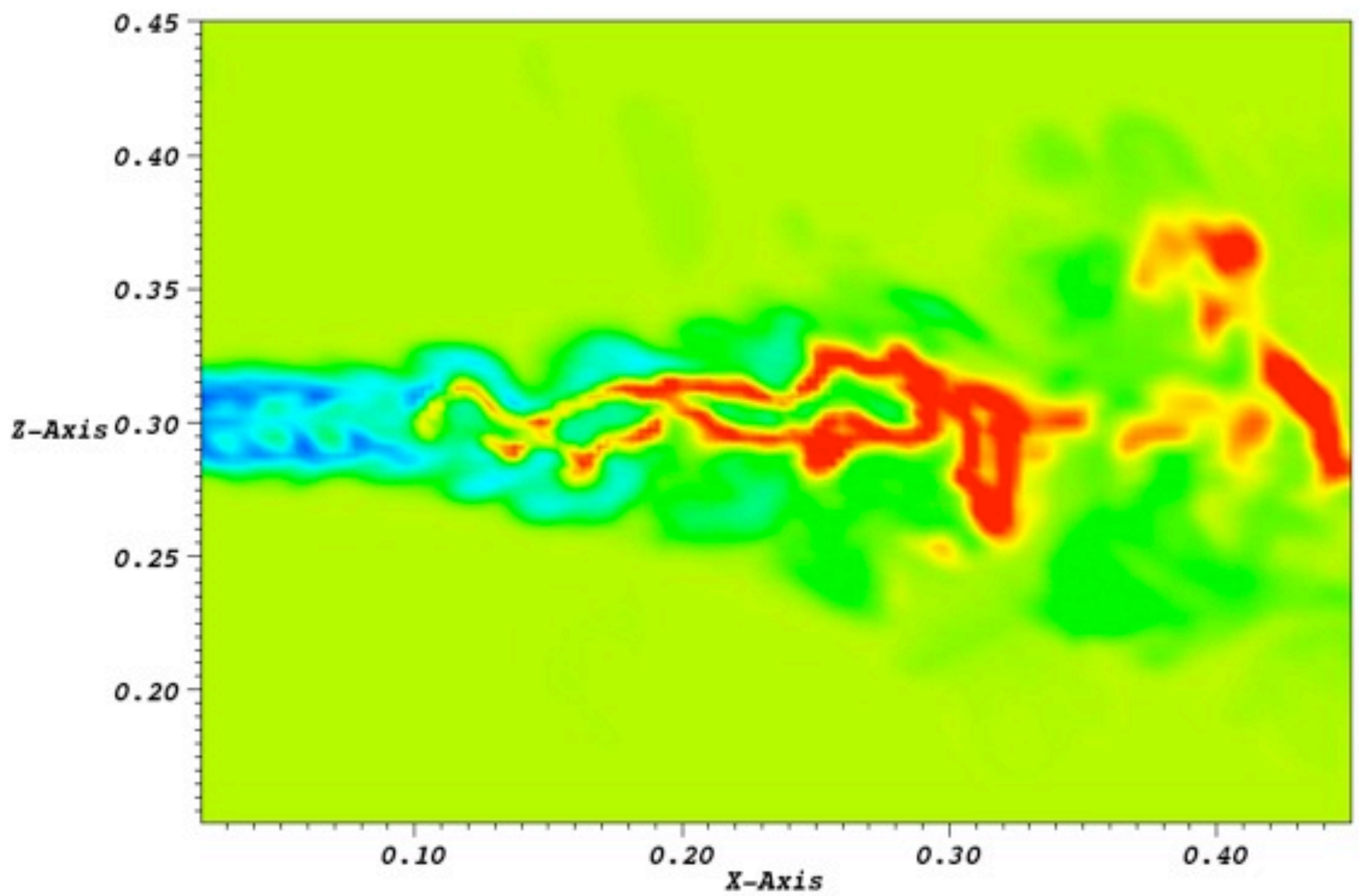
P_{O_2} primary	Wall temperature (K)	Measured mean stand-off distance	Predicted mean stand-off distance
0% +/- 1%	1283 +/- 150 K (bias error)	30 +/- 1.5 cm	31 +/- 2 cm
20.9% +/- 1%	1283 +/- 150 K (bias error)	12 +/- 1.5 cm	10 +/- 2 cm

predicted flame stand-off distance shows high sensitivity to wall temperature

simulation observations: Gas Temperature



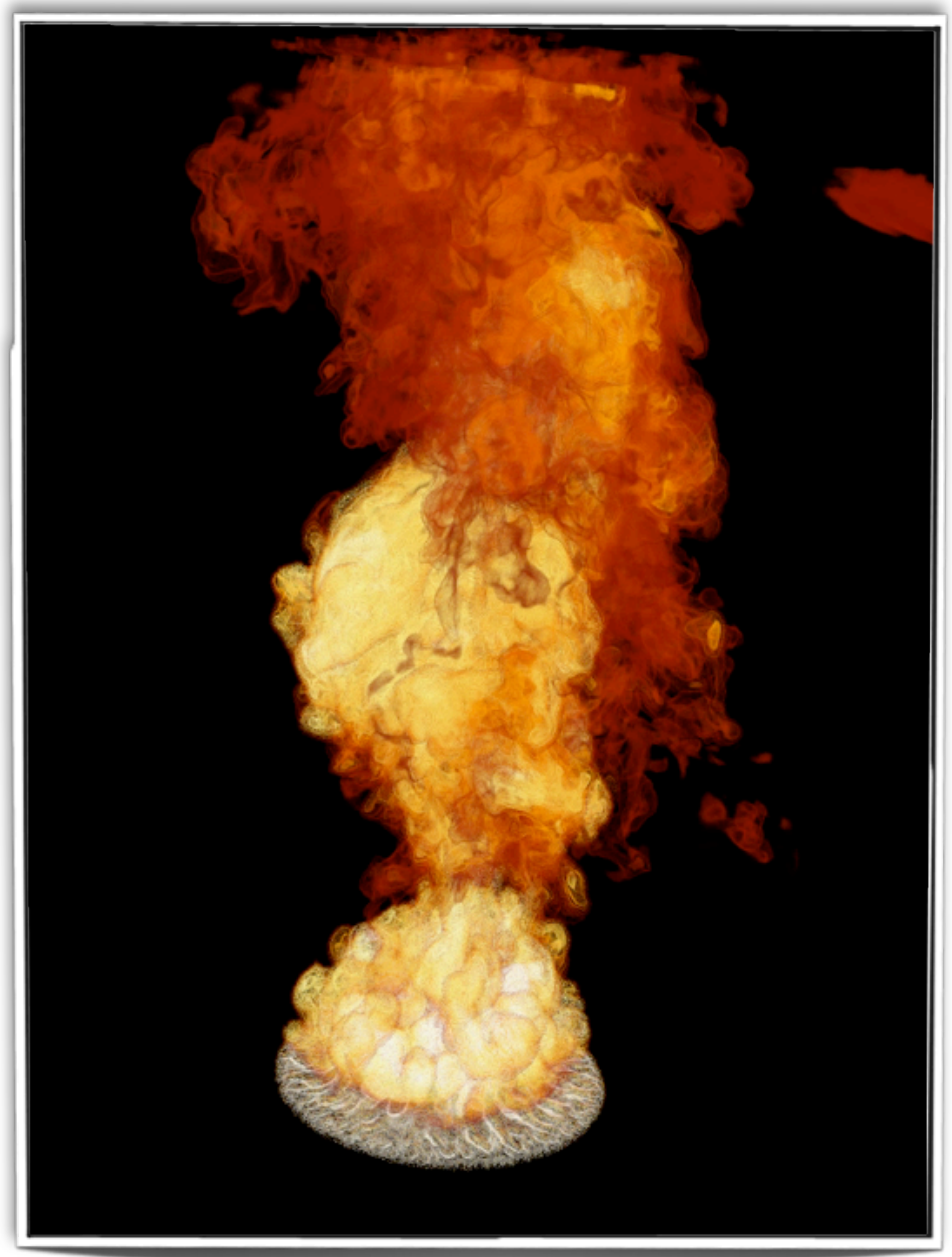
$P_{O_2,primary} = 0\%$

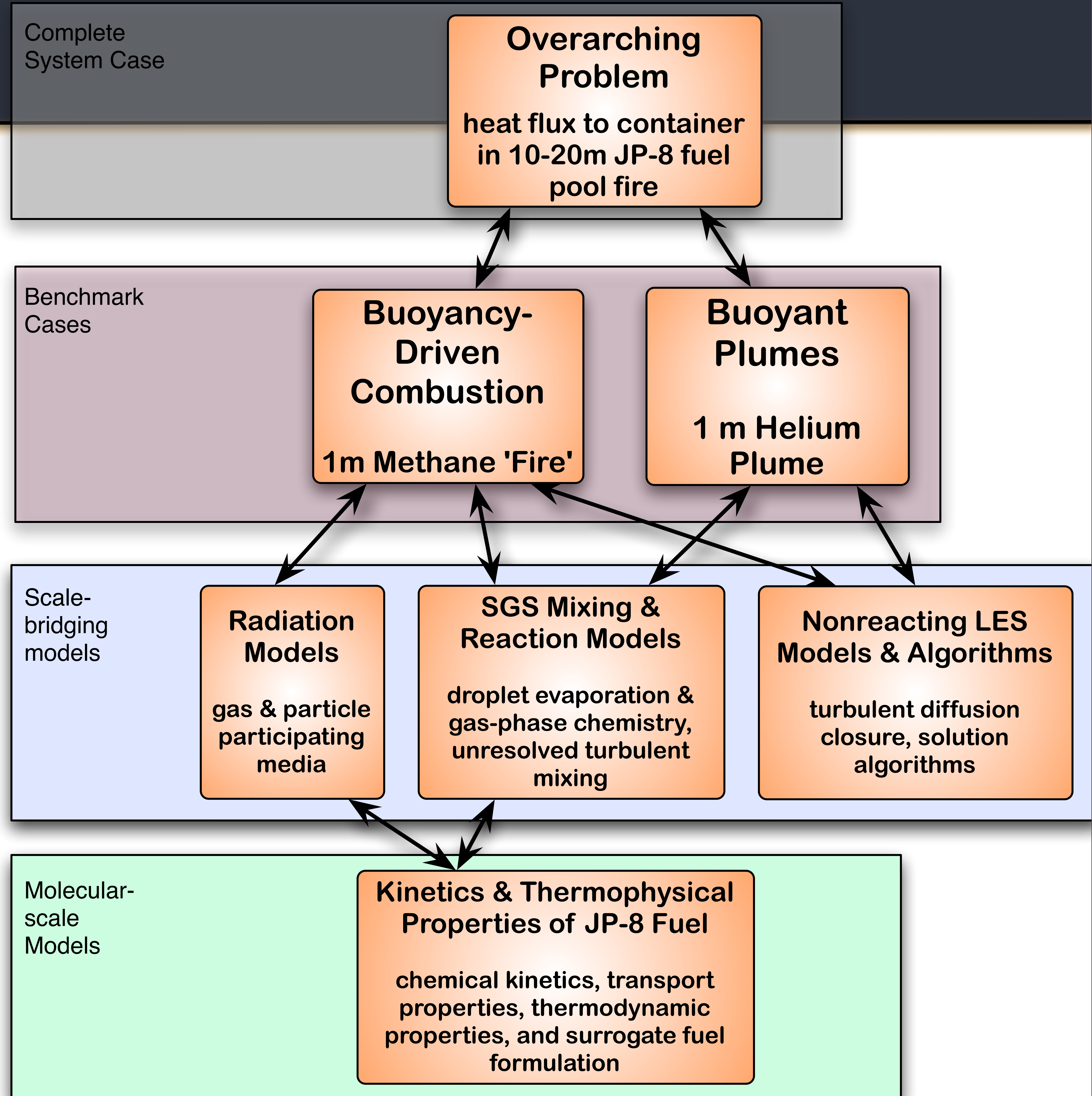


$P_{O_2,primary} = 21\%$

Hierarchical V/UQ

$$u \geq [y_m(\mathbf{x}) - y_e] \geq l$$





UQ-Predictive Validation Framework for Combustion Applications

V/UQ provides:

- formal hierarchical consistency between experiment and simulation

- reduced uncertainty

- increased physics

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information gain