Multi-Scale Chemical Process Modeling with Bayesian Nonparametric Regression

Evan Ford,[1] Fernando V. Lima[2] and David S. Mebane[1]
[1]Mechanical and Aerospace Engineering
[2]Chemical Engineering
West Virginia University

CCSI
Carbon Capture Simulation Initiative

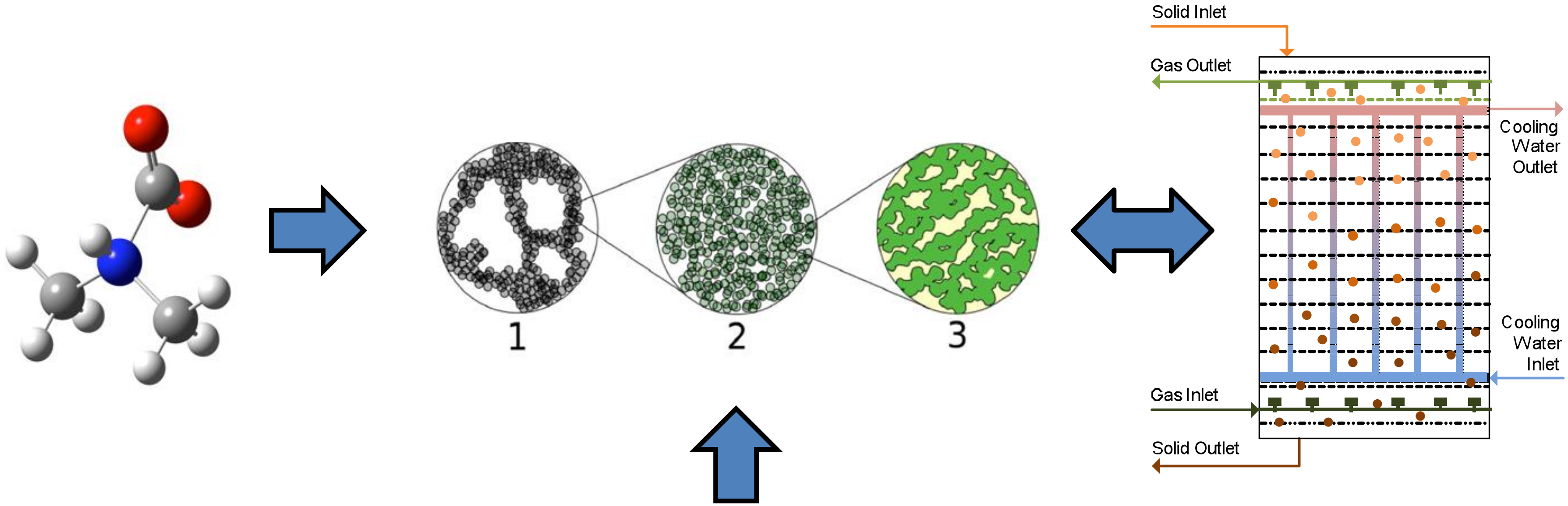
AIChE Annual Meeting, Salt Lake City
November 10th, 2015

Energy Systems and Materials Simulation

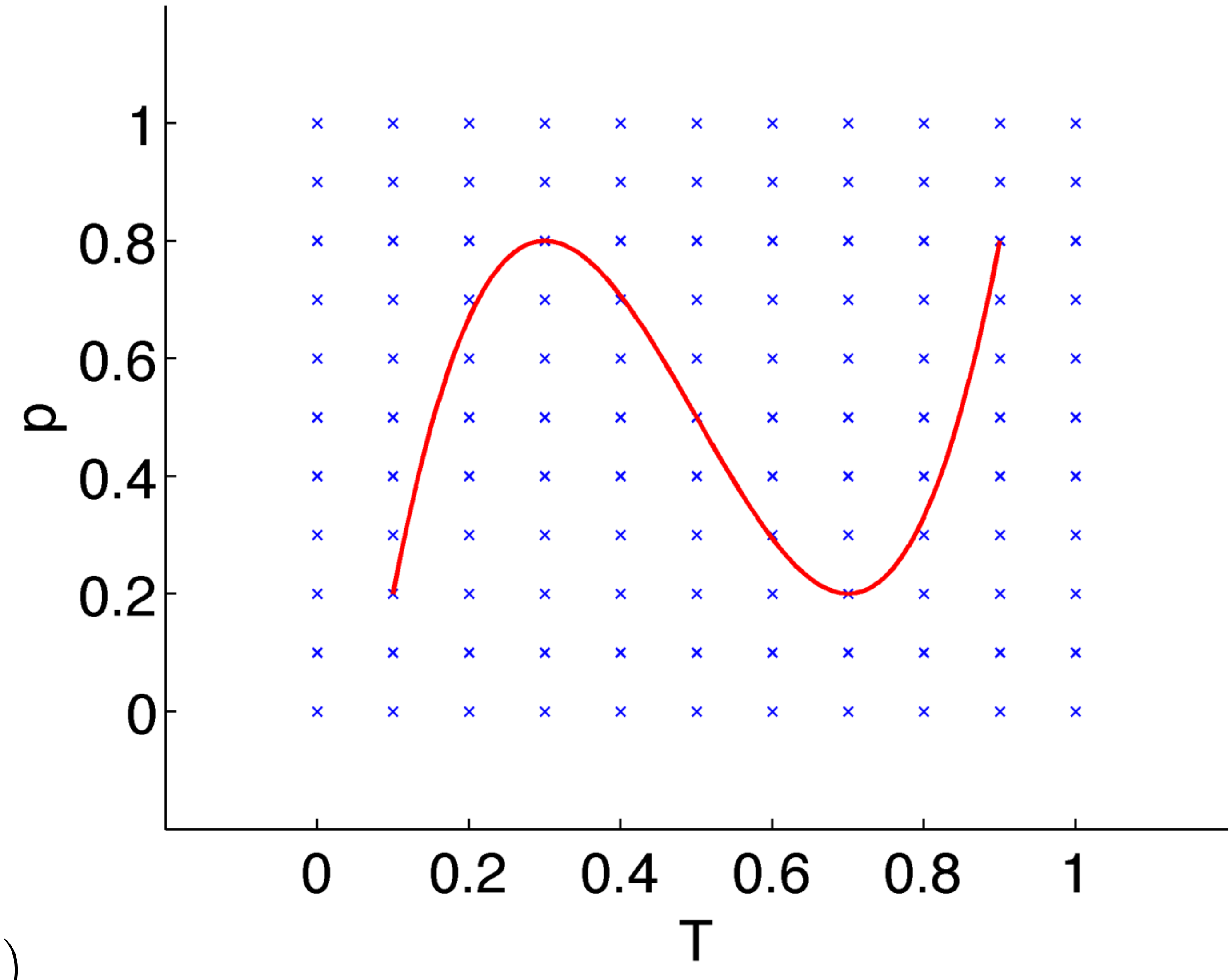
West Virginia University

outline

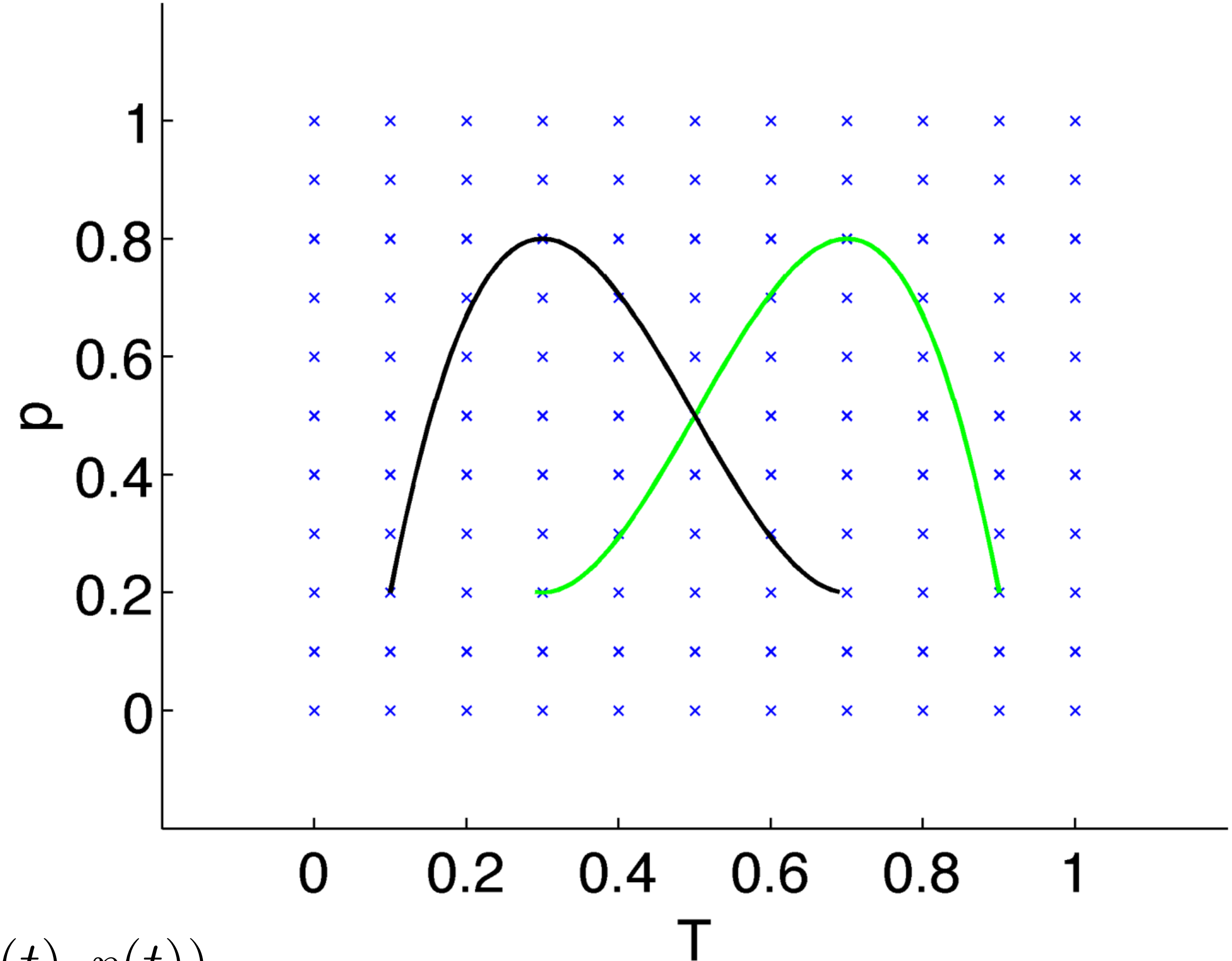
- Reduced modeling and prediction in dynamic systems ➔ uncertainty quantification
- Bayesian calibration and BSS-ANOVA Gaussian processes
- Results in carbon capture: two-state reaction; calibration with propagation from TGA to BFB adsorber
- Results in catalytic steam reformation: 16-state reaction; calibration with propagation from lab-scale CSTR to industrial-scale PFR



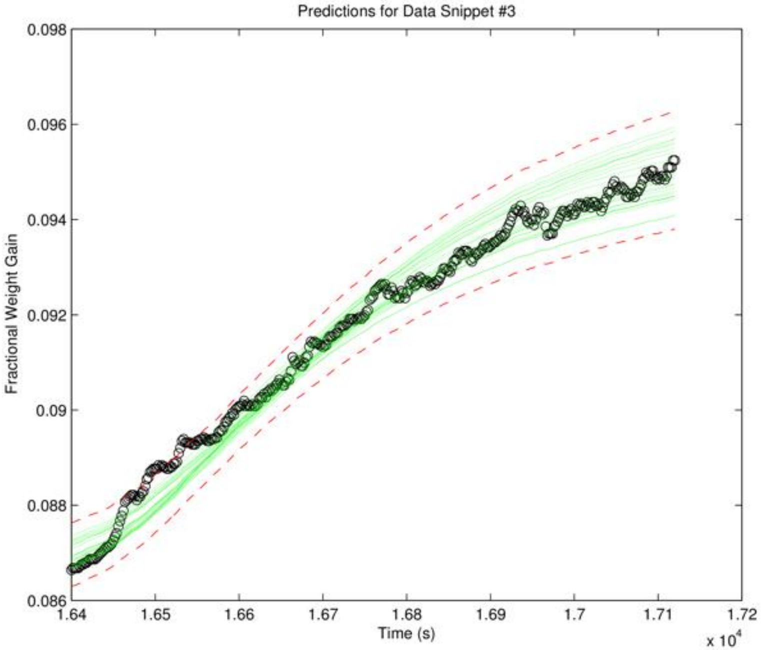
Bench-scale data: TGA, fixed bed, etc.

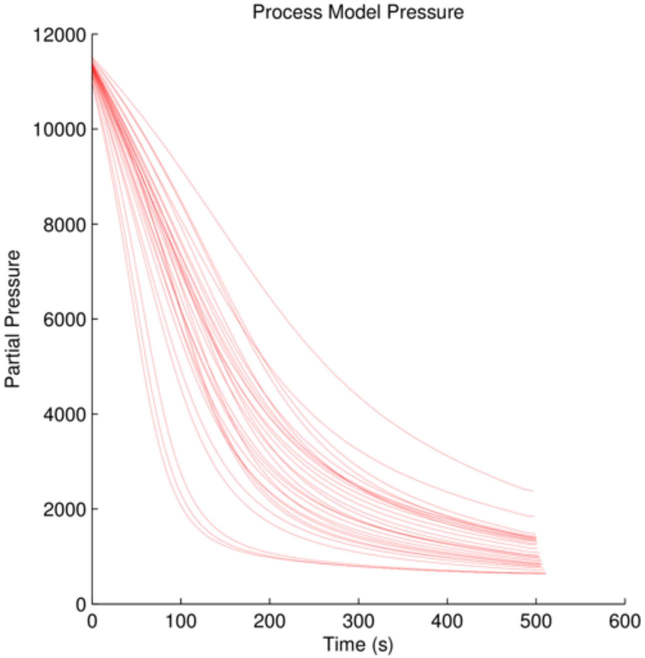


$$x = f(T, p)$$



$$\dot{x} = f(x, T(t), p(t))$$





K.S. Bhat, DSM, *et al.*, submitted, arXiv:1411.2578.

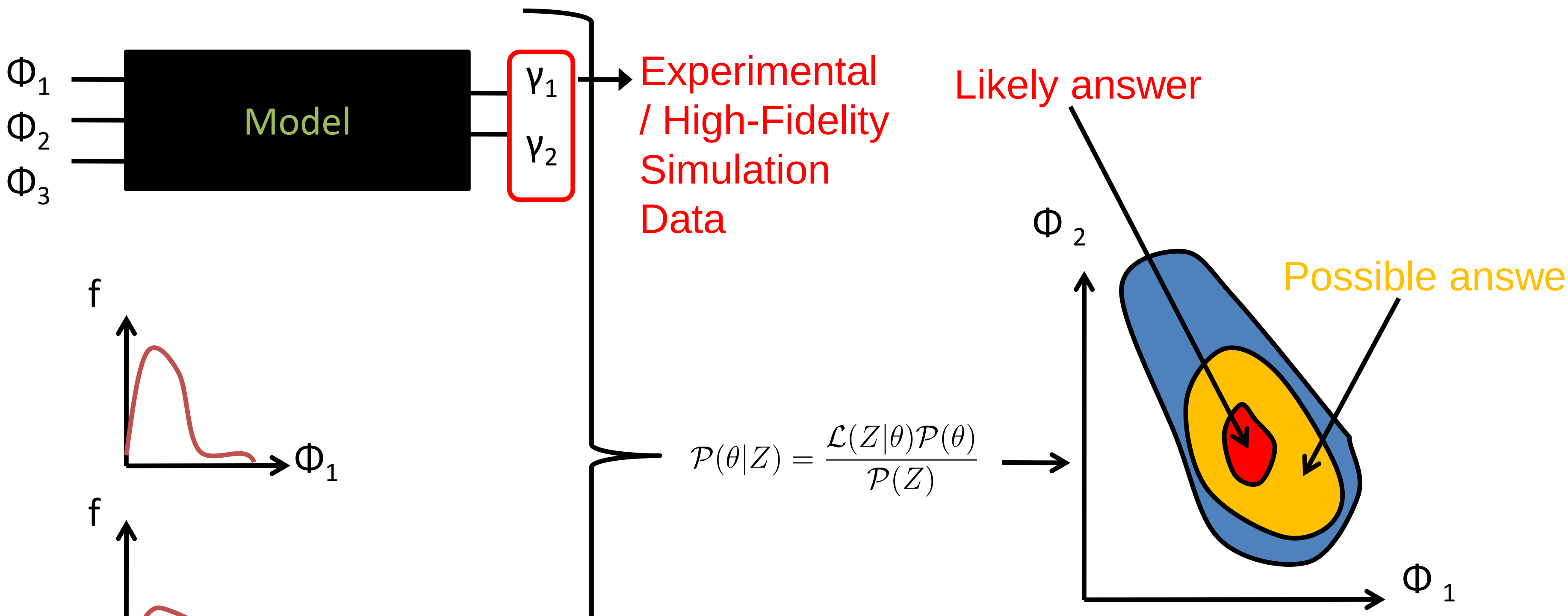
what is Bayesian statistics?

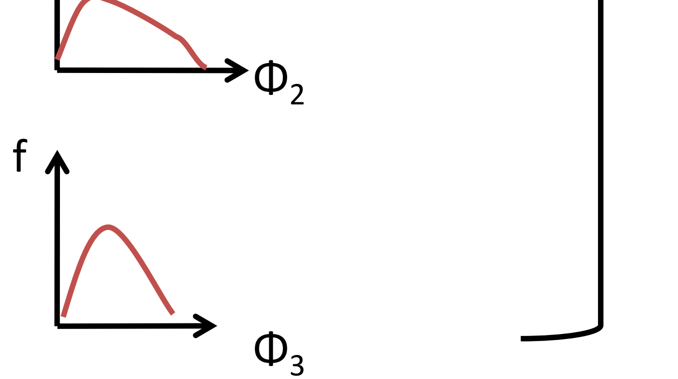
- Two ways to think about probability:
  - Stuff is really random (rainfall) ➔ aleatory uncertainty
  - Stuff is not really random, we just don't know what it is (oddsmaking) ➔ epistemic uncertainty
- Bayesian statistics handles both kinds.
- Things that we think of as fixed values can now have probability distributions.
- How do these probability distributions evolve in light of evidence?
- Bayes' theorem:

$$\mathcal{P}(\theta|Z) = \frac{\mathcal{L}(Z|\theta)\mathcal{P}(\theta)}{\mathcal{P}(Z)}$$

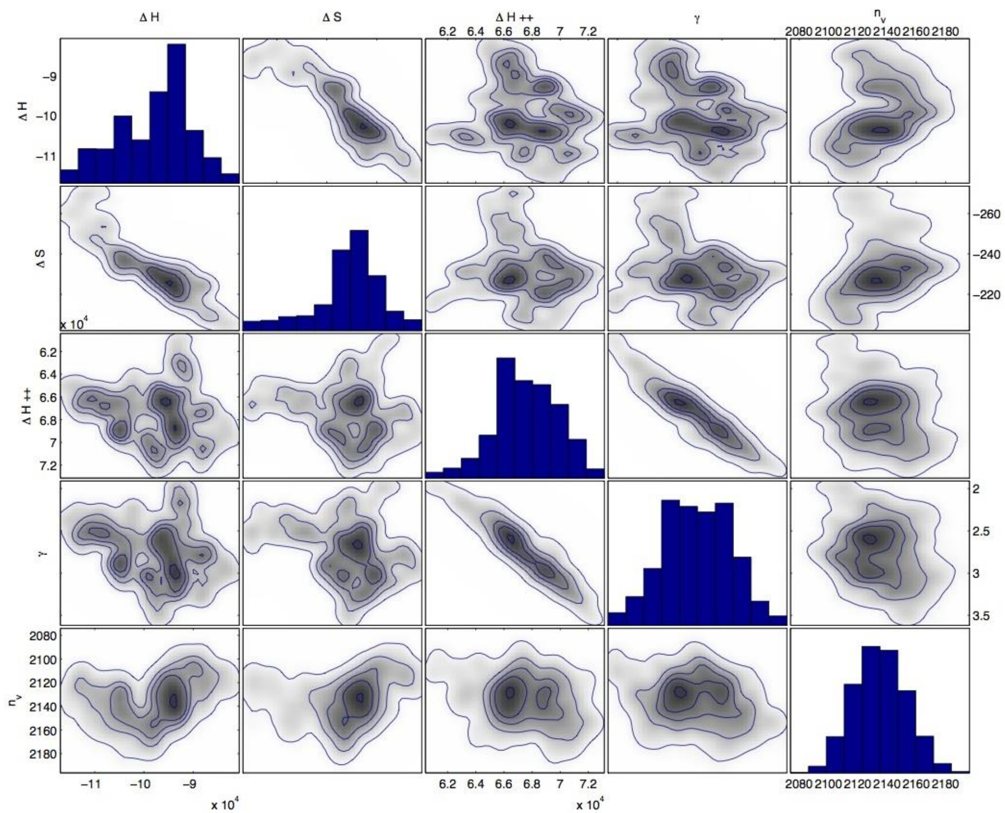
new odds = (old odds)(evidence adjustment)

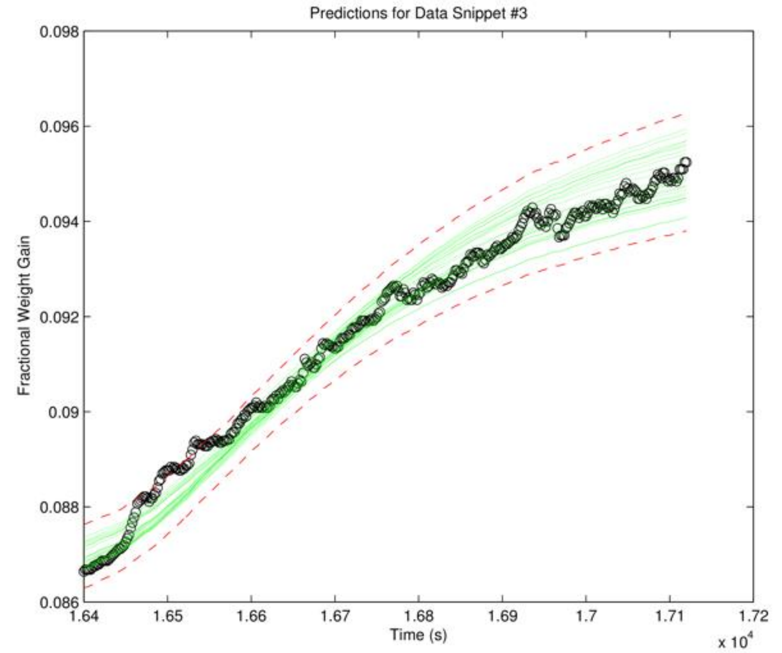
Bayesian model-based analysis

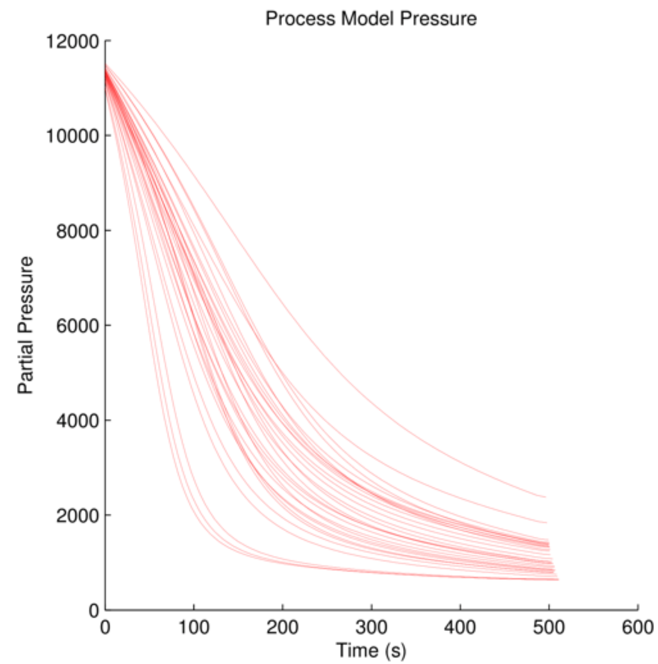




The result of Bayesian calibration is a probability distribution on the parameter space.







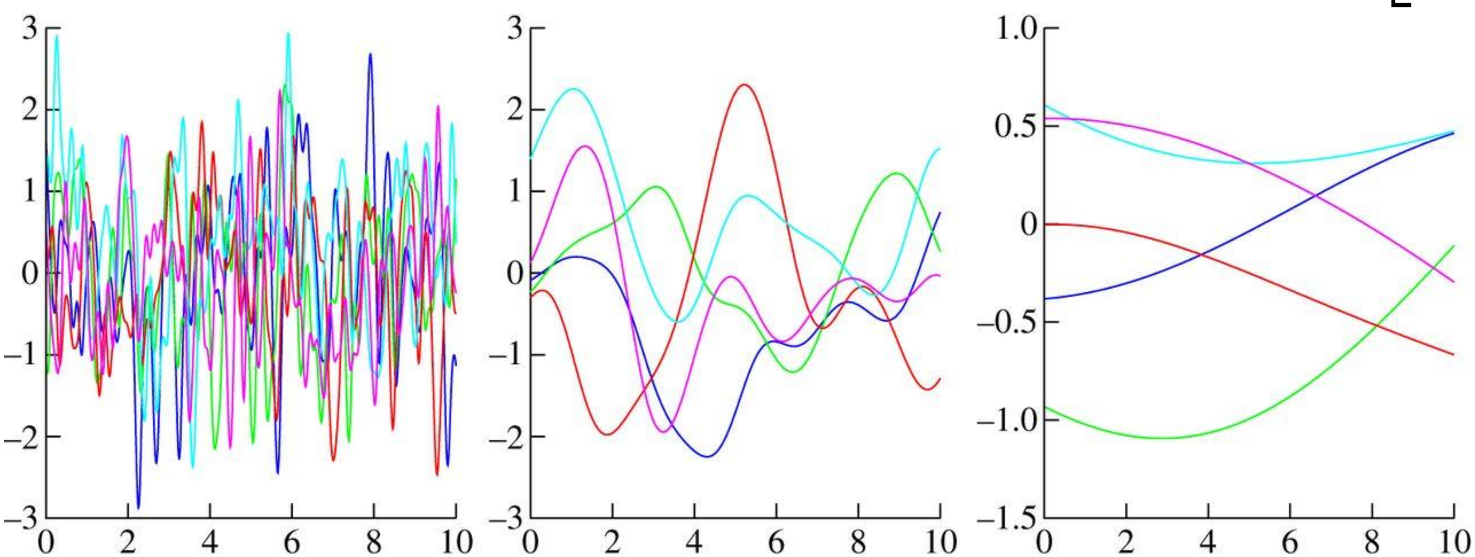
K.S. Bhat, DSM, *et al.*, submitted, arXiv:1411.2578.

$$\dot{x} = f(x, T(t), p(t))$$

- What is the form of *f* ?
  - flexible
  - easy for calibration
  - physically constrained

Gaussian process $f = f(\theta, \delta)$ $\delta \sim MVN(0, \Gamma)$

$$\Gamma_{ij} = \sigma^2 \exp\left[\frac{(\vartheta_i - \vartheta_j)^2}{\phi}\right]$$



S. Roberts, *et al.*, *Phil. Trans. A* **371** (2013) 20110550.

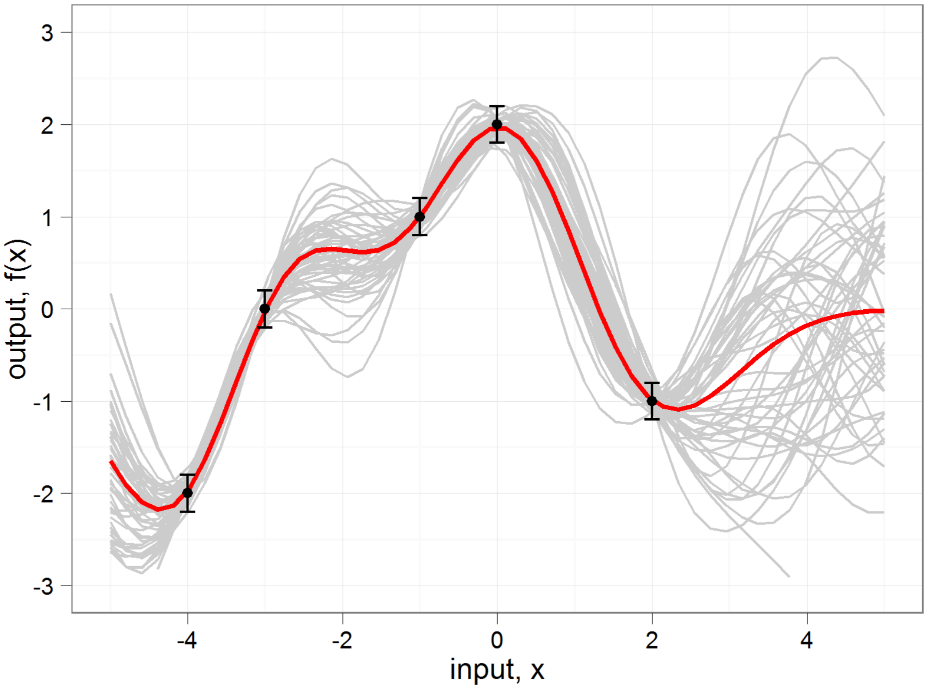
$$\dot{x} = f(x, T(t), p(t))$$

- What is the form of *f* ?
  - flexible
  - easy for calibration
  - physically constrained

Gaussian process

$$f = f(\theta, \delta) \qquad \delta \sim MVN(0, \Gamma)$$

$$\Gamma_{ij} = \sigma^2 \exp\left[\frac{(\vartheta_i - \vartheta_j)^2}{\phi}\right]$$



James Keirstead, Imperial College

$$\delta \sim MVN(0, \Gamma)$$

$$\Gamma(\vartheta, \vartheta') = \sigma_0^2 + \sum_{k=1}^{K} \sigma_k^2 \Gamma_1(\vartheta_k, \vartheta_k') + \sum_{k=1}^{K-1} \sum_{l=k}^{K} \sigma_{kl}^2 \Gamma_2([\vartheta_k, \vartheta_l], [\vartheta_k', \vartheta_l']) + \cdots$$

$$\Gamma_1(\vartheta_k, \vartheta_k') = \mathcal{B}_1(\vartheta_k)\mathcal{B}_1(\vartheta_k') + \mathcal{B}_2(\vartheta_k)\mathcal{B}_2(\vartheta_k') - \frac{1}{4!}\mathcal{B}_4(|\vartheta_k - \vartheta_k'|)$$

$$\Gamma_2([\vartheta_k, \vartheta_l], [\vartheta_k', \vartheta_l']) = \Gamma_1(\vartheta_k, \vartheta_k')\Gamma_1(\vartheta_l, \vartheta_l')$$

$$\delta(\vartheta; \beta) = \beta_0 + \sum_{k=1}^{K} \sum_{m=1}^{M} \beta_{mk} \varphi_{m1}(\vartheta_k) + \sum_{k=1}^{K-1} \sum_{l=k+1}^{K} \sum_{m=1}^{M} \beta_{mkl} \varphi_{m2}(\vartheta_k, \vartheta_l) + \cdots$$

$$\beta_{mk} \sim N(0, \lambda_{m1}\sigma_k^2)$$

$$\beta_{mkl} \sim N(0, \lambda_{m2}\sigma_{kl}^2)$$

$$\dot{x}_i = f_i(x_i, x_j; k_i, \kappa_i)$$

$$k_i = k_i^0 \exp\left[\delta_{k_i}(x_i, x_j, T; \beta_{kijT})\right]$$

$$\kappa_i = \kappa_i^0 \exp\left[\delta_{\kappa_i}(x_i, x_j, T; \beta_{\kappa ijT})\right]$$

B.J. Reich, *et al.*, *Technometrics* **51** (2009) 110.

K.S. Bhat, DSM, *et al.*, submitted, arXiv:1411.2578.

- All draws belong to a 2nd-order Sobolev space.
- Orthogonal basis functions ➔ ordered set for model building.
- Dynamics physically constrained as chemical rate expressions.
- *betas* block proposed in calibration.

$$\delta(\vartheta;\beta) = \beta_0 + \sum_{k=1}^{K}\sum_{m=1}^{M}\beta_{mk}\varphi_{m1}(\vartheta_k) + \sum_{k=1}^{K-1}\sum_{l=k+1}^{K}\sum_{m=1}^{M}\beta_{mkl}\varphi_{m2}(\vartheta_k,\vartheta_l) + \cdots$$

$$\beta_{mk} \sim N(0,\lambda_{m1}\sigma_k^2)$$

$$\beta_{mkl} \sim N(0,\lambda_{m2}\sigma_{kl}^2)$$

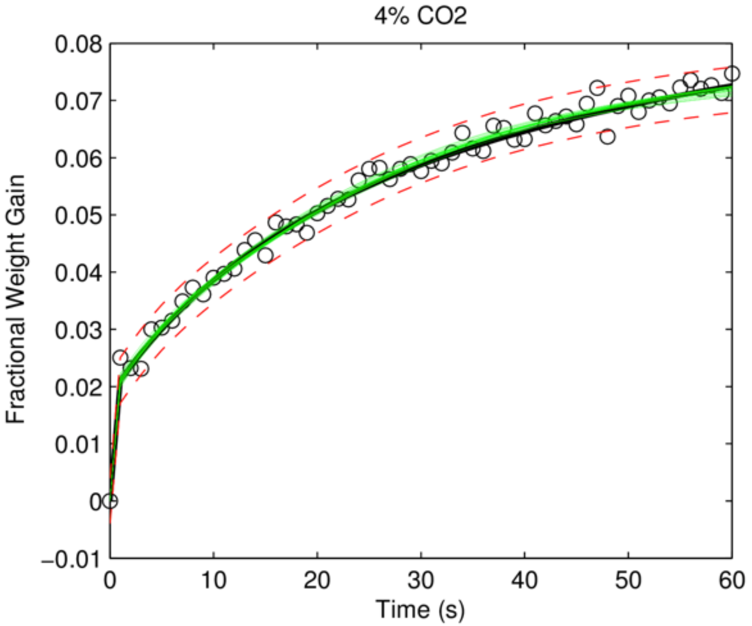
$$\dot{x}_i = f_i(x_i, x_j; k_i, \kappa_i)$$

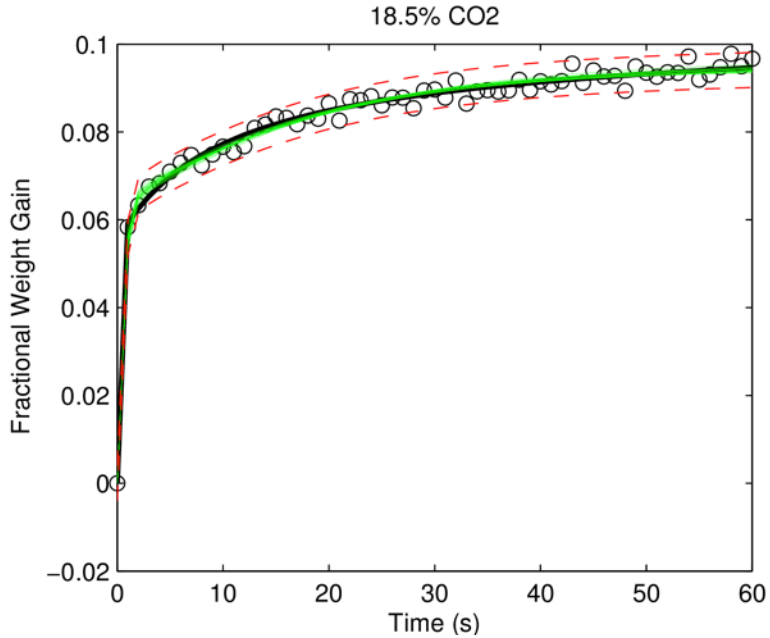
$$k_i = k_i^0 \exp\left[\delta_{k_i}(x_i, x_j, T; \beta_{kijT})\right]$$

$$\kappa_i = \kappa_i^0 \exp\left[\delta_{\kappa_i}(x_i, x_j, T; \beta_{\kappa ijT})\right]$$

B.J. Reich, et al., *Technometrics* **51** (2009) 110.

K.S. Bhat, DSM, *et al.*, submitted, arXiv:1411.2578.



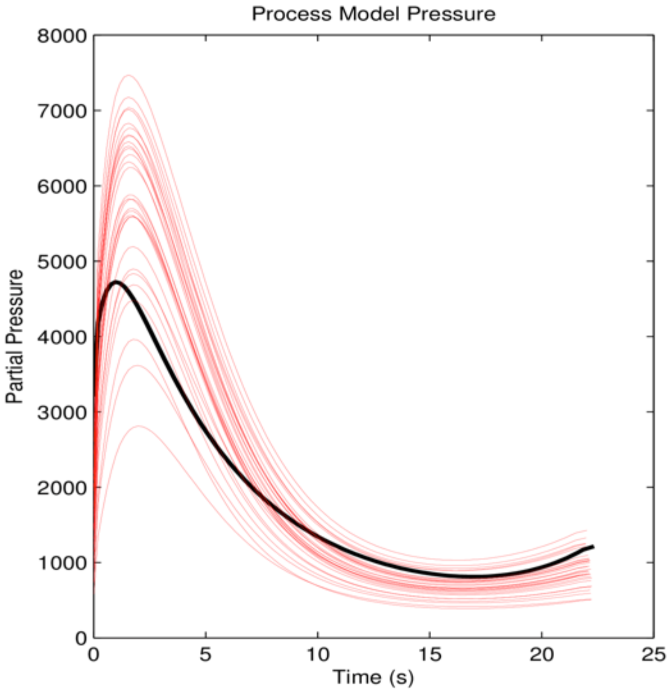


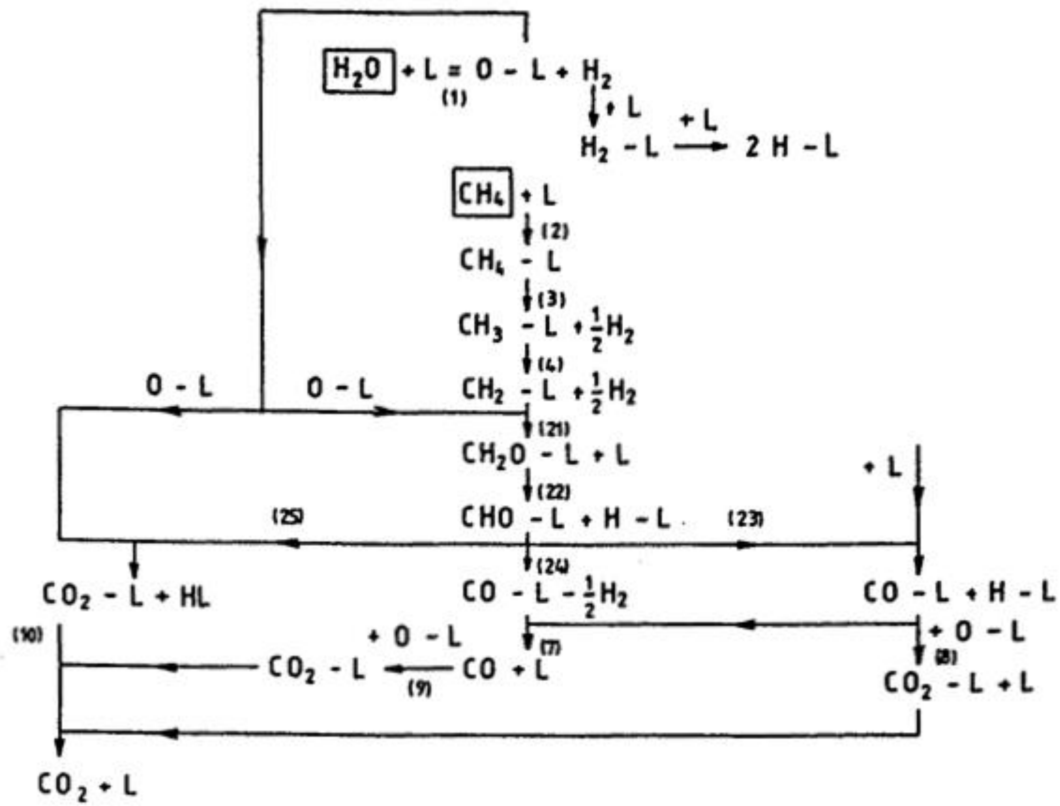
$$\dot{z} = k_{\mathrm{z}}\Big[p(1-2x) - z/\kappa_{\mathrm{z}}\Big] - k_{\mathrm{x}}\Big[z(1-2x) - x^2/\kappa_{\mathrm{x}}\Big]$$

$$\dot{x} = k_{\mathrm{x}}\Big[z(1-2x) - x^2/\kappa_{\mathrm{x}}\Big]$$

$$\dot{x} = k^0 \exp\left[\delta_{\mathrm{k}}(x,p,T)\right]\Big\{p(1-2x)^2 - x^2/\kappa^0 \exp\left[\delta_{\mathrm{K}}(p,T)\right]\Big\}$$

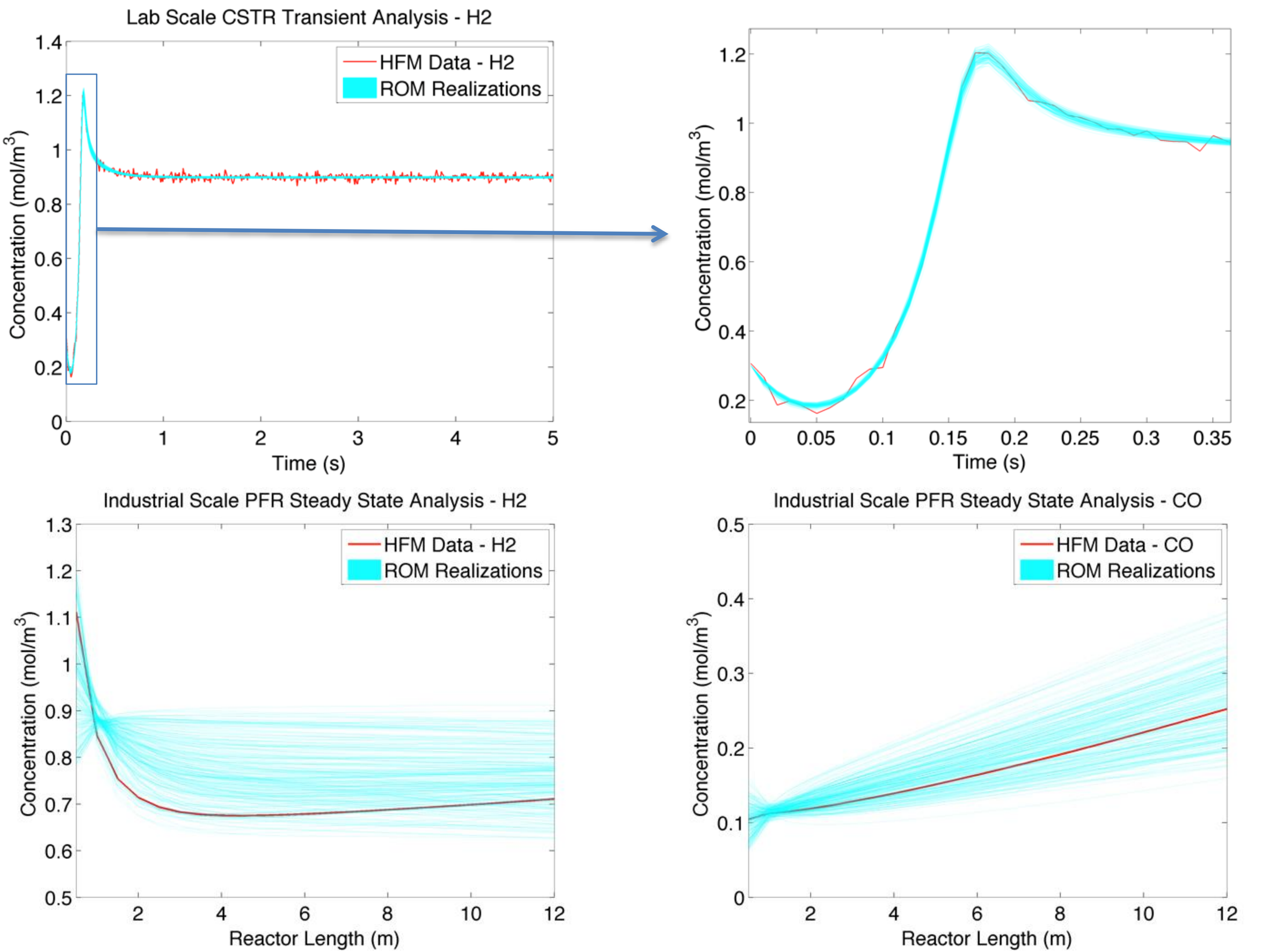
K.S. Bhat, DSM, *et al.*, submitted, arXiv:1411.2578.





J. Xu and G.F. Froment, *AIChE J.* **35** (1989) 88.

$$CH_4 + H_2O \Rightarrow CO + 3H_2$$
$$H_2O + CO \Rightarrow CO_2 + H_2$$
$$CH_4 + 2H_2O \Rightarrow CO_2 + 4H_2$$


Lab Scale CSTR Transient Analysis - H2
HFM Data - H2
ROM Realizations
Concentration (mol/m^3)
Time (s)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
1
2
3
4
5
Concentration (mol/m^3)
Time (s)
0.2
0.4
0.6
0.8
1
1.2
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
Industrial Scale PFR Steady State Analysis - H2
HFM Data - H2
ROM Realizations
Concentration (mol/m^3)
Reactor Length (m)
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
2
4
6
8
10
12
Industrial Scale PFR Steady State Analysis - CO
HFM Data - CO
ROM Realizations
Concentration (mol/m^3)
Reactor Length (m)
0
0.1
0.2
0.3
0.4
0.5
2
4
6
8
10
12

what's next?

- Harder and harder problems: Fischer-Tropsch is up next.
- Solutions for optimization and design under uncertainty
- Solutions for machine learning-based control
- Automated model building for dynamic systems

CCSI
Carbon Capture Simulation Initiative

Accelerating Technology Development

Rapidly synthesize optimized processes to identify promising concepts → Better understand internal behavior to reduce time for troubleshooting → Quantify sources and effects of uncertainty to guide testing & reach larger scales faster → Stabilize the cost during commercial deployment

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory EST. 1943
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin

Industry

- ADA Environmental Solutions
- ALSTOM
- B&W the babcock&wilcox company
- GE
- EPRI Electric Power Research Institute
- FLUOR
- Phillips 66
- AEP American Electric Power
- Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
- Southern Company
- ExxonMobil
- Chevron
- URS
- Air Products
- EASTMAN
- aspentech
- ANSYS
- Schneider Electric
- PSE

acknowledgements

K. Sham Bhat	Los Alamos National Lab
Curtis B. Storlie	Mayo Clinic
Priyardashi Mahapatra	National Energy Technology Lab
David C. Miller	National Energy Technology Lab

Questions? Want software?

david.mebane@mail.wvu.edu