# A Multi-model Predictive Control Approach Based on Dynamic Discrepancy Reduced Order Modeling

Session: Advances in Process Control

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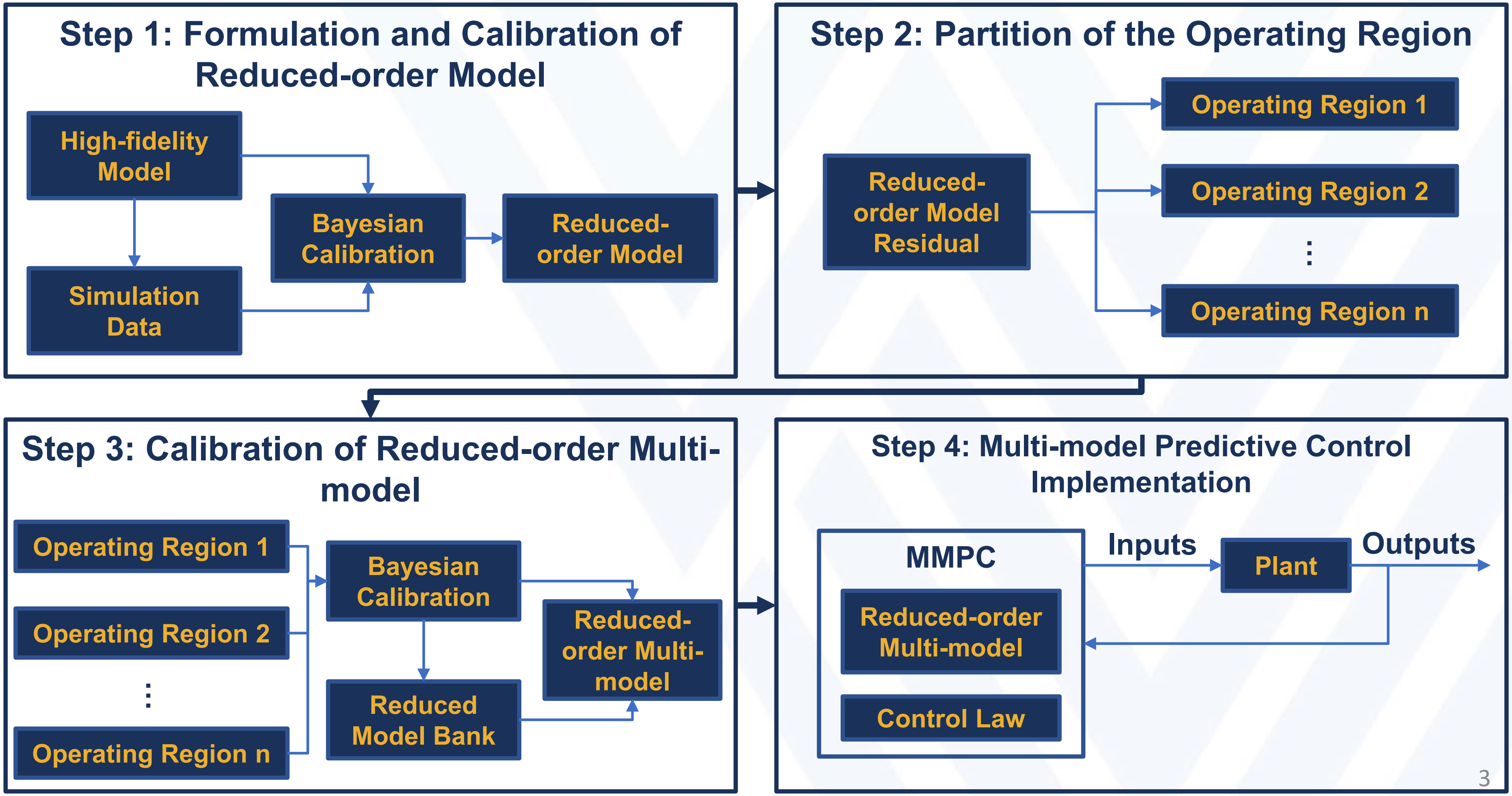
# Background

- Challenges and motivation:
  - Online implementation of Nonlinear Model Predictive Control (NMPC) requires a simplified dynamic model for real-time control
  - Multiple different models may be needed at different operating regions to reduce plant-model mismatch
  - Parameter estimation for dynamic modeling may not reflect the uncertainty propagation from model inputs to the model outputs
- Objectives:
  - Formulate and calibrate reduced-order multi-model
  - Implement the multi-model for NMPC

# Proposed Framework



# Bayesian Calibration

Let $u$ be the model input, $y(u)$ be the real measurement of the output, $\theta$ be the uncertainty vector, $\eta(u, \theta)$ be the model, $\sigma(u)$ be the discrepancy term (plant-model mismatch), and $\epsilon(u)$ be the measurement noise

$$y(u) = \eta(u, \theta) + \sigma(u) + \epsilon(u)$$

Bayesian calibration: Given the set of measurements $\{y(u)\}$, calculate the probability distribution of $\theta$

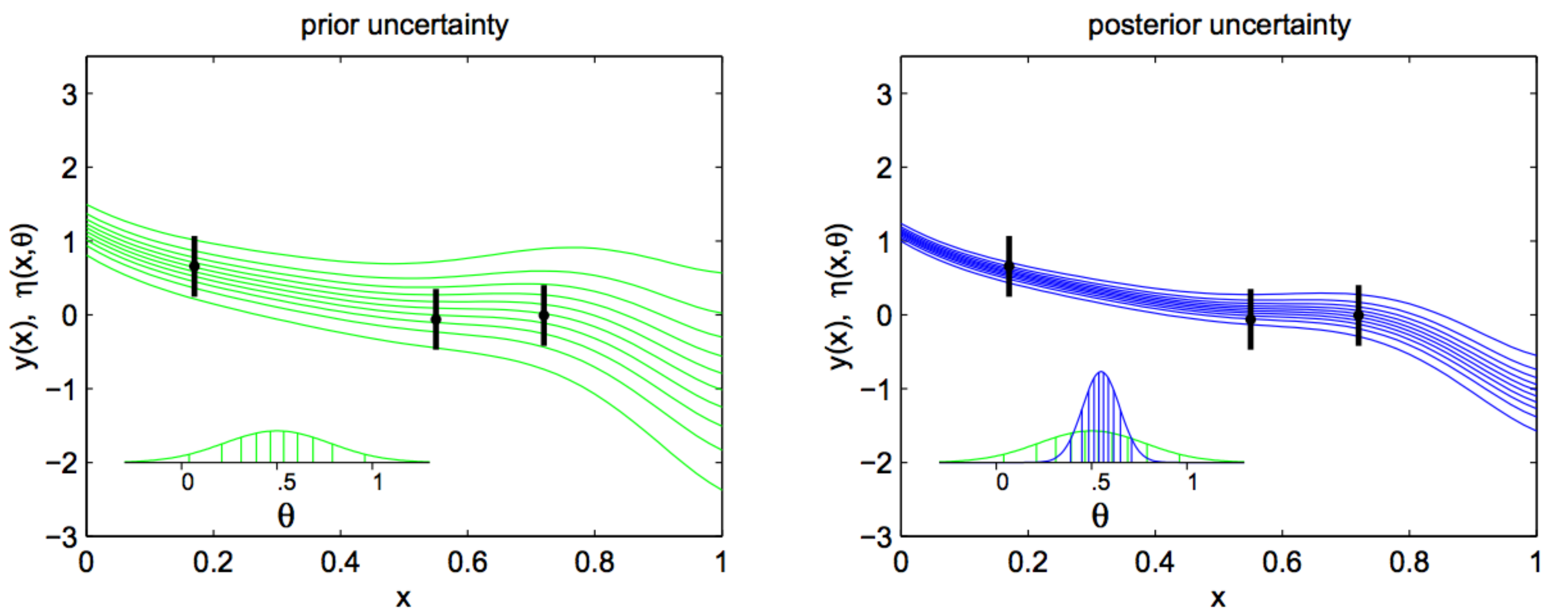





Image source: Higdon, Kennedy, Cavendish, Cafeo, Ryne (2004)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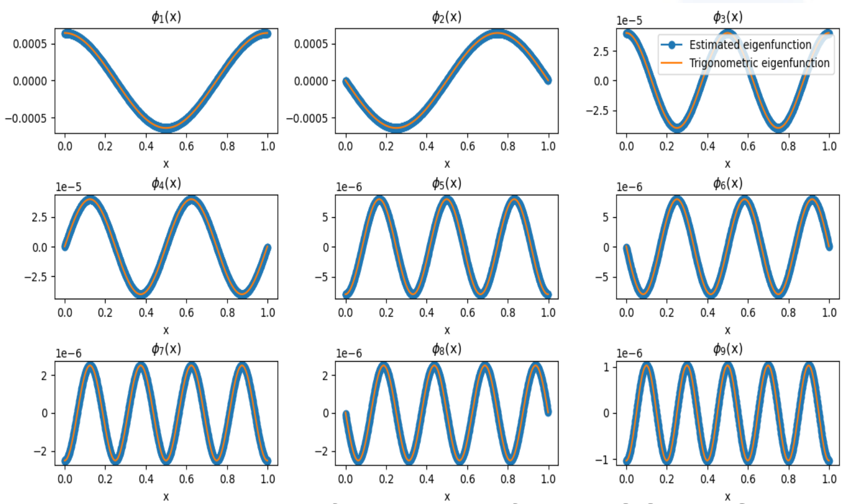
# Dynamic Discrepancy with Bayesian Smoothing Spline Analysis of Variance

Reducing the order of the high-fidelity model introduces uncertainty into the model representation:

$$\dot{x} = f_{reduced}\big(x, u, \sigma(x, u, \theta)\big) = f_{high-fidelity}(x, u)$$

The discrepancy function to characterize such uncertainty is chosen to be a Bayesian Smoothing Spline Analysis of Variance (BSS-ANOVA) model:

$$\sigma(u) = \theta_0 + \sum_{r=1}^{R} \underbrace{\sum_{l=1}^{\infty} \theta_{r,l} \times \phi_l(u_r)}$$




First 9 basis functions of the BSS-ANOVA

The effect of each input is represented by the sum of orthogonal functions $\phi_l$, and the stochastic parameters $\theta$ are calibrated

The basis functions are added one at a time to increase accuracy of the discrepancy function

# Calibration with Approximated Bayesian Computation

Given by propagating the uncertainty through the model $f_{reduced}$

Initial guess of the parameter distribution (Prior distribution)

Bayes' theorem:

$$\mathbb{P}(\theta|x) = \frac{\mathbb{L}\boldsymbol{ikelyhood}(\boldsymbol{x}|\boldsymbol{\theta}) \times \mathbb{P}(\boldsymbol{\theta})}{\int \mathbb{L}\boldsymbol{ikelyhood}(\boldsymbol{x}|\boldsymbol{\theta}) \times \mathbb{P}(\boldsymbol{\theta})\boldsymbol{dxd\theta}}$$

Normalization constant; will be canceled out if using Markov Chain Monte Carlo for calibration

Approximated Bayesian Computation for likelihood function's approximation:

Matching the <u>first</u> moment of the reduced-order model to the high-fidelity model

Matching the <u>second</u> moment of the reduced-order model to the high-fidelity model

$$\mathbb{L}\boldsymbol{ikelyhood}(\boldsymbol{x}|\boldsymbol{\theta}) = \frac{\mathbf{1}}{\boldsymbol{\varepsilon}\sqrt{\mathbf{2}\boldsymbol{\pi}}}\prod_{\boldsymbol{i}} \boldsymbol{exp}\left(-\frac{(\boldsymbol{\mu_i}(\boldsymbol{\theta}) - \boldsymbol{x_i})^2 + (\boldsymbol{\sigma_i}(\boldsymbol{\theta}) - \boldsymbol{\gamma}|\boldsymbol{\mu_i}(\boldsymbol{\theta}) - \boldsymbol{x_i}|)^2}{\mathbf{2}\boldsymbol{\varepsilon}^2}\right)$$



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# Multi-model Representation

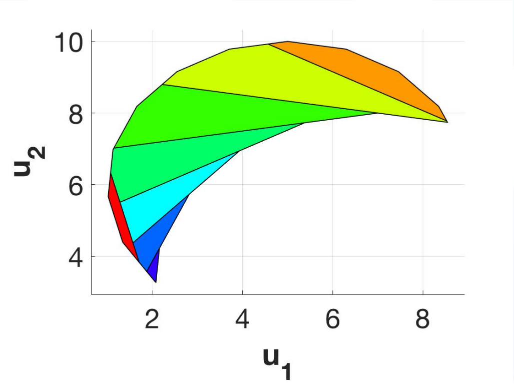
- To increase accuracy, the structure of the reduced-order model remains constant, but its parameters are calibrated at different operating regions
- The reduced-order multi-model parameters, $\theta$, are defined as:

$$\theta(u) = \sum_{i=1}^{number\ of\ model} I_{i^{th}\ region}(u)\theta_{i^{th}\ region}$$

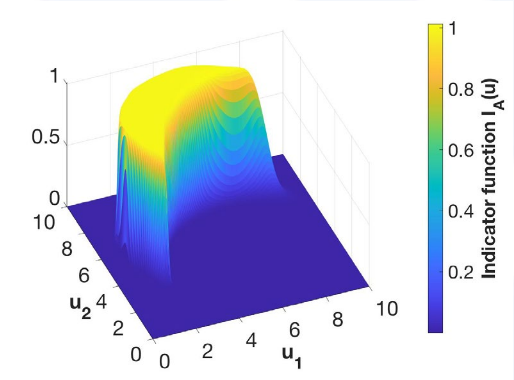
- If each region is represented as a union of a set of polyhedra $S = \cup\{A_i u \geq b_i\}_{i=1}^{N}$, let $A_i(j), b_i(j)$ be the $j^{th}$ row of $A_i, b_i$ respectively. The sigmoid indicator function with smoothing constant $k_s$ is defined as:

$$I_S(u) = \sum_i \prod_j \frac{1}{1 + e^{-k_s(A_i(j)u - b_i)}}$$

- $I_S(u)$ are smooth, continuous functions, and the closed form derivatives are available for optimization packages




**Example**: Non-convex region is represented by a union of 8 convex polyhedra




**Example**: Indicator function



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# Nonlinear Model Predictive Control Formulation

- Steady-state model is solved to find the terminal constraints:

$$0 = f(x_{sp}, u_{sp})$$
$$y_{sp} = h(x_{sp}, u_{sp})$$

- The initializations of the current time step is the optimal solution of the previous time
- Continuous form Nonlinear Model Predictive Control (NMPC) formulation:

Setpoint Tracking

Terminal Constraint

$$\min \int_{t_0}^{t_0+P} \left(y(t) - \boldsymbol{y_{sp}}\right)^T Q\left(y(t) - \boldsymbol{y_{sp}}\right)dt + \int_{t_0}^{t_0+P} u'(t)^T R u'(t) dt + \left(u(P) - \boldsymbol{u_{sp}}\right)^T R_f\left(u(P) - \boldsymbol{u_{sp}}\right)$$

$$s.t \qquad \dot{x}(t) = f(x(t), u(t)) \qquad (1)$$
$$y(t) = h(x(t), u(t)) \qquad (2)$$
$$y_{min} \leq y(t) \leq y_{max} \ \forall\, t \in [t_0, t_0 + P] \qquad (3)$$
$$u_{min} \leq u(t) \leq u_{max} \ \forall\, t \in [t_0, t_0 + P] \qquad (4)$$

- Reduced-order multi-model is used in (1) and (2) for the NMPC implementation

# Fischer-Tropsch Synthesis Reaction

**Reaction stoichiometry:**

$$nCO + 2nH_2 \rightarrow (-CH_2-)_n + nH_2O$$

- **CO/$\gamma$Al$_2$O$_3$ catalyst: assume the water gas shift and oxidation reactions are negligible(*)**
- **Langmuir-Hinshelwood type reaction, mass transfer effect is neglected**
- **Reaction rate = rate(Temperature, Partial Pressure of $CO$ and $H_2$)**

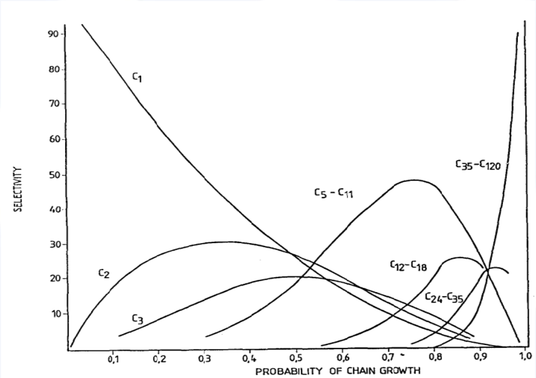
**Selectivity : $\alpha$ = $\alpha$(Temperature, Partial Pressure of $CO$ and $H_2$)**

**Probability of chain growth: $\alpha$**

$$(-CH_2-)_n \xrightarrow{\alpha} (-CH_2-)_{n+1}$$

$$(-CH_2-)_n \xrightarrow{1-\alpha} \text{Termination to Hydrocarbons} \rightarrow C_nH_{2n},\ C_nH_{2n+2}$$

**Anderson-Schulz-Flory Distribution(**)**




Low $\alpha$, high light hydrocarbons concentration

High $\alpha$, high heavy hydrocarbons concentration



(*) Azadi, Brownbridge, Kemp, Mosbach, Dennis, Kraft (2015)
(**) Dry, M.E. (1990)

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# Fischer-Tropsch Slurry Bubble Column

Slurry bubble column reactor with internal cooling tubes is used for industrial Fischer-Tropsch synthesis because of its thermal management capability(*).

- Manipulated variables: coolant flow rate, superficial gas velocity
- Controlled variables: temperature, chain growth probability

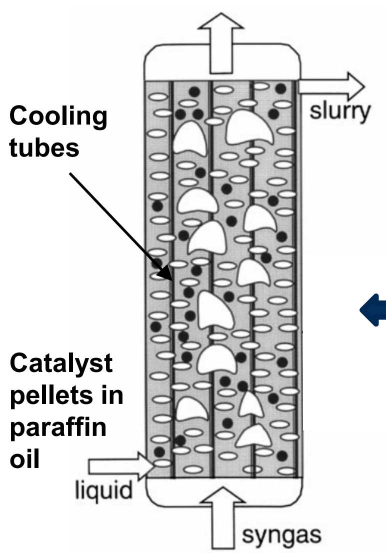



Image source: (*)

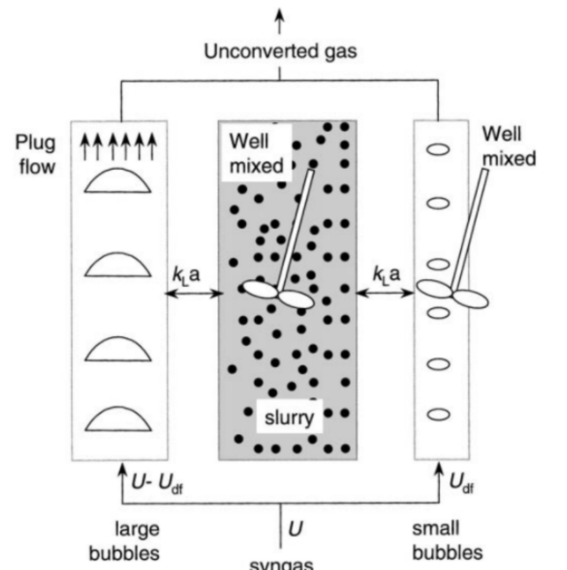



Image source: (*)

**Dynamic model assumptions:**

Hydrodynamic:
- Large & small bubbles holdup
- Large & small bubbles velocity
- Heat transfer coefficient

Mass balance
- Large bubble: PFR
- Small bubble: CSTR
- Liquid slurry: CSTR with reaction
- VLE between bubbles and liquid

Energy balance
- Quasi steady-state for gas phase
- Liquid phase for reactor temperature



(*) Maretto, C., & Krishna, R. (1999).

# Reduced-order Model of Fischer-Tropsch Reactor

**High-fidelity Model**

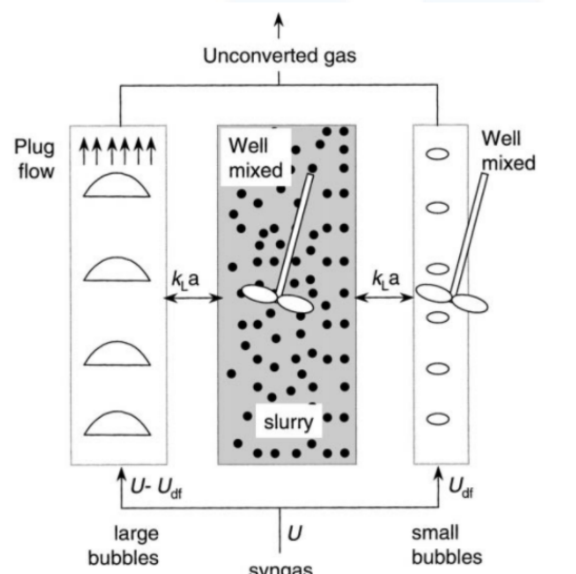
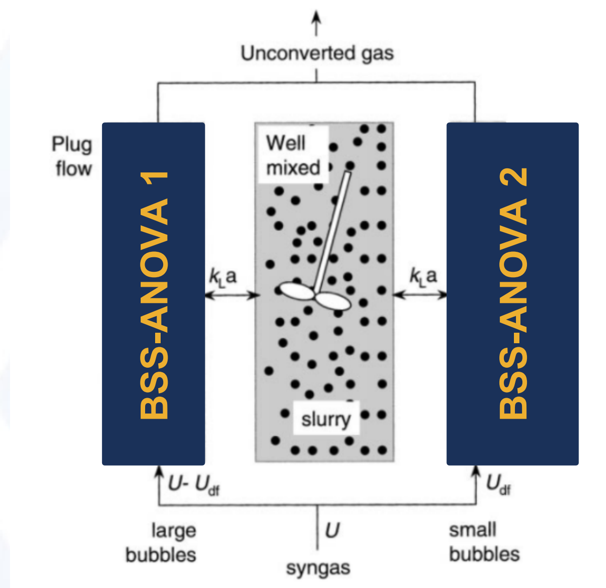



Image source: (*)

**Reduced-order Model**




- 2 CSTR and 1 PFR at equilibrium
- 25 state variables
- Hydrodynamics and VLE are derived from experiments(*)

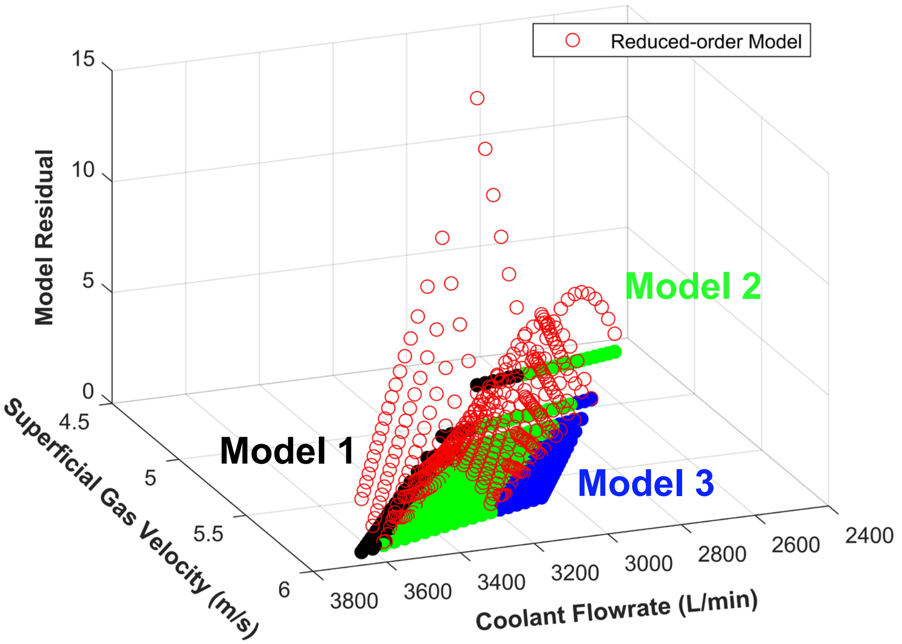
- 1 CSTR
- 3 state variables
- Hydrodynamics and VLE are calibrated using BSS-ANOVA

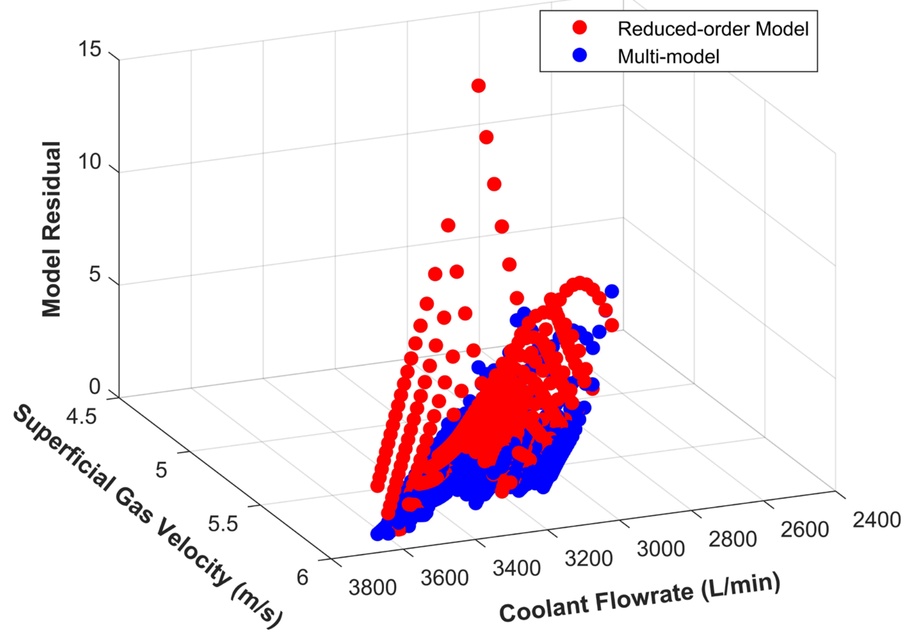


(*) Maretto, C., & Krishna, R. (1999).

# Multi-model representation of Fischer-Tropsch Reactor

- Input set is divided based on residual of reduced-order model at desired steady-states
- The combined reduced-order of the multi-models with indicator functions is formulated from the reduced-order models in each region



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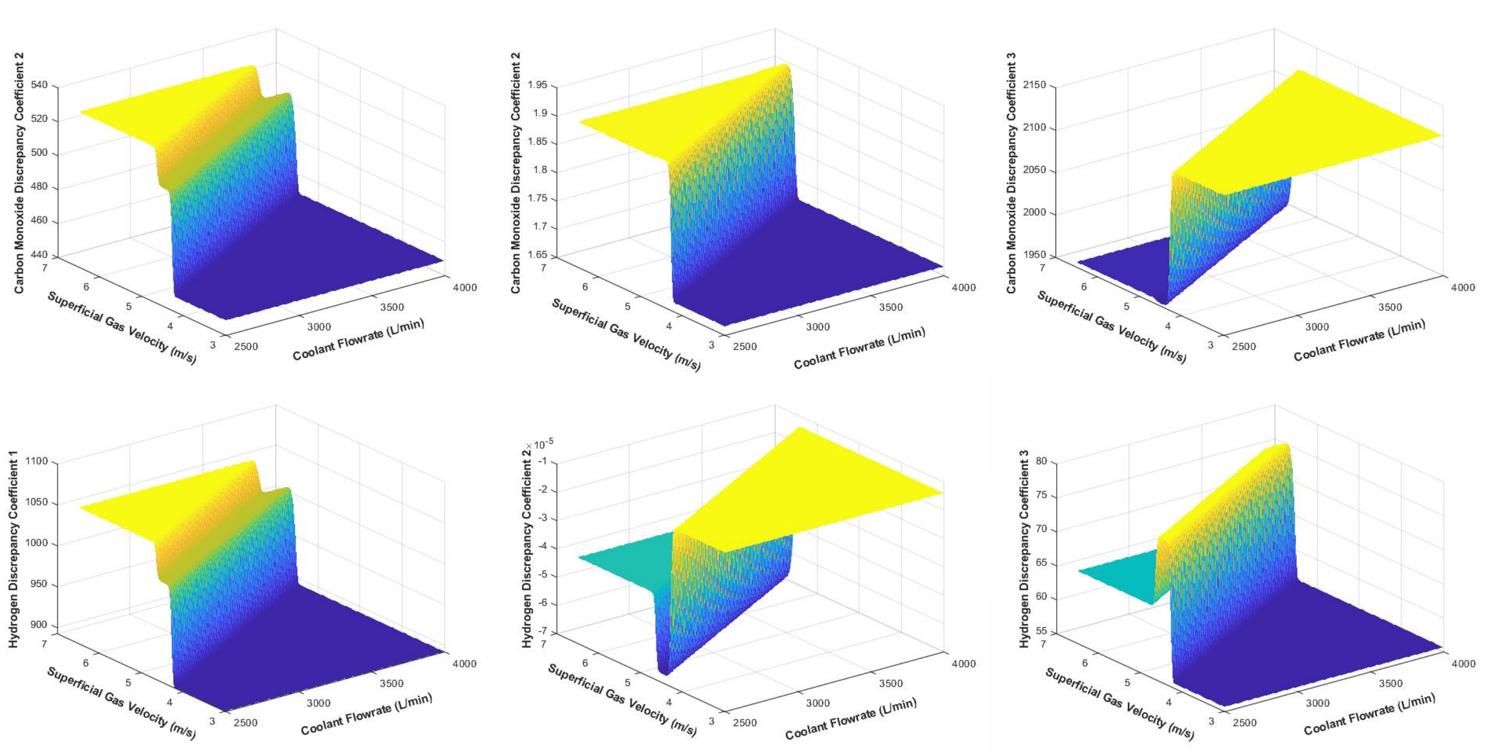
# Calibration Results of Fischer-Tropsch Reactor

- The discrepancy functions are recalibrated within each operating region. Each discrepancy function contains the first 5 eigenfunctions of the Karhunen-Loeve expansion.
- The smoothing constant of 0.1 is chosen for the indicator function of the multi-model representation to ensure the convergence of the reduced-order model




First 3 parameters of the discrepancy functions representing the VLE of Hydrogen and Carbon Monoxide



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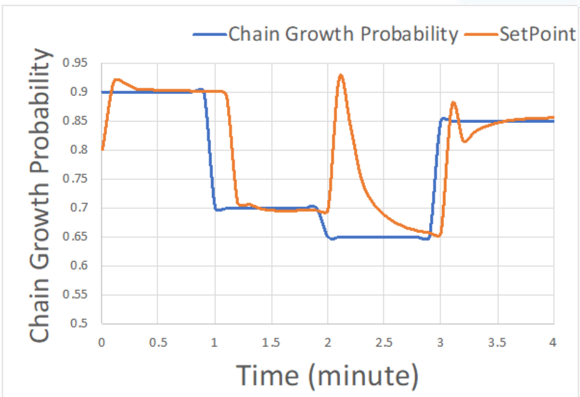
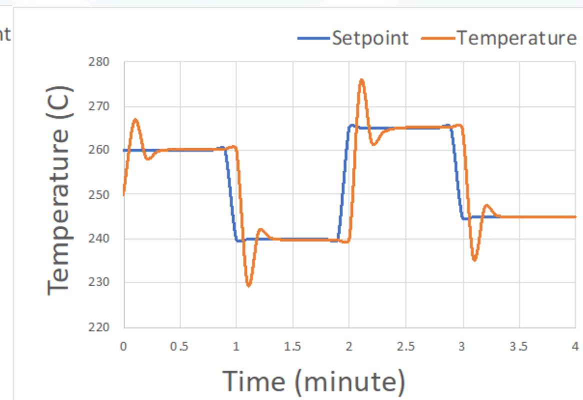
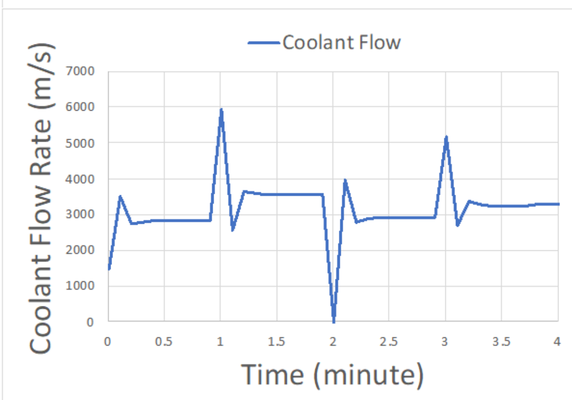
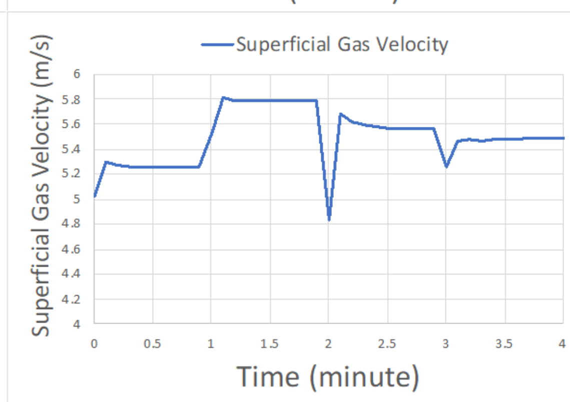
# Online Implementation of NMPC

- The high-fidelity model is used as the real process to test the NMPC with 6 second controller step size
- NMPC successfully brings the process to the new setpoints without violating the input constraints




| NMPC Model | Computation Time/ Step (Seconds) |
|---|---|
| High-fidelity | 29.4 |
| Reduced-order | 5.6 |
| Reduced-order Multi-model | 3.4 |

- Even though the reduced-order multi-model has some additional indicator functions, smaller model mismatch leads to faster online computational time than the reduced-order model



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# Conclusions and Acknowledgments

**Conclusion:**

- Online implementation shows that the developed reduced-order multi-model is applicable for NMPC
- Future work involves online calibration of reduced-order model for online control

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Other research directions:
https://fernandolima.faculty.wvu.edu/

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