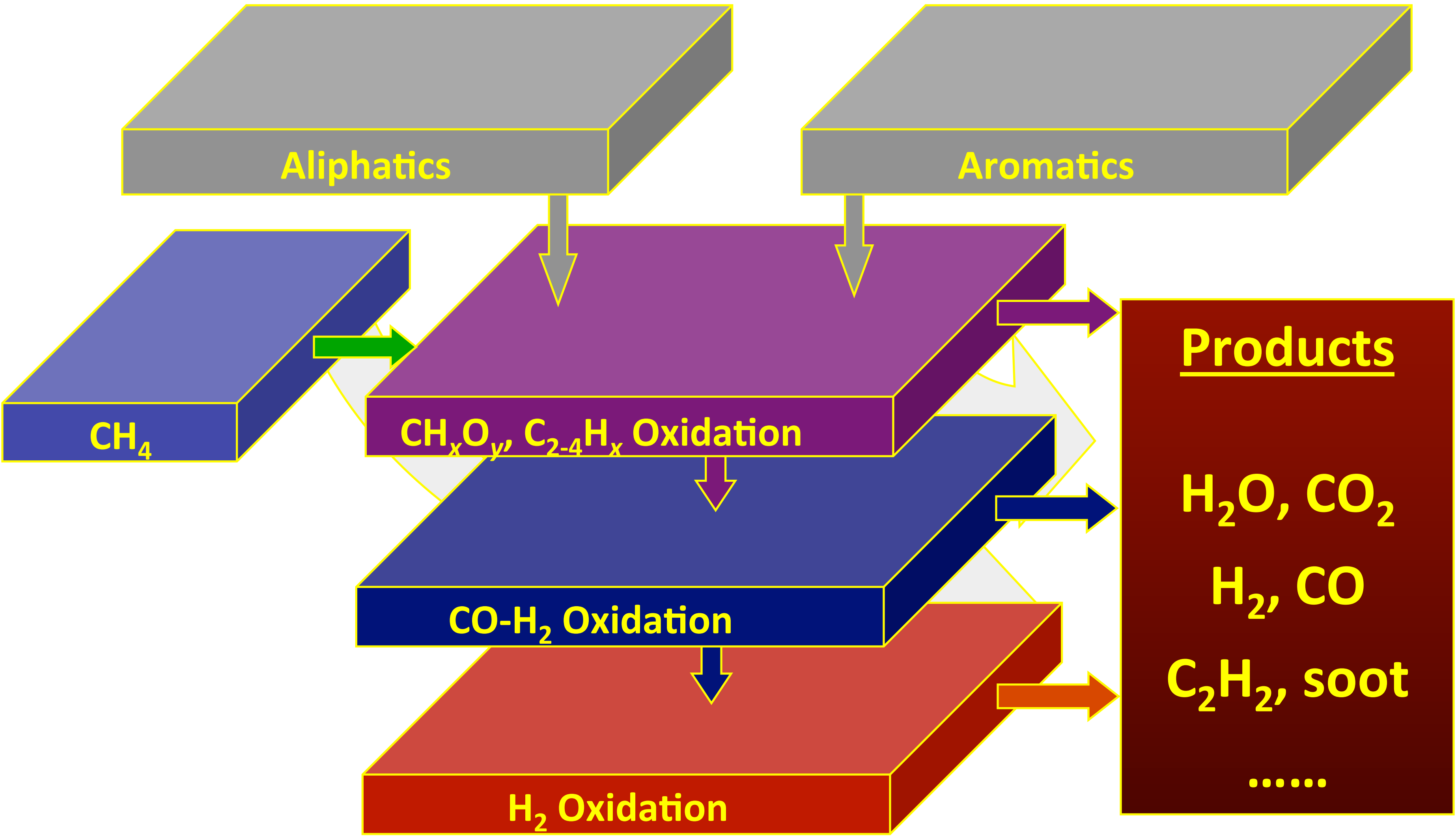
Towards a predictive combustion chemistry model – Uncertainty propagation and minimization

Hai Wang and David A. Sheen

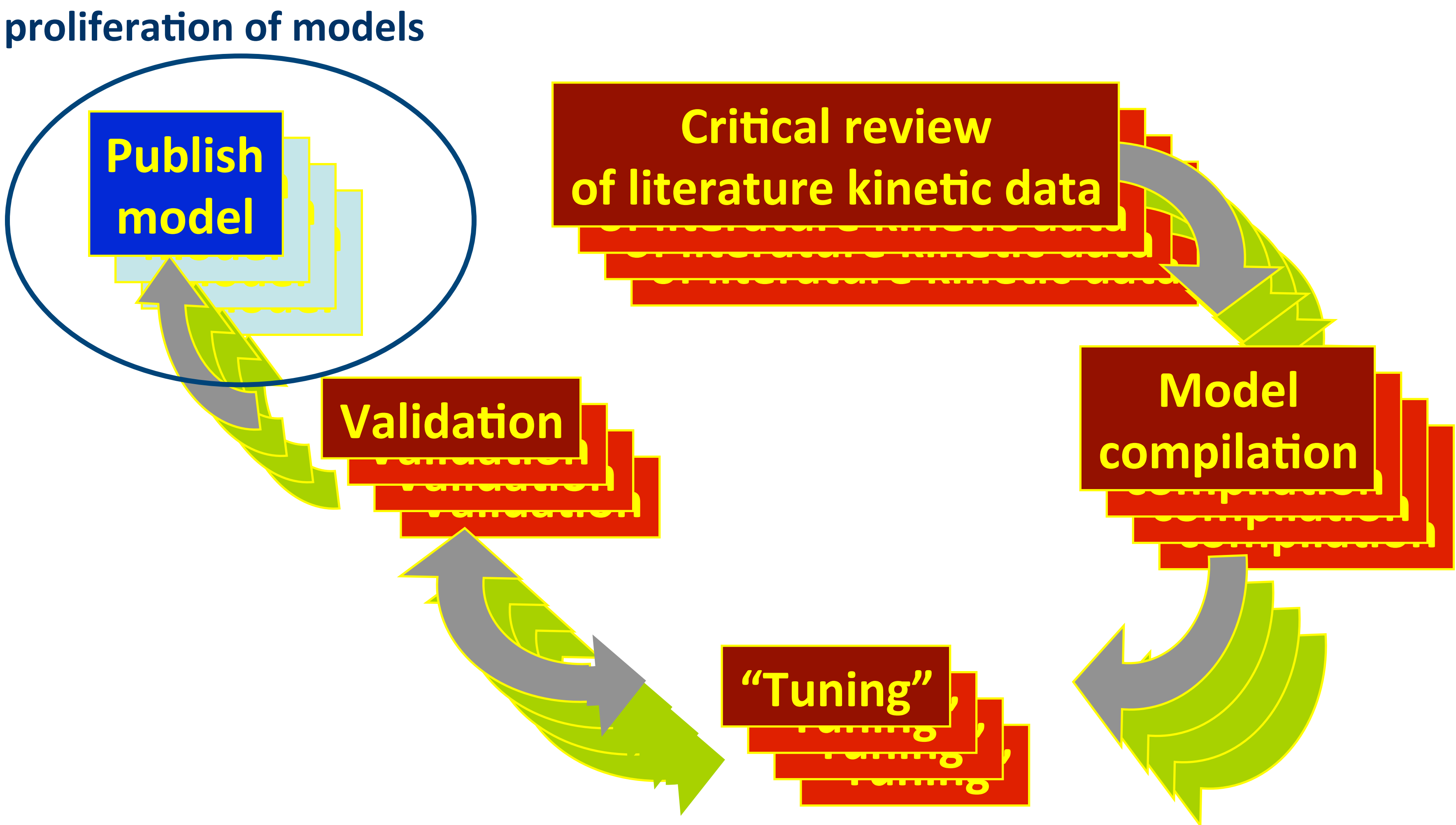
University of Southern California, Los Angeles, California, USA

Model Hierarchy



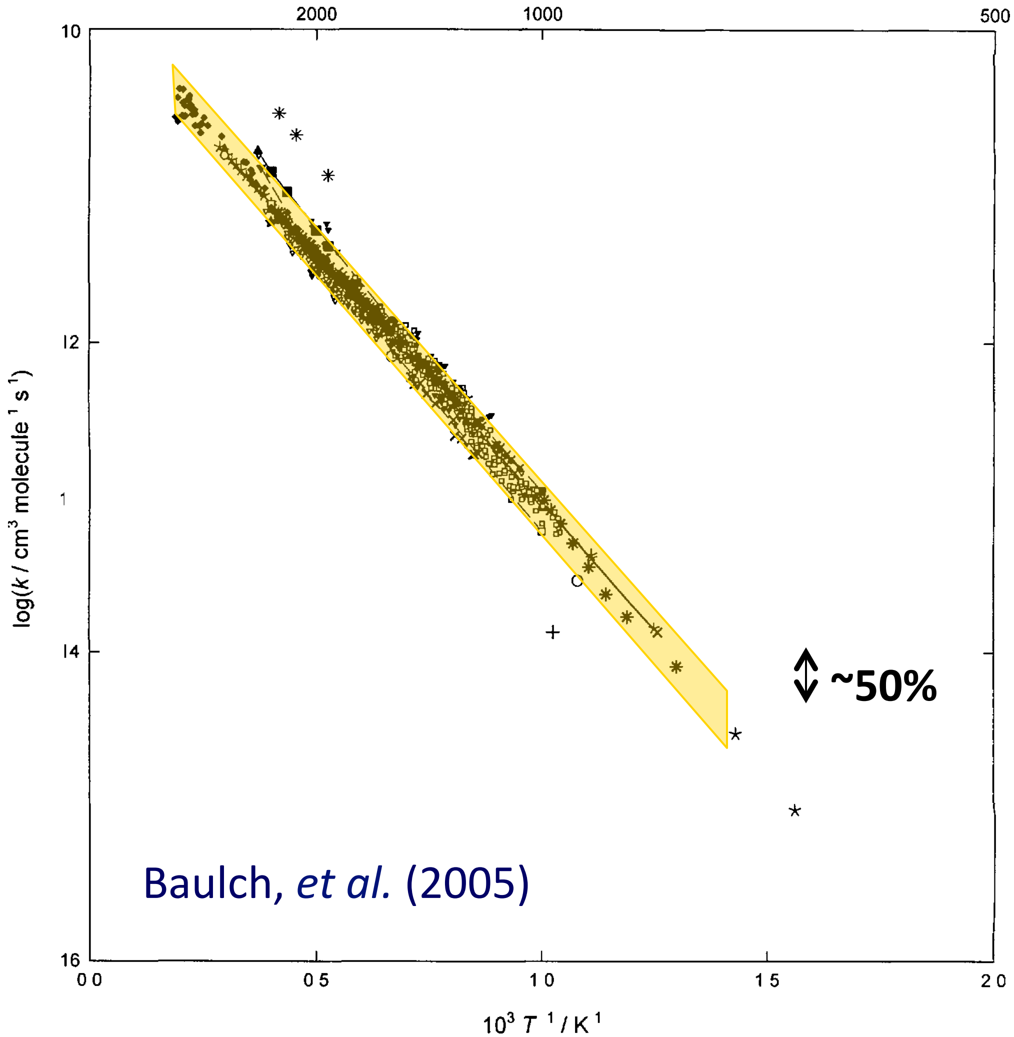
Reaction Model Development

The Current Approach



Kinetic Rate Parameter Uncertainties

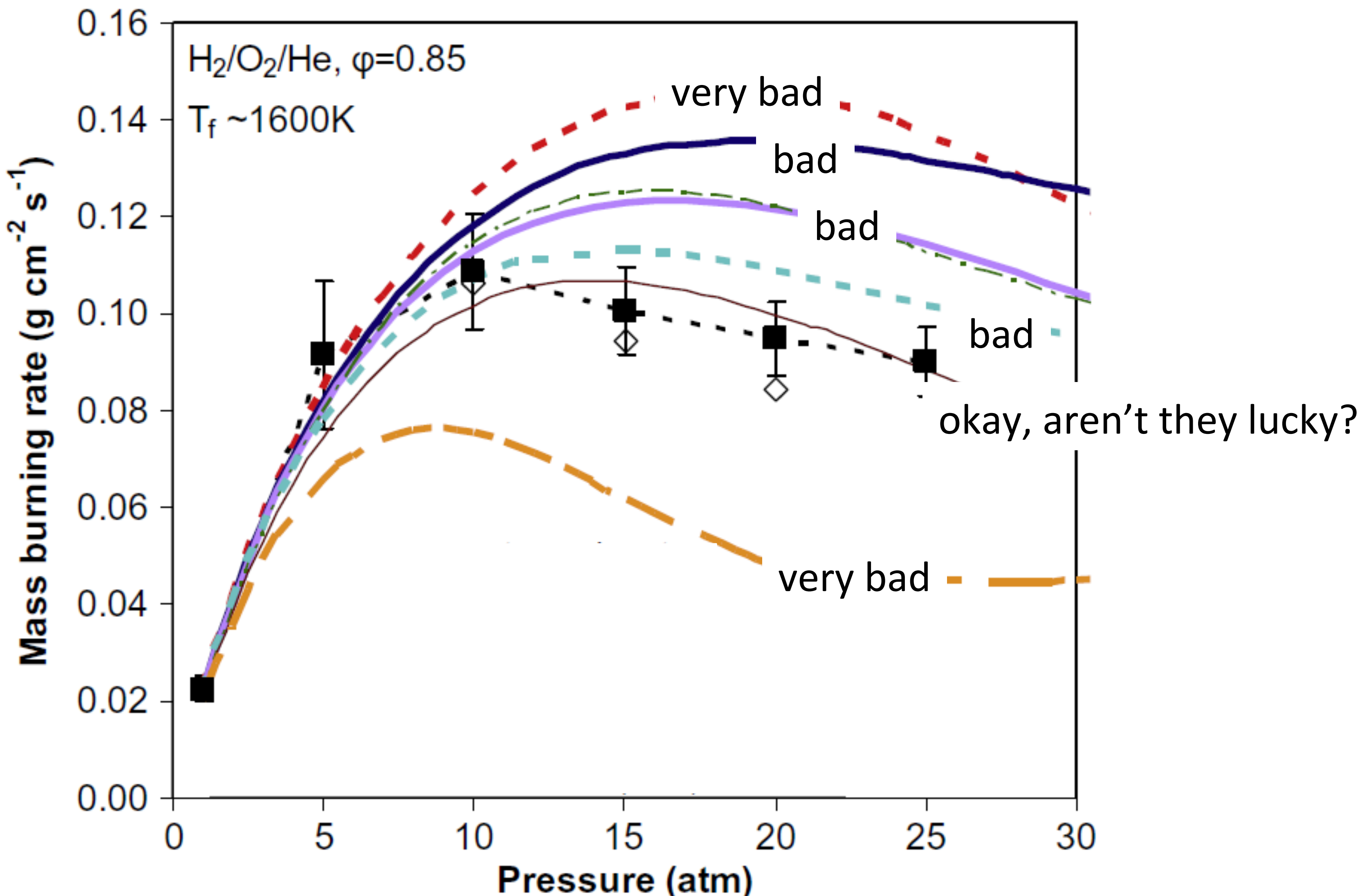
$H + O_2 \leftrightarrow OH + O$ (R1)



- **Uncertainty factor ~1.25**
- **Logarithmic sensitivity coefficient = 0.24 (ethylene-air, *f* = 1, *p* = 1 atm)**

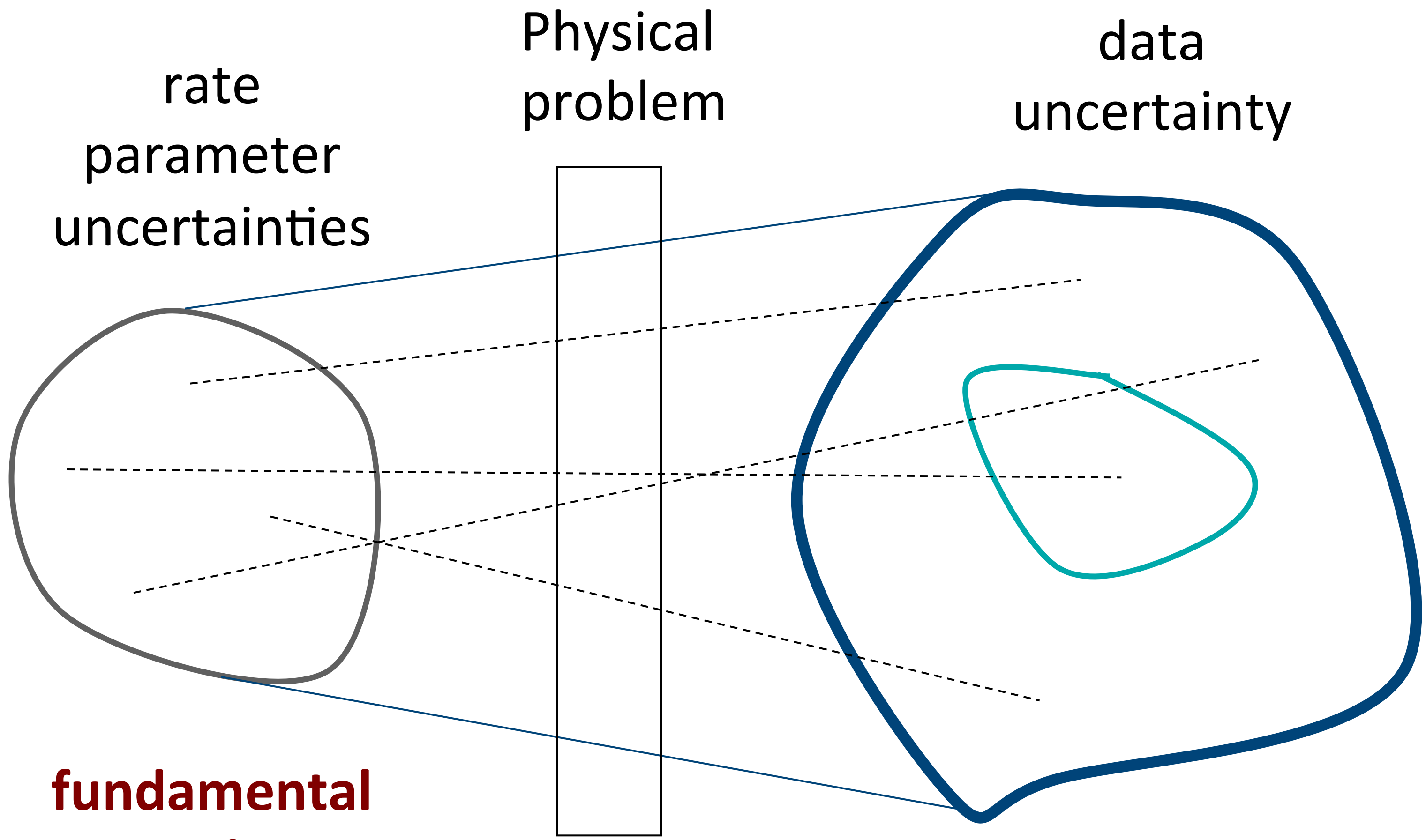
- **±5% (±4 cm/s) uncertainty in predicted flame speed due to R1 alone**
- **Key question: How do we propagate uncertainties in rate constants in combustion simulations?**

Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty



Burke, *et al.* (2010)

Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty

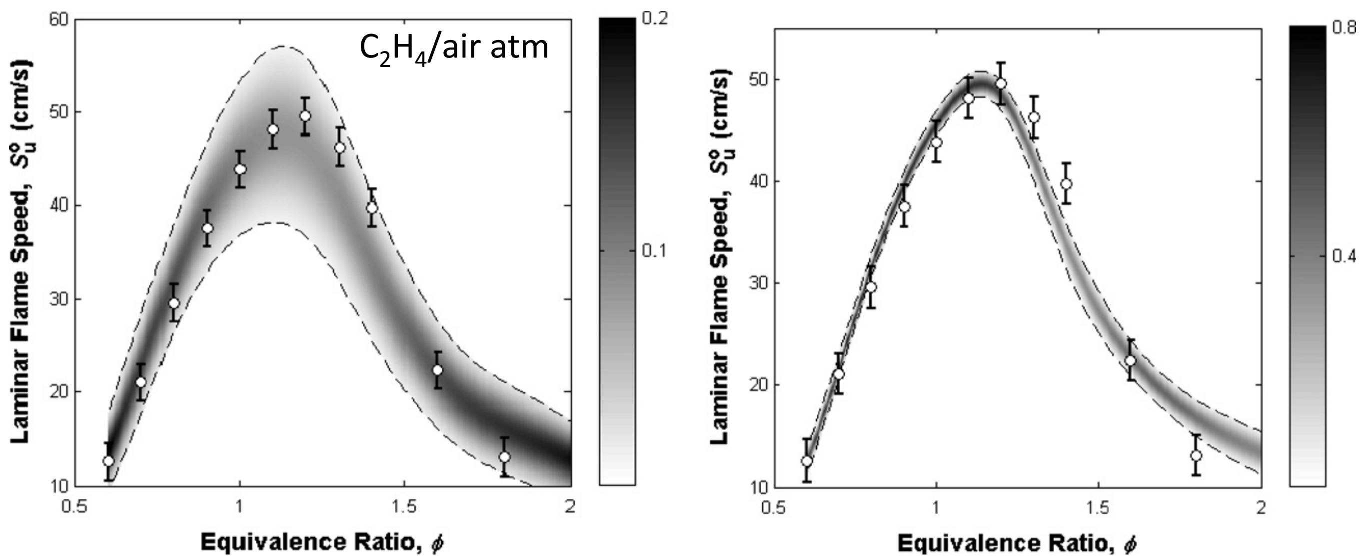


fundamental reaction kinetics expt + calc

fundamental combustion expt.

MUM-PCE

- Method of Uncertainty Minimization – Polynomial Chaos Expansions
  - Mathematical foundation and numerical methods: Sheen & Wang "Kinetic uncertainty quantification and minimization using polynomial chaos expansions," *Combustion and Flame*, DOI:10.1016/j.combustflame.2011.05.010.



  - Model prediction presented as a (2-*s*) band of uncertainty resulting from kinetic parameter uncertainties.
  - Model uncertainty may be constrained by experimental data (ignition delay, species-time history, flame speeds etc)

MUM-PCE: Methods

- **Stochastic Spectral Expansion:** express kinetic parameter *x_i* as a polynomial expansion of basis random variables

$$x_i = x_i^{(0)} + \sum_{j=1}^{m} \alpha_{ij}\xi_j + \sum_{k=1}^{m}\sum_{j=k}^{m} \beta_{ijk}\xi_j\xi_k + \ldots$$

Following N. Wiener (1938), D.B. Xiu, *et al.* (2002)

- **Solution Mapping**: use polynomial response surface to express the relation between a combustion response *h* and **x**

$$\eta_r(\mathbf{x}) \cong \eta_{r,0} + \sum_{i=1}^{N} a_{r,i}x_i + \sum_{i=1}^{N}\sum_{j\geq i}^{N} b_{r,ij}x_i x_j$$

Forward Uncertainty Propagation

$$\eta_r(\mathbf{x}) = \eta_{r,0} + \sum_{i=1}^{n} a_i x_i + \sum_{i=1}^{n}\sum_{j\geq i}^{n} b_{ij} x_i x_j$$

Response surface from solution mapping

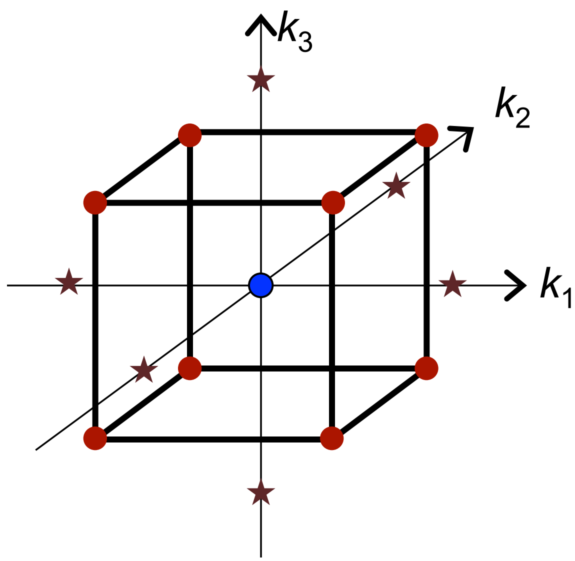
$$x_i = {}^1\!/_2\, \xi_i$$

Spectral representation of uncertainty in x's
(mean = 0, s = 0.5, each indep't of others)

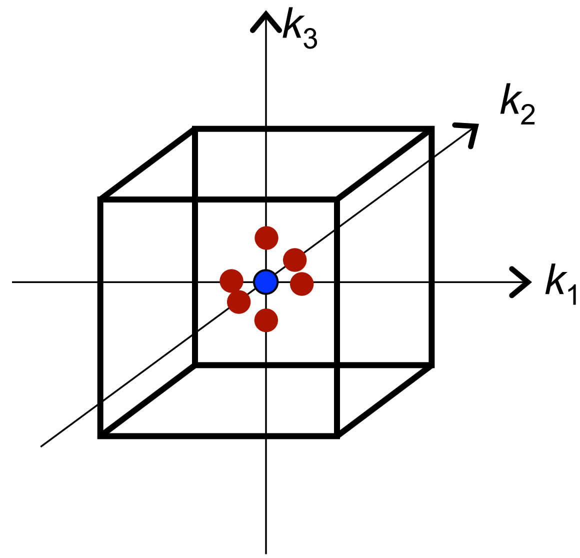
$$\eta_r(\mathbf{x},\boldsymbol{\xi}) = \eta_r\left(\mathbf{x}^{(0)}\right) + \sum_{i=1}^{M} \hat{\alpha}_{r,i}\xi_i + \sum_{i=1}^{M}\sum_{j=i}^{M} \hat{\beta}_{r,ij}\xi_i\xi_j$$

Solution Mapping Method

- **Fit a response surface to the model**



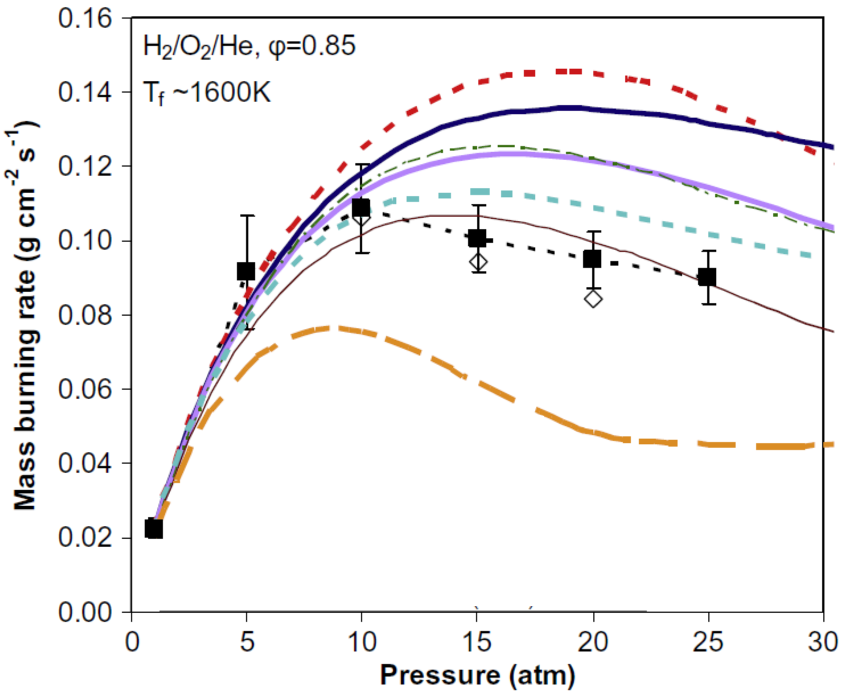
Central-Composite Factorial Design

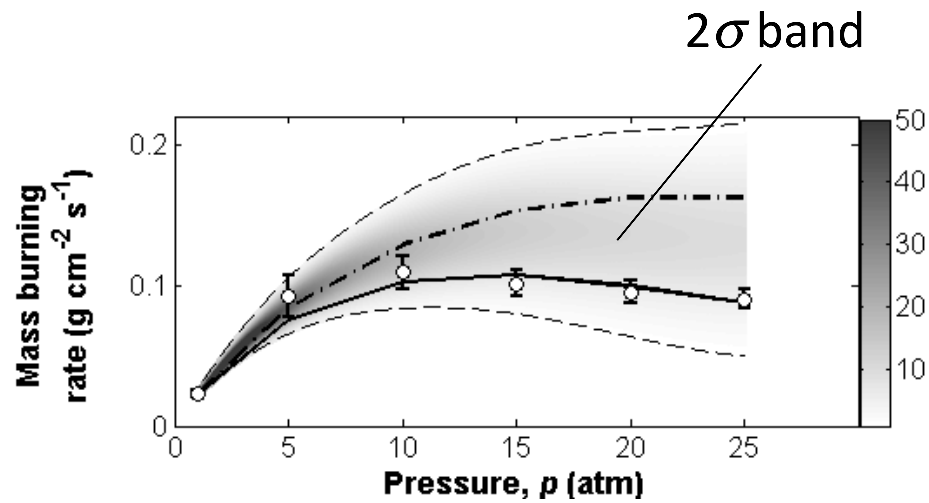


Sensitivity Analysis Based Design

G.E.P. Box, *et al.* (1978), Frenklach *et al*. (1992), S.G. Davis *et al.* (2004)

MUM-PCE – Application in H_2/O_2 Combustion





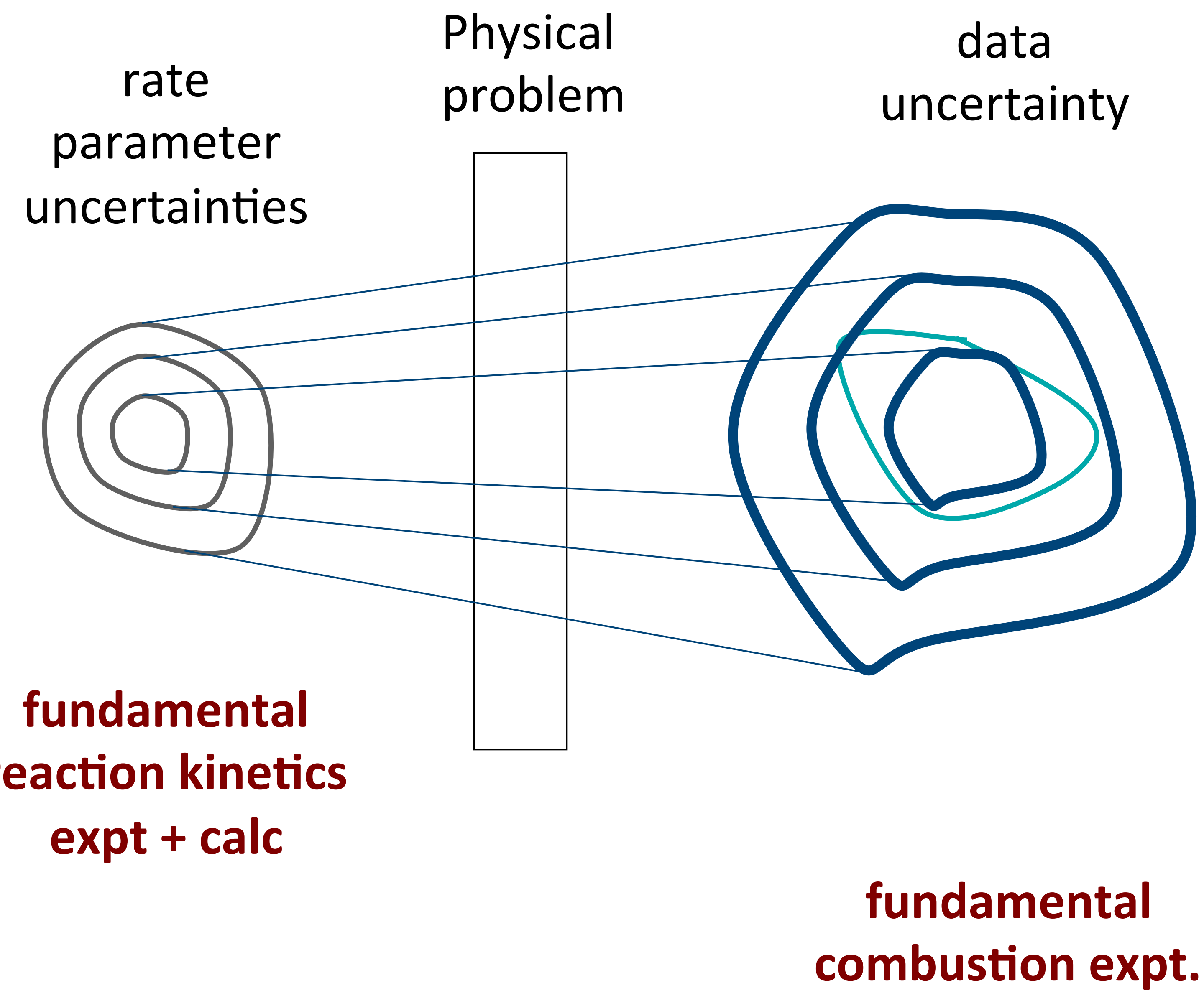
- High-pressure data sensitize kinetics of hydrogen oxidation.
- A large number of models outside experimental uncertainty at high pressures.

Burke, *et al.* (2010)

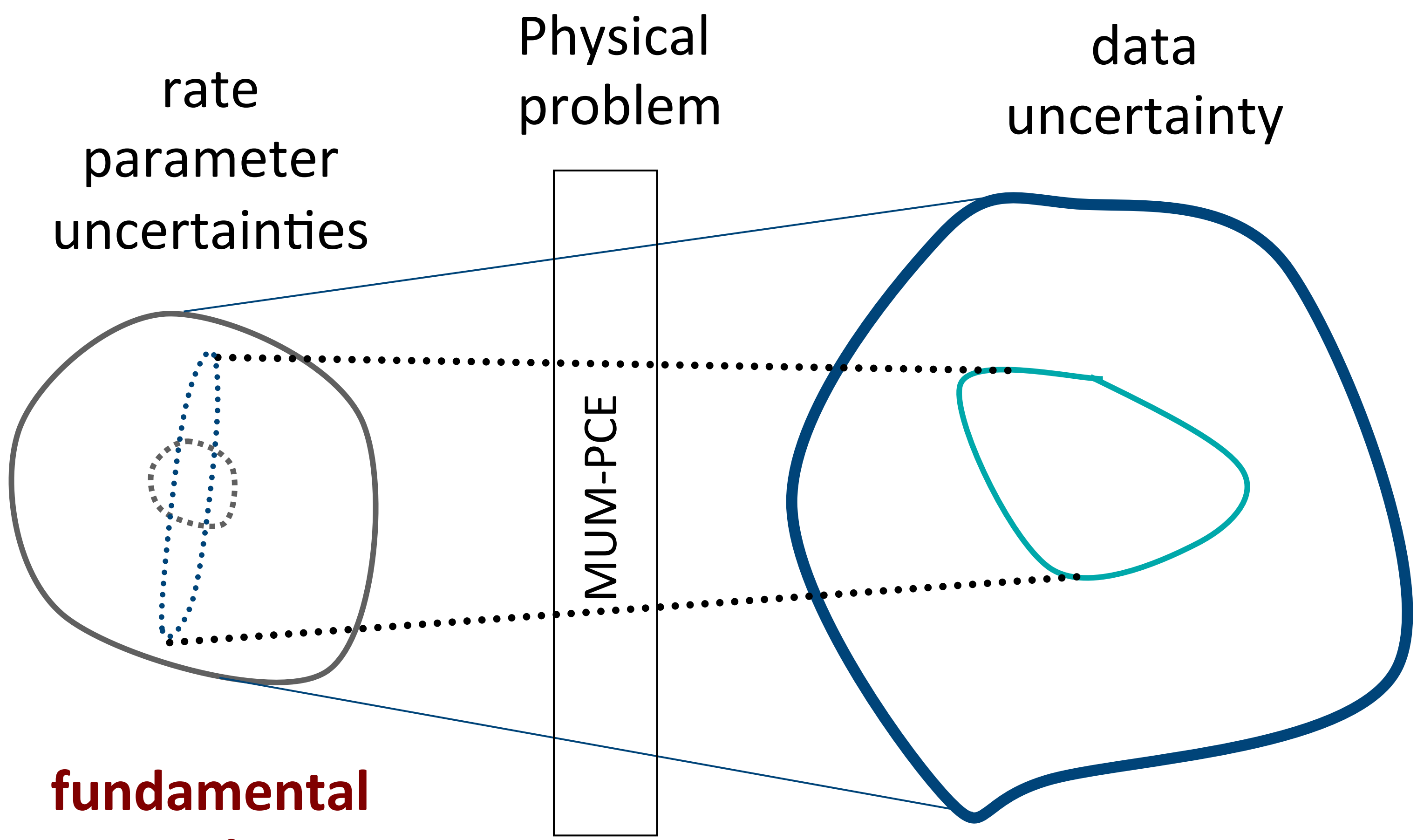
- 2σ uncertainty band calculated by MUM-PCE, based on rate parameter uncertainties.
- Models are statistical samples of parameter uncertainties.

Sheen & Wang (2011)

Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty Uncertainty



MUM-PCE



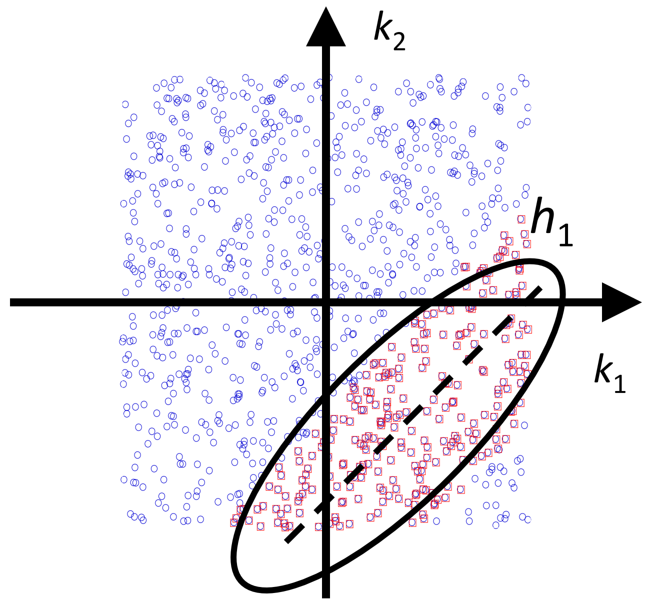
**fundamental
reaction kinetics
expt + calc**

**fundamental
combustion expt.**

Method of Uncertainty Minimization

$$\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\alpha}\boldsymbol{\xi}$$

Chemical model
+ associated uncertainty



$$\eta_r(\mathbf{x}) \cong \eta_{r,0} + \sum_{i=1}^{N} a_{r,i} x_i + \sum_{i=1}^{N} \sum_{j \geq i}^{N} b_{r,ij} x_i x_j$$

Physics model

$$\Phi\left(\mathbf{x}_0^*\right) = \min_{\mathbf{x}_0} \left\{ \sum_{r=1}^{M} \frac{\left[\eta_{r,0}^{\text{obs}} - \eta_r\left(\mathbf{x}_0\right)\right]^2}{\left(\sigma_r^{\text{obs}}\right)^2} + \sum_{n=1}^{N} \frac{\left(x_{0,n}\right)^2}{\left(\sigma_n\right)^2} \right\}$$

$$\eta_r(\mathbf{x}, \boldsymbol{\xi}) = \eta_r\left(\mathbf{x}^{(0)}\right) + \sum_{i=1}^{m} \hat{\alpha}_{r,i} \xi_i + \sum_{i=1}^{m} \sum_{j=i}^{m} \hat{\beta}_{r,ij} \xi_i \xi_j$$

$$\Sigma = \left[\sum\nolimits_{r=1}^{n} \frac{1}{\left(\sigma_r^{\text{obs}}\right)^2} \left(\mathbf{b}\mathbf{x}_0^* \mathbf{x}_0^{*T} \mathbf{b} + \mathbf{a}\mathbf{x}_0^{*T} \mathbf{b} + \mathbf{b}^T \mathbf{x}_0^* \mathbf{a}^T + \mathbf{a}\mathbf{a}^T \right) + 4\mathbf{I} \right]^{-1}$$

$$\boldsymbol{\alpha}^* = \Sigma^{1/2}$$

Predictions
+ associated uncertainty

MUM-PCE – Application in H_2/O_2 Combustion

- Model uncertainty constraining
- JetSurF 2.0 H2/CO submodel
  - 14 species, 41 reactions

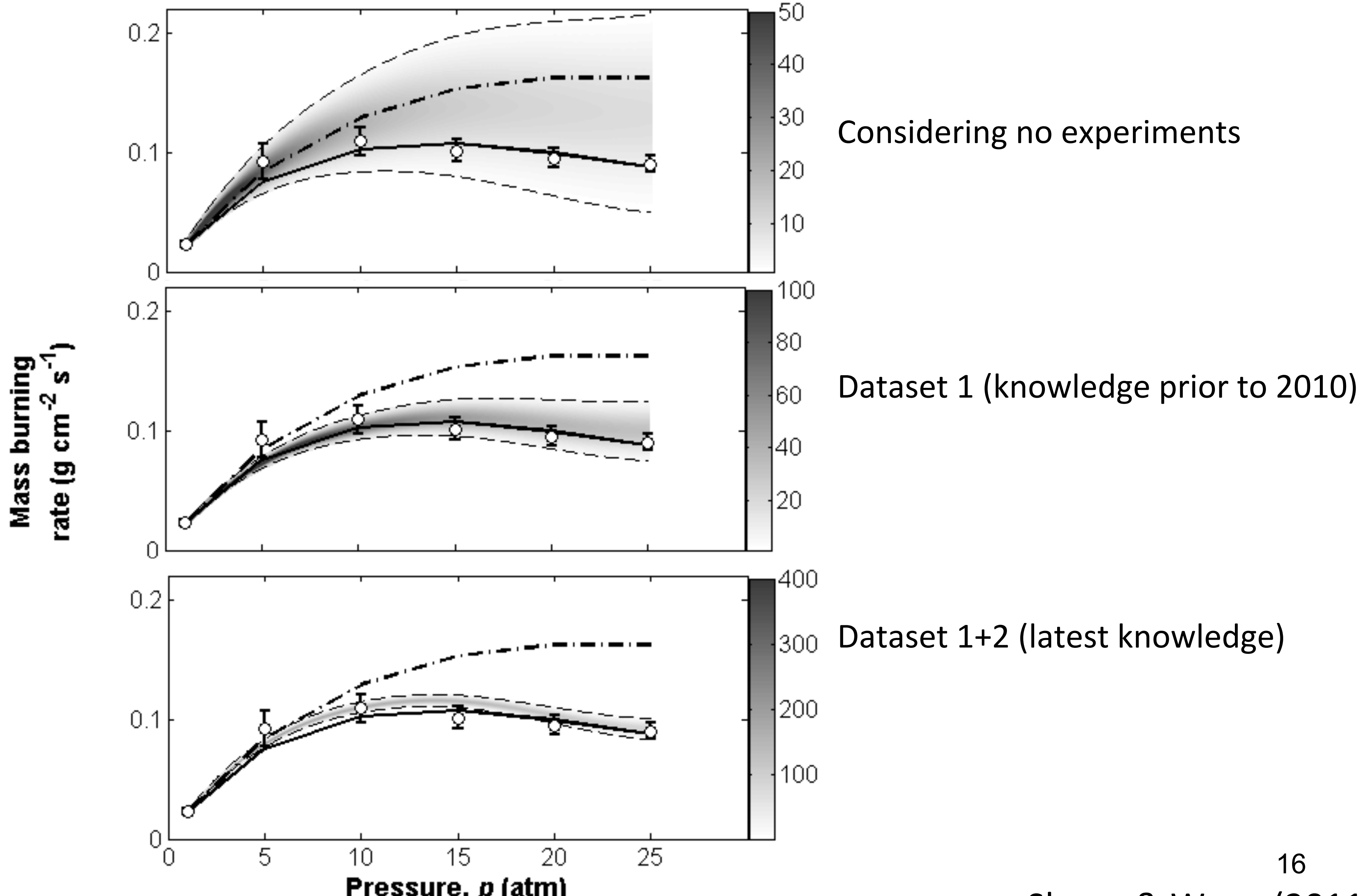
Dataset 1: From Davis, *et al.* (2005):

	No.	P_0, P_5 (atm)	T_0, T_5 (K)	f
Laminar Flame Speeds	12	1-15	298	1.0-3.0
Ignition Delay Times	13	0.5-33	1000-2600	1.0-6.1
Flow Reactor Profiles	9	1.0-16	915-1040	0.3-1.0
Laminar Flame Profiles	2	0.047	400	1.9

Dataset 2:

From Burke, *et al.* (2010):	No.	P_0, P_5 (atm)	T_0, T_5 (K)	f
Laminar Flame Speeds	18	15-25	298	0.85-2.5

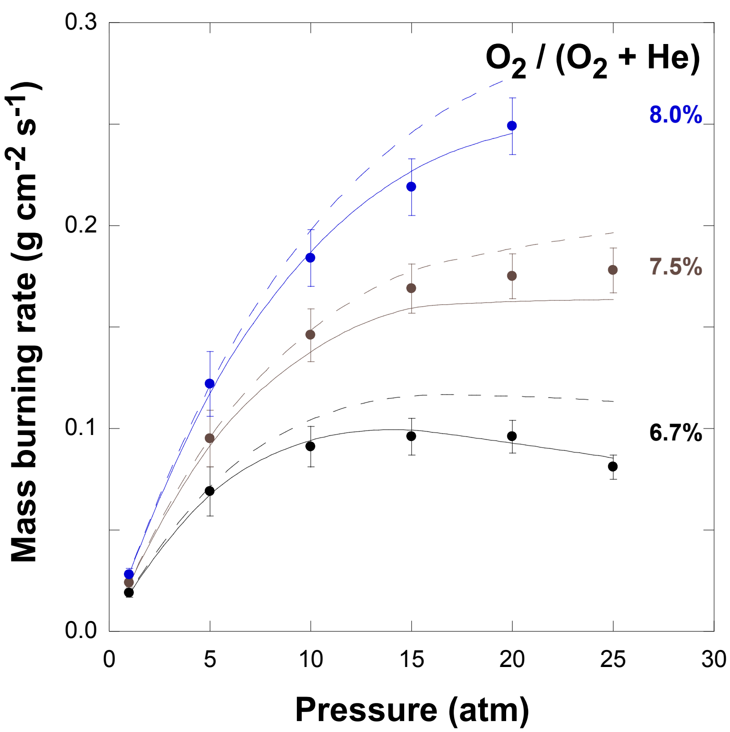
MUM-PCE – Application in H_2/O_2 Combustion



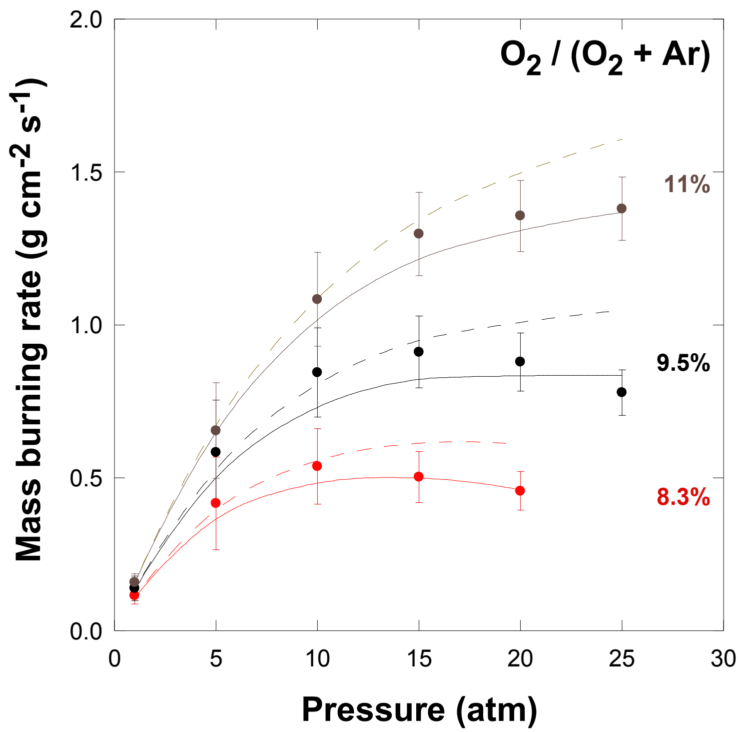
Sheen & Wang (2011)

MUM-PCE – Application in H_2/O_2 Combustion

H_2/O_2/He mixtures at equivalence ratio 1



H_2/O_2/Ar mixtures at equivalence ratio 2.5

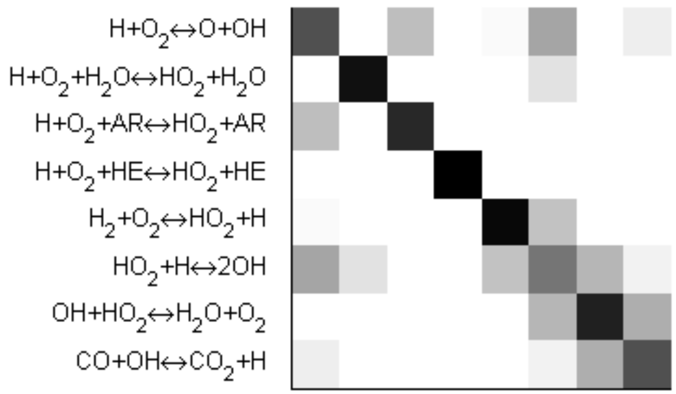


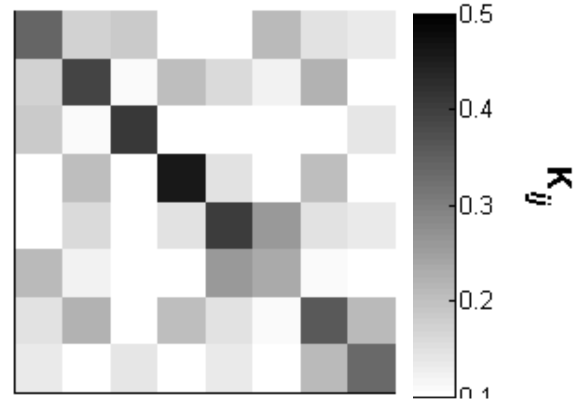
Sheen & Wang (2011)

MUM-PCE – Application in H_2/O_2 Combustion

Dataset 1
Knowledge prior to 2010

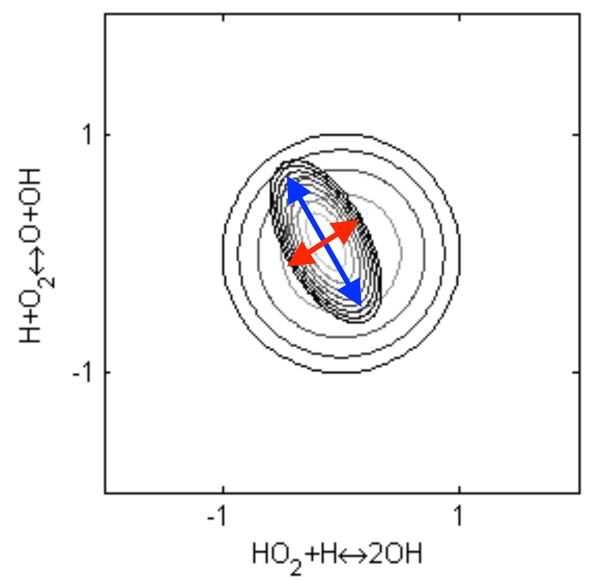
+ Burke, *et al.* (2010)
Current knowledge





Weak constraint by experiments

Strong constraint by experiments



JetSurF - A Jet Surrogate Fuel Model

Page Safety Tools

JetSurF – A Jet Surrogate Fuel Model

JetSurF is a detailed chemical reaction model for the combustion of jet-fuel surrogate. The model is being developed through a multi-university research collaboration and is funded by the Air Force Office of Scientific Research. Project participants include

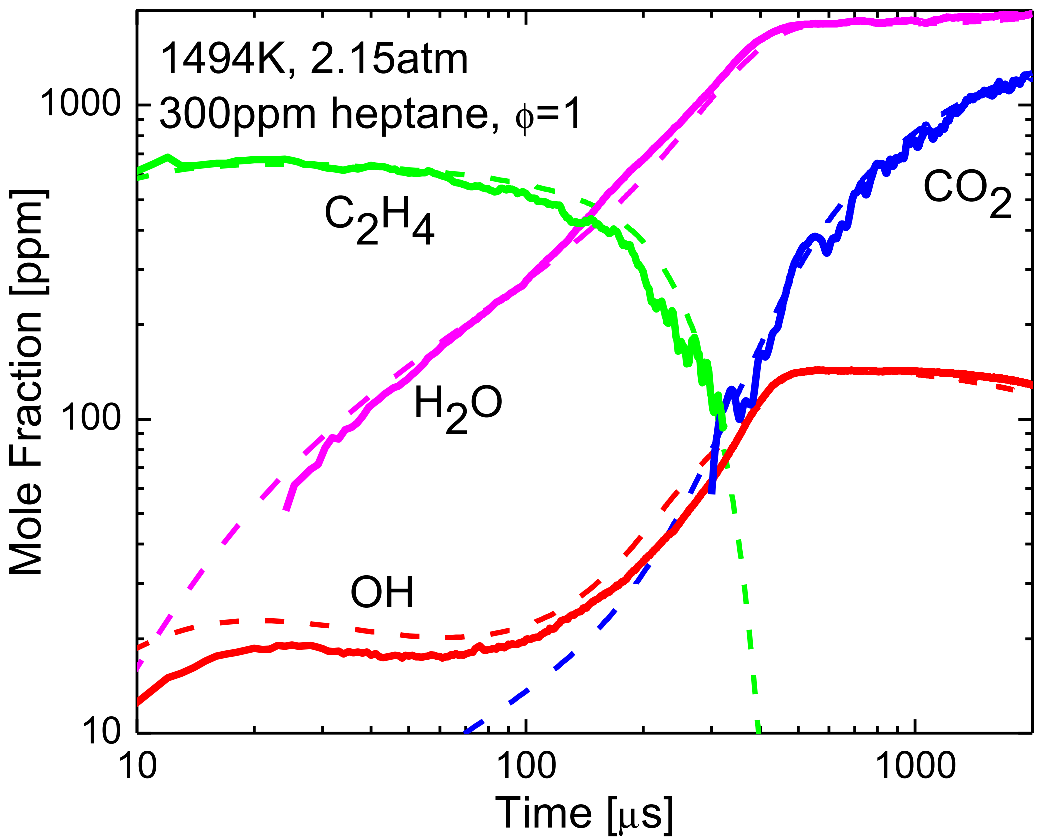
F. N. Egolfopoulos, Hai Wang	*University of Southern California*
R. K. Hanson, D. F. Davidson, C. T. Bowman, H. Pitsch	*Stanford University*
C. K. Law	*Princeton University*
N. P. Cernansky, D. L. Miller	*Drexel University*
W. Tsang	*National Institute of Standards and Technology*
R. P. Lindstedt	*Imperial College, London*
A. Violi	*University of Michigan*

New Release: **JetSurF Version 2.0 – A working model for the combustion of *n*-alkane up to *n*-dodecane, cyclohexane, and mono-alkylated cyclohexane up to *n*-butyl-cyclohexane**
(Release Date: September 19, 2010)

Old Releases: **JetSurF Version 1.1 – A interim model for the combustion of *n*-butyl-, *n*-propyl-, ethyl-, and methyl-cyclohexane and cyclohexane**
(Release Date: September 15, 2009)

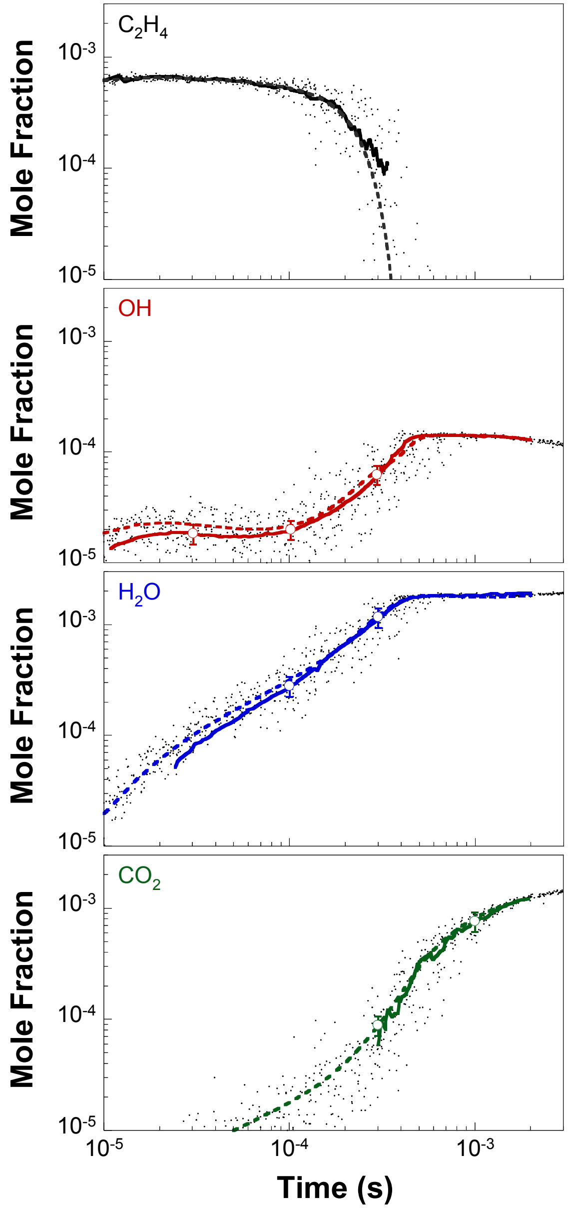
JetSurF Validation – Species Concentrations behind reflected shock waves

B. Sirjean, E. Dames, D. A. Sheen, X.-Q. You, C. Sung, A. T. Holley, F. N. Egolfopoulos, H. Wang, S. S. Vasu, D. F. Davidson, R. K. Hanson, H. Pitsch, C. T. Bowman, A. Kelley, C. K. Law, W. Tsang, N. P. Cernansky, D. L. Miller, A. Violi, R. P. Lindstedt, A high-temperature chemical kinetic model of n-alkane oxidation, JetSurF version 1.0, September 15, 2009 (http://melchior.usc.edu/JetSurF/Version1_0/Index.html).



Plot stolen from Ron Hanson. Solid line: experiments; dashed line: JetSurF

Prediction Uncertainties in As-Compiled Model



Good nominal prediction with significant uncertainty!

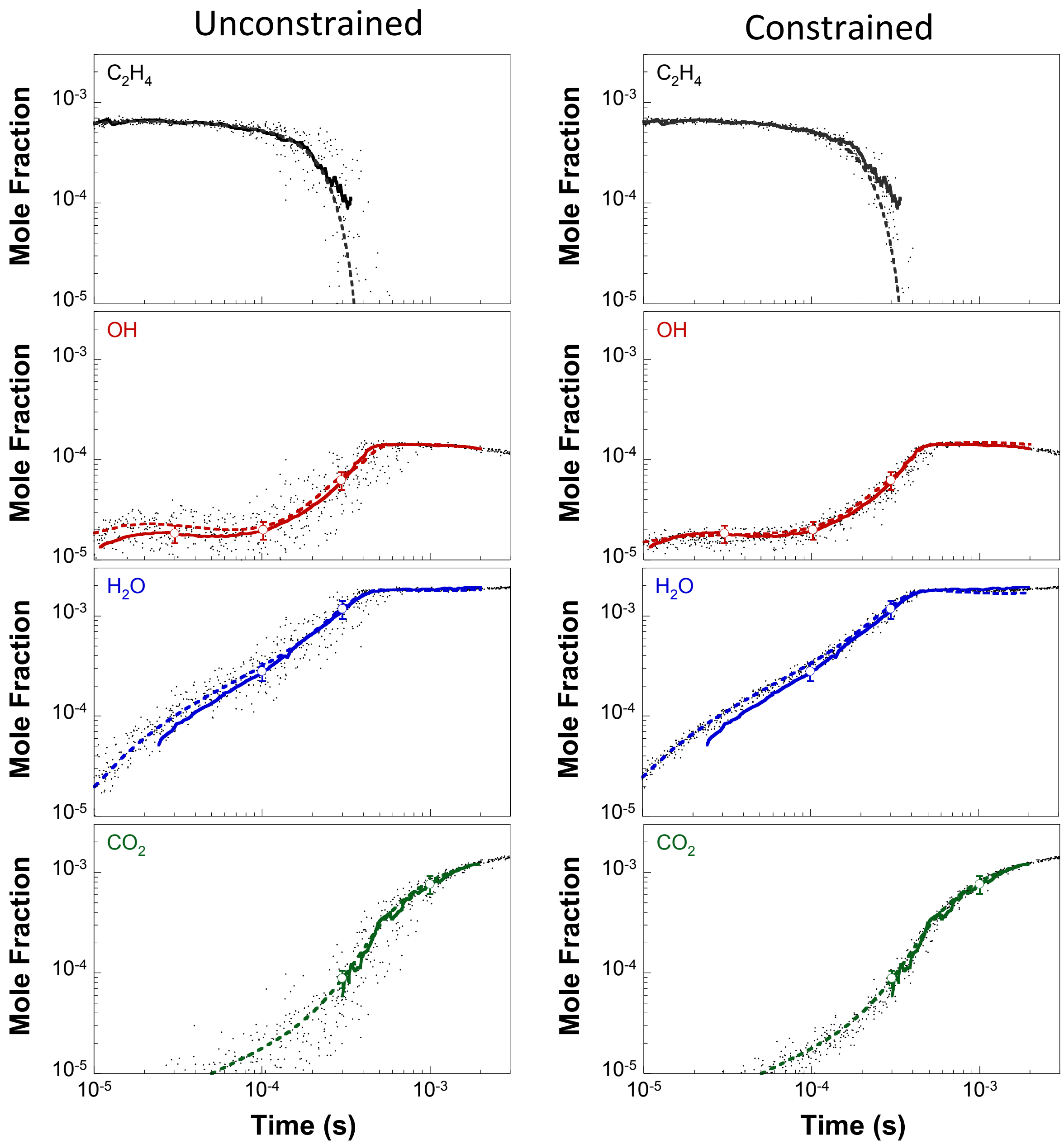
Chemistry Model & Experimental Targets

- Modified JetSurF 1.0
  - 196 species, 1478 reactions

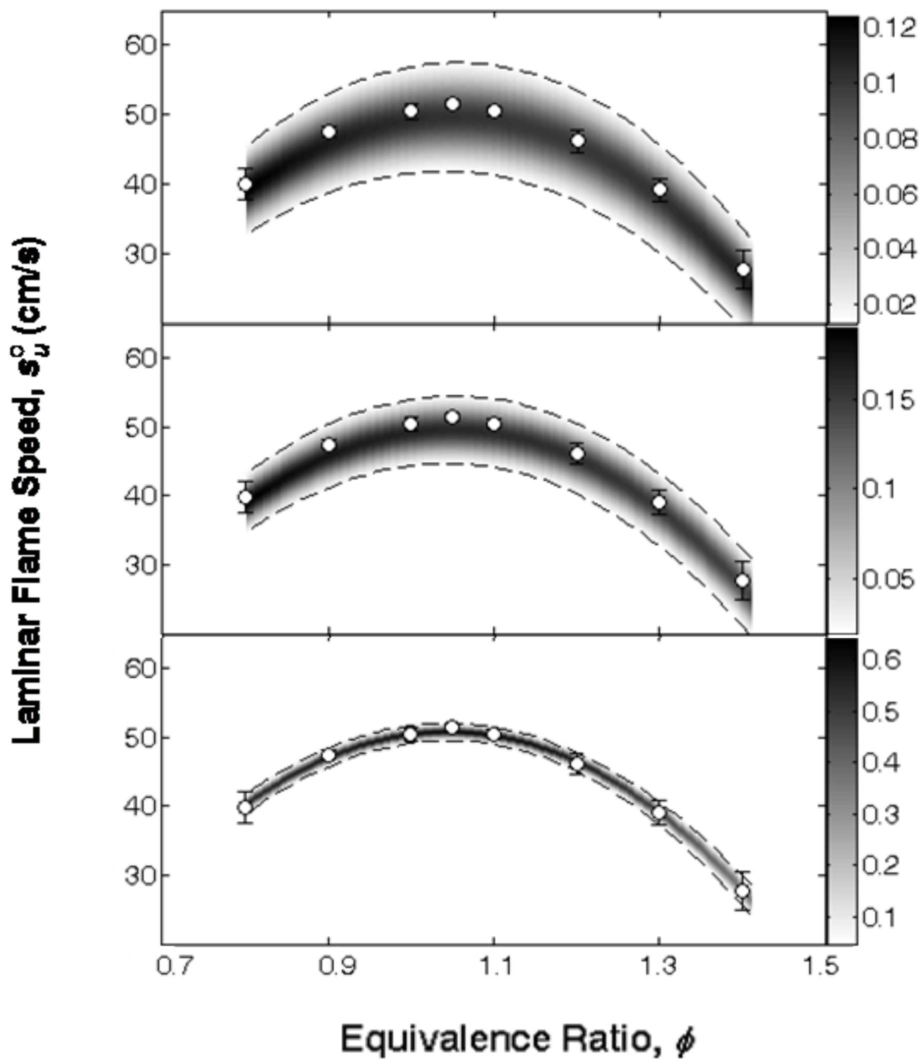
	No.	P_0, P_5 (atm)	T_0, T_5 (K)	f
Laminar Flame Speeds	4	1	353	0.8-1.4
Ignition Delay Times	11	1-4	1000-2600	0.5-2

	No.	P_5 (atm)	T_5 (K)	f
OH, H_2O, CO_2, C_2H_4, CH_3 Species Profiles	11	1.6-2.4	1365-1545 K	1

Predictions of As-Compiled and Uncertainty-Minimized Models



Effect on Flame Speed Predictions

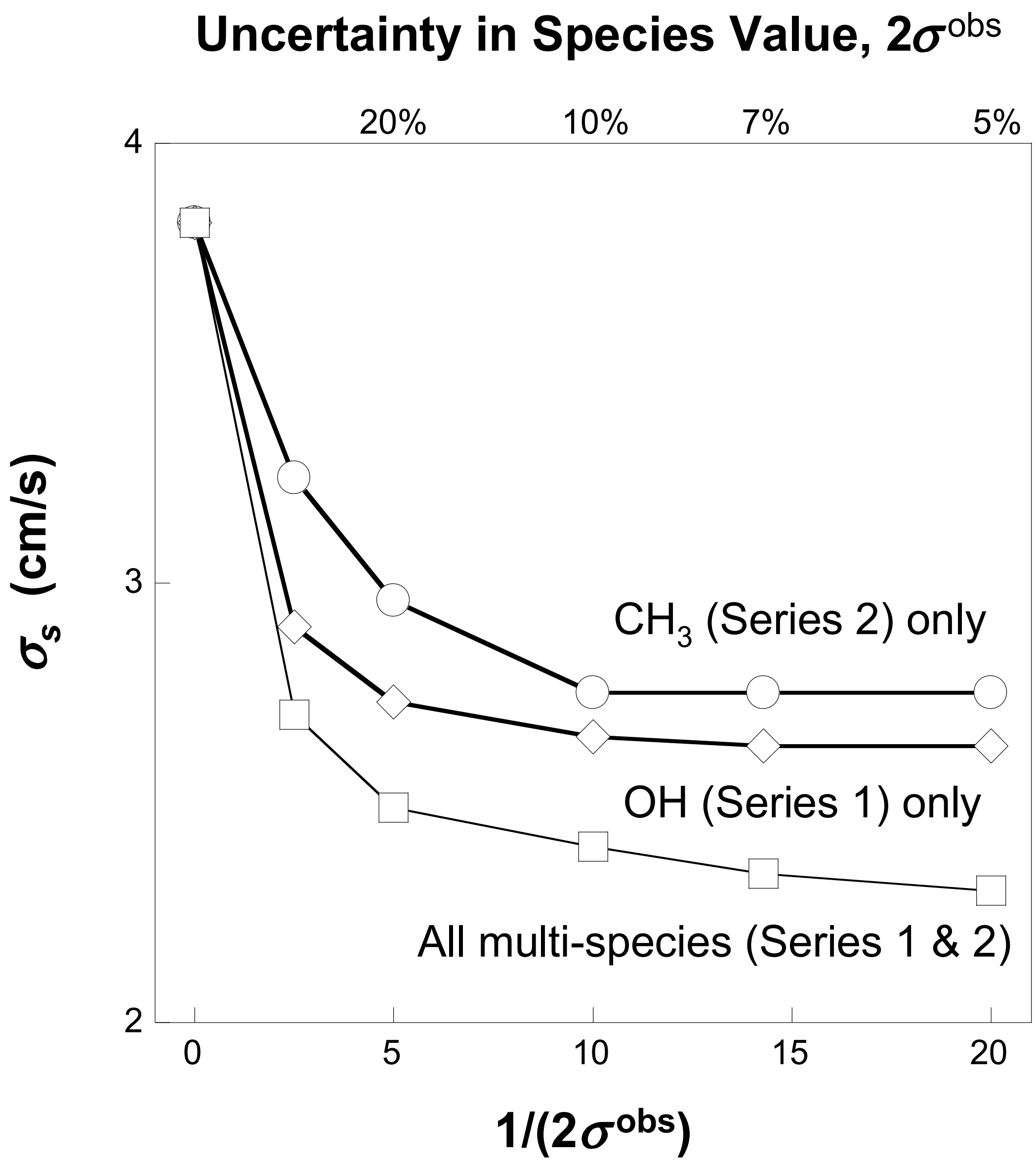


Considering no experiments

Model constrained by species profiles

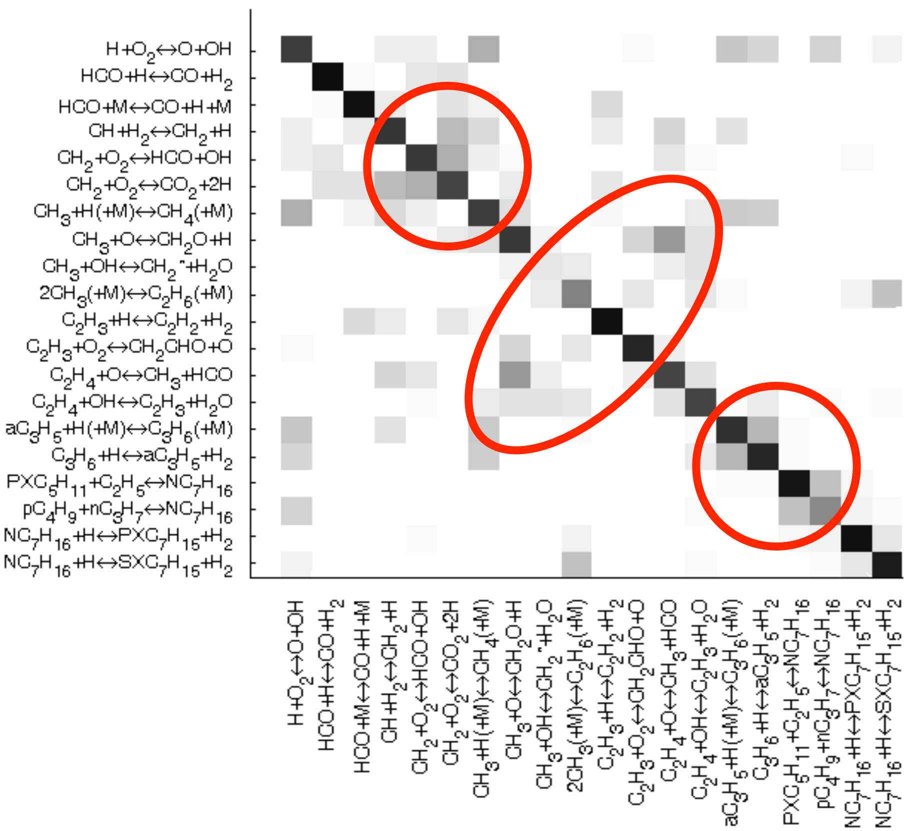
Model constrained by species profiles
+ flame speeds

Effect on Flame Speed Predictions

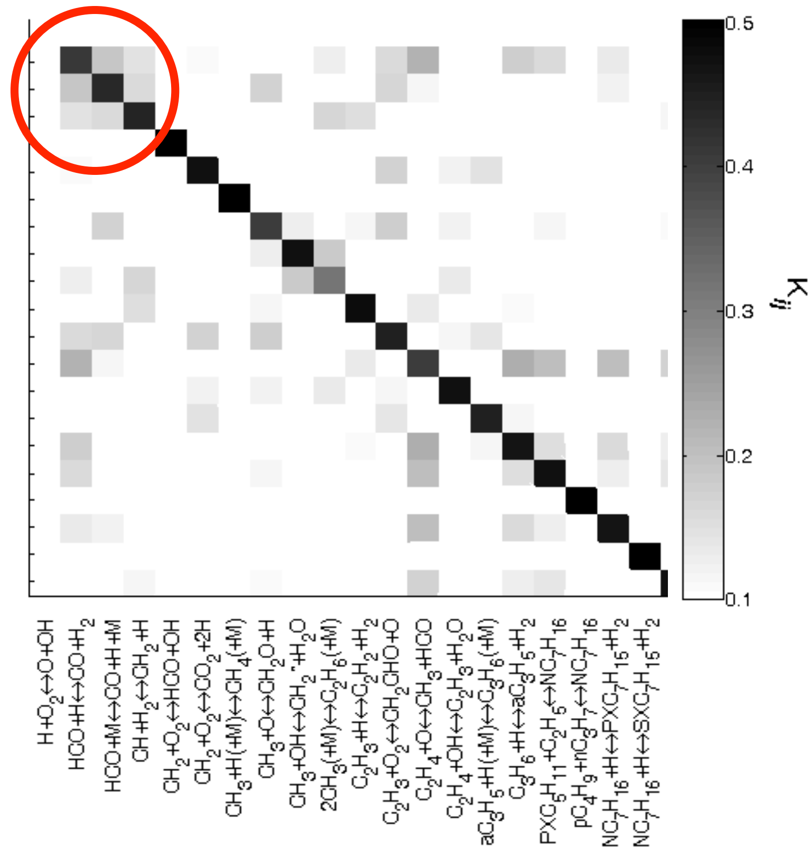


What did uncertainty minimization do?

Model constrained by species profiles



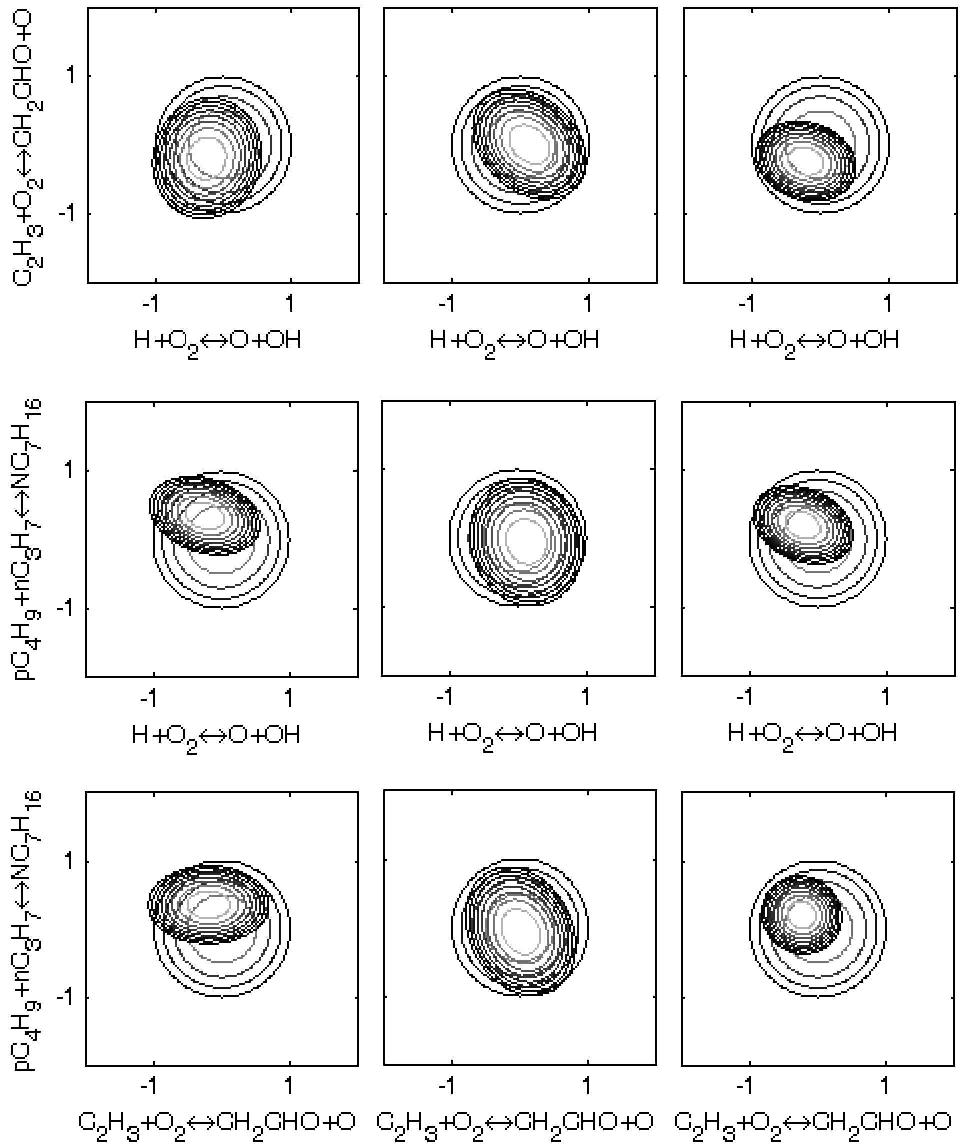
Model constrained by flame speeds



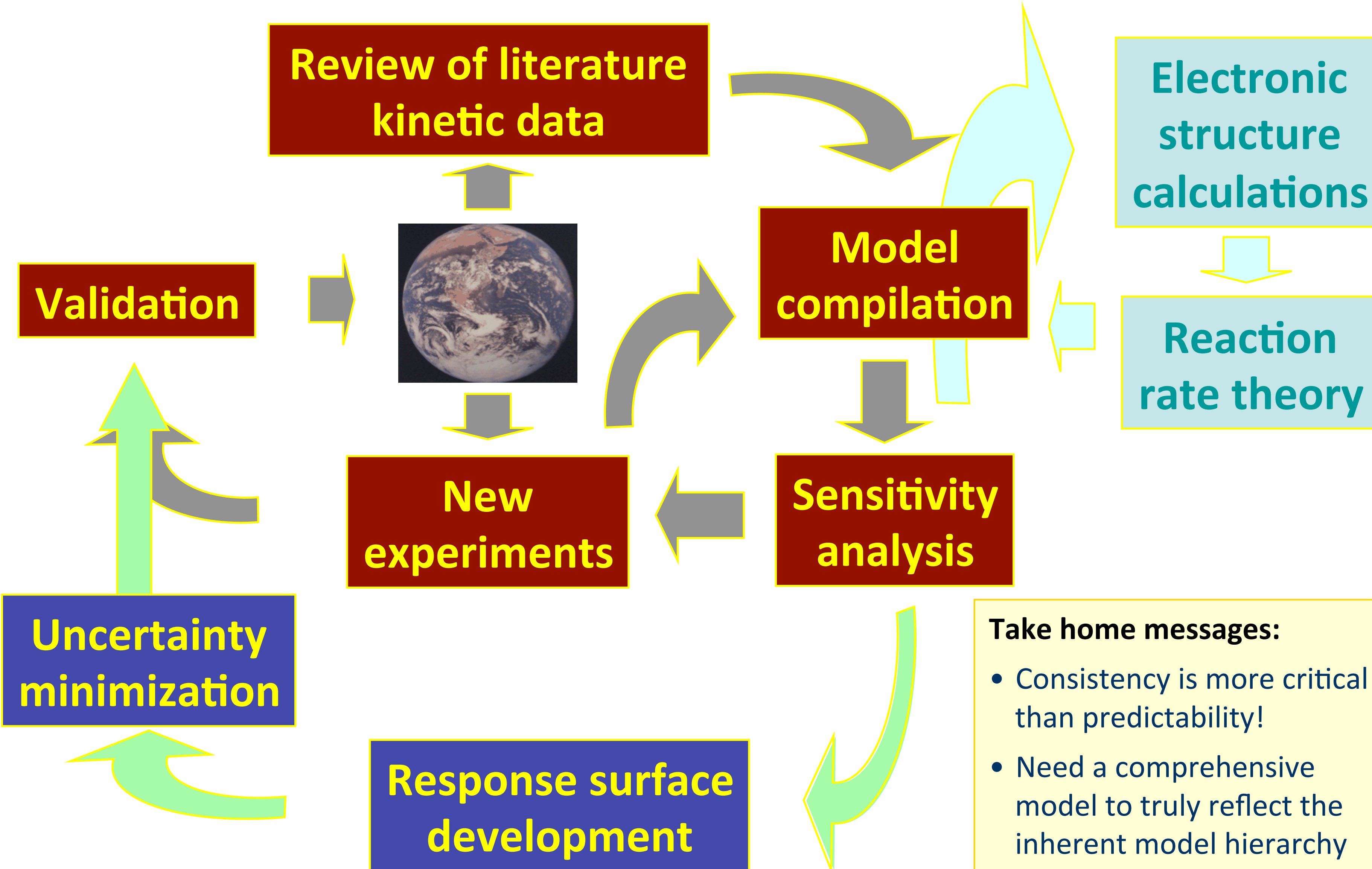
CH_3, CH_2, secondary chain branching, fuel breakup

H chain branching

What did uncertainty minimization do?



"Our" Approach



Take home messages:

- Consistency is more critical than predictability!
- Need a comprehensive model to truly reflect the inherent model hierarchy and uncertainty.

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- Bing yang

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- Chung-King Law (Princeton)
- Fokion Egolfopoulos (USC)
- Elke Goos (DLR)

The JetSurF team

Ron Hanson (Stanford)
Tom Bowman (Stanford)
Heinz Pitsch (Stanford)
Wing Tsang (NIST)
Angela Violi (UMich)
Peter Lindstedt (Imperial Col.)
Nick Cernansky (Drexel)
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