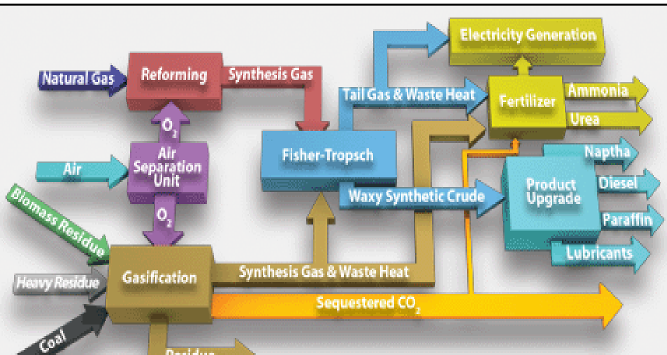
A Process Systems Framework for Design, Optimization and Control of Modular Energy Systems

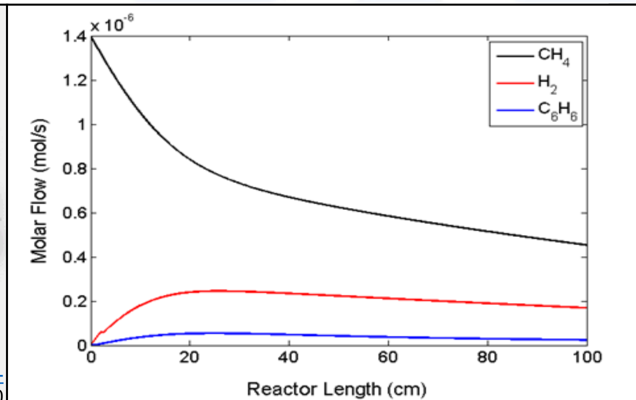
Fernando V. Lima
Department of Chemical and Biomedical Engineering
West Virginia University
Visiting Faculty, Carnegie Mellon University

January 14, 2022

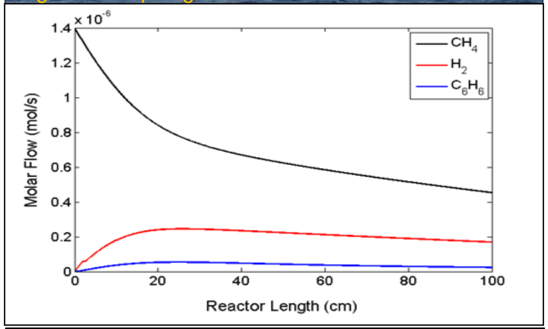
CAPD Energy Systems Initiative (ESI) Seminar

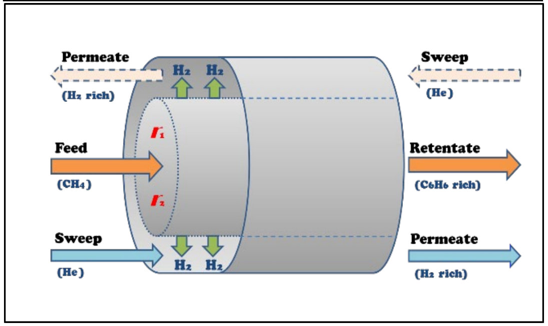


http://www.dreamstime.com/stock-photo-sinopec-group-natural-gas-processing-plant-model-image27735070



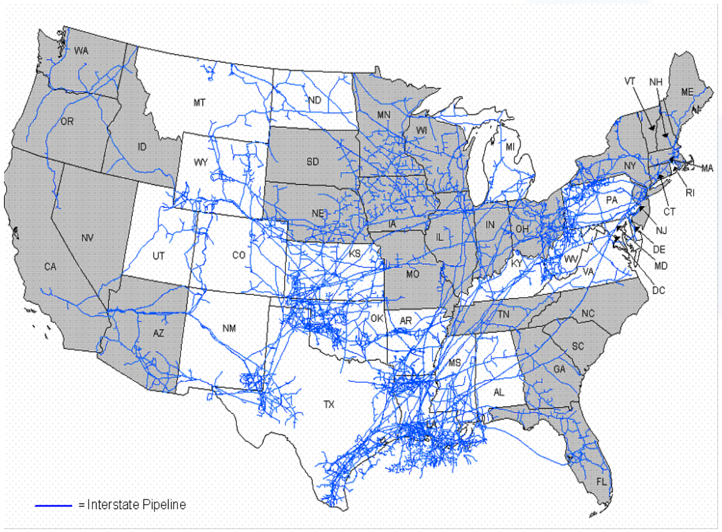
Presentation Outline





- **Introduction and Background**
  - ✓ Challenges and Opportunities for Natural Gas Utilization
  - ✓ Process Intensification
  - ✓ Process Systems Framework
  - ✓ Process Operability Concepts
- **Proposed Approach**
  - ✓ Membrane Reactor Application
  - ✓ Operability App for Design and Intensification
- **Strategies for High-D Modular Systems**
  - ✓ Parallel Computing and Natural Gas Combined Cycle Example
  - ✓ Machine Learning (Gaussian Process) Mapping
- **Operability for Control and Estimation**
- **Next Steps and Conclusions**

Challenges and Opportunities



http://www.eia.gov/pub/oil_gas/natural_gas/analysis_publications/ngpipeline/dependstates_map.html

- ✓ After the shale gas revolution, according to the U.S. EIA, ***Appalachian region provided about 34% (2021)*** of the U.S. natural gas production*
- ✓ ***Specialized software tools*** that can assess technical and economic feasibility of natural gas utilization processes are needed

* Energy Information Administration, 2021

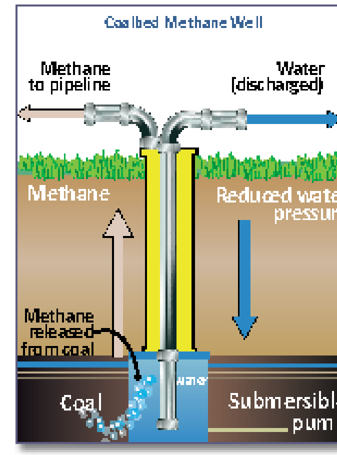
Challenges and Opportunities

Methane Rich Gases Not Utilized

Flare Gas
($100 million per month is burned at Bakken, ND)

Refinery Off Gas

Shale Gas

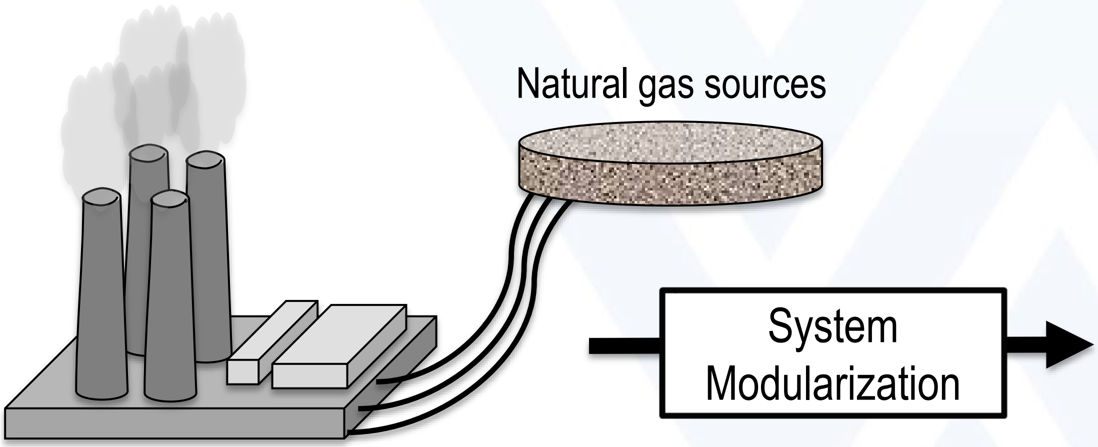


Coal-Bed Methane

- ✓ These gases, which have been discovered but some remain untapped due to physical or economic reasons, are stranded
- ✓ Effective utilization of these gases will have strong impact on science, economy, and environment

Challenges and Opportunities

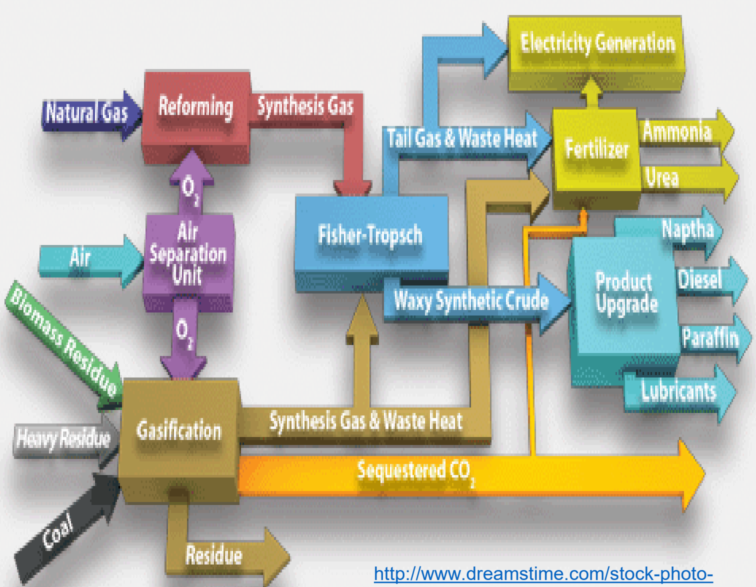
Conventional vs. Modular Natural Gas Utilization



http://www.oil-gasportal.com/gtl-small-scale-and-modular-technologies-for-gas-to-liquid-industry/

- ✓ Explore distributed characteristics of feedstock (e.g., natural gas)
- ✓ Transport and/or assemble modular units or skids on site
- ✓ Need to address challenges associated with design and operation of modular plants

Challenges and Opportunities

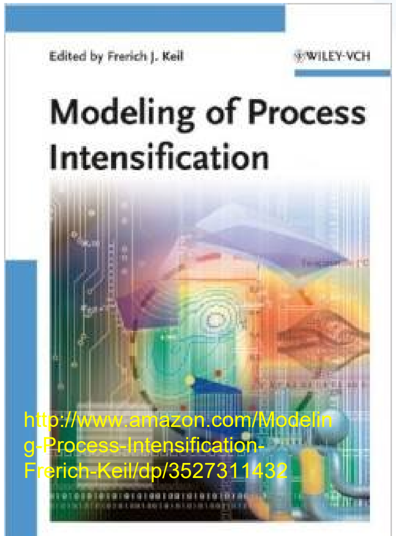


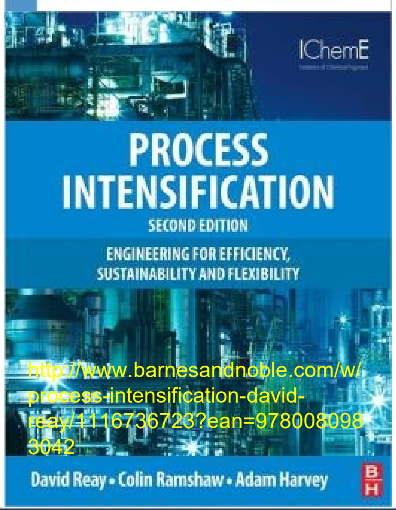
http://www.dreamstime.com/stock-photo-sinopec-group-natural-gas-processing-plant-model-image27735070

- ✓ Modular energy processes are operated in a ***highly constrained*** and integrated environment that is represented by complex ***large-scale and nonlinear models***

- ✓ There is an ***opportunity*** to employ ***process systems*** approaches to enable the ***design, intensification, and control*** of complex energy systems towards modularity

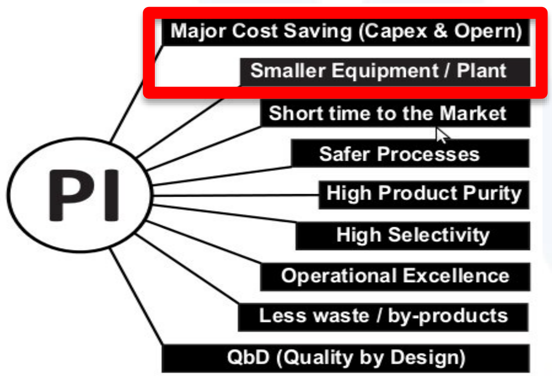
Process Intensification (PI)



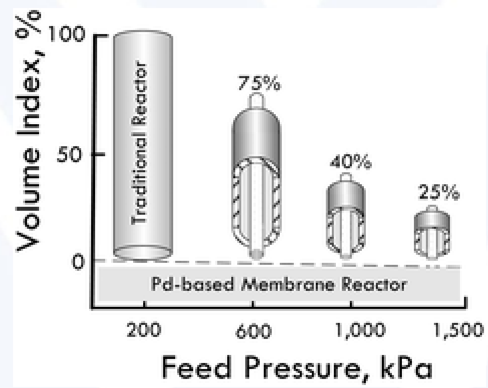


Emerging equipment, … promise spectacular improvements in process plants, markedly shrinking their size and dramatically boosting their efficiency*

PI is a strategy for making dramatic reductions in the size of a chemical plant so as to reach a given production objective**



http://pi-inc.co/services.html

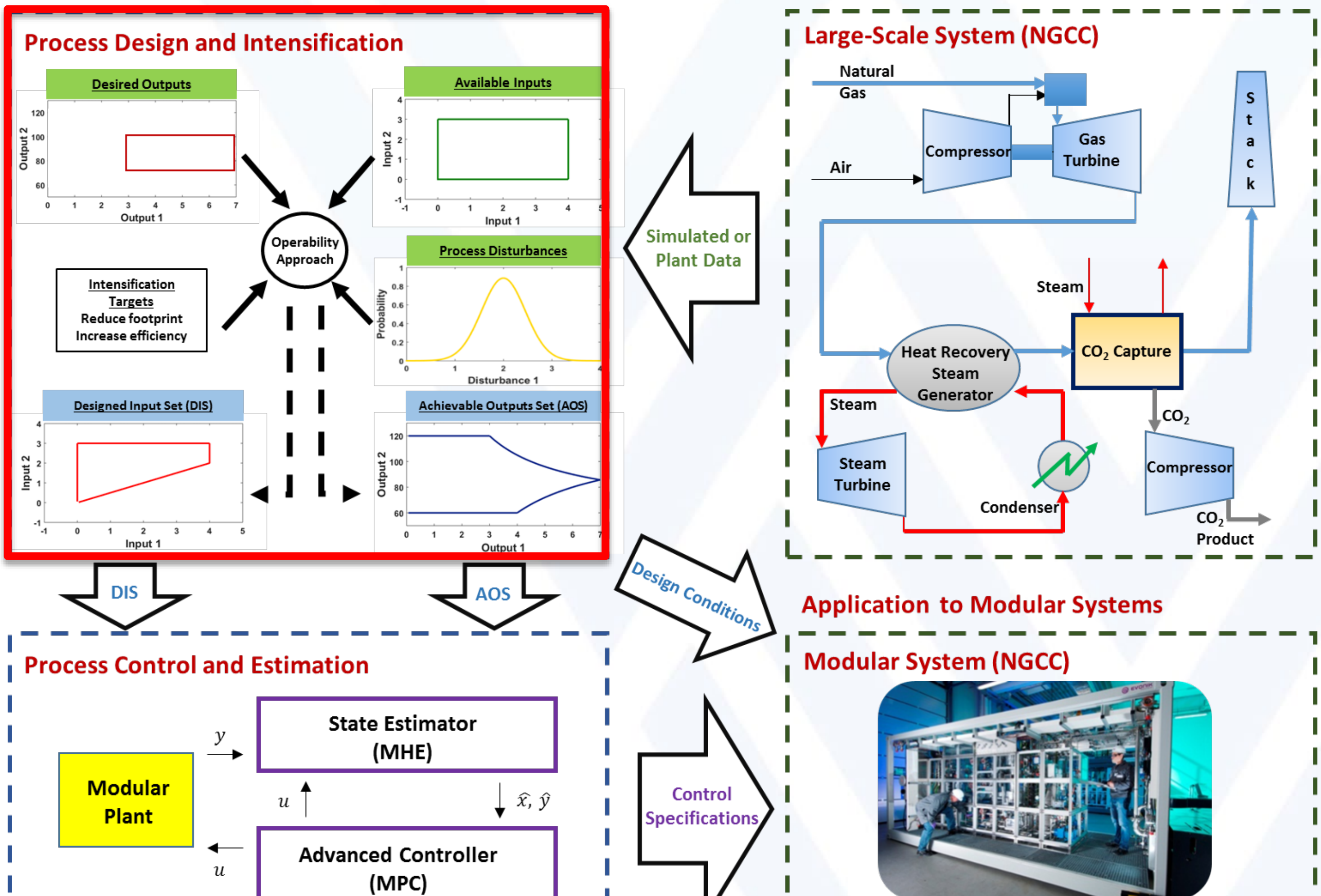


http://pubs.rsc.org/en/Content/ArticleLanding/2012/GC/C2GC16668B#!divAbstract

*Stankiewicz & Moulijn, Chemical Engineering Progress, 2000
**Ranshaw, Proceedings -1st Intl. Conf. Proc. Intensif. for Chem. Ind., 1995

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Process Systems Framework



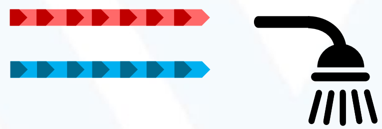
Modular Facility Framework Schematic (F[3] Factory Project, 2014)

WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Operability Definition

Operability Analysis[*,**]: Address operability challenges at the design phase

($u_{op,1}$) hot flow
($u_{op,2}$) cold flow



(y_1) Total flow
(y_2) Temperature

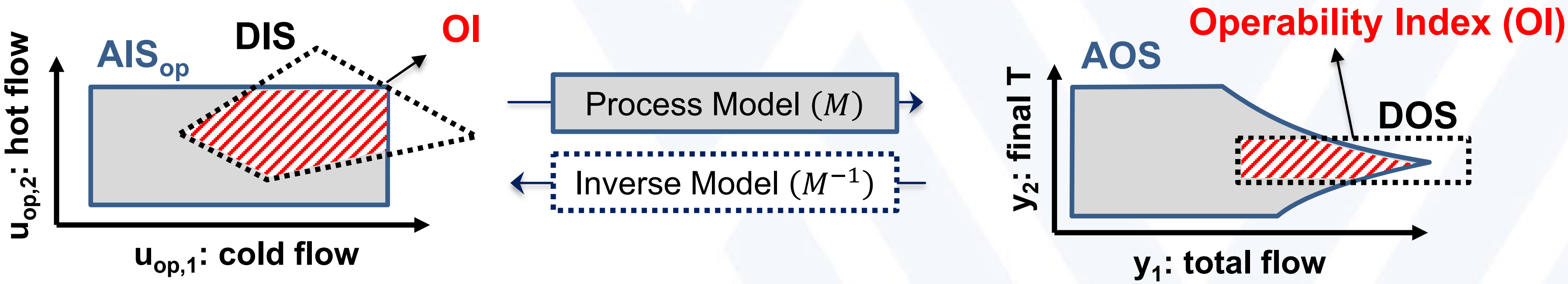
Shower Problem

Available Input Set (AIS_{op})
Manipulated variables (MVs)

Desired Input Set (DIS)
Desired input operation

Achievable Output Set (AOS)
Controlled variables (CVs)

Desired Output Set (DOS)
Desired output operation



Challenges:

- M^{-1} may not be straightforward to obtain
- High number of function evaluations (M and M^{-1})
- Operability approaches are usually tailored for specific applications

* Vinson D. R. and Georgakis C., *J. Process Control*, 2000
** Gazzaneo V., Carrasco J.C., Vinson D. R., Lima F. V., *Ind. Eng. Chem. Res.*, 2020

Specific Objectives

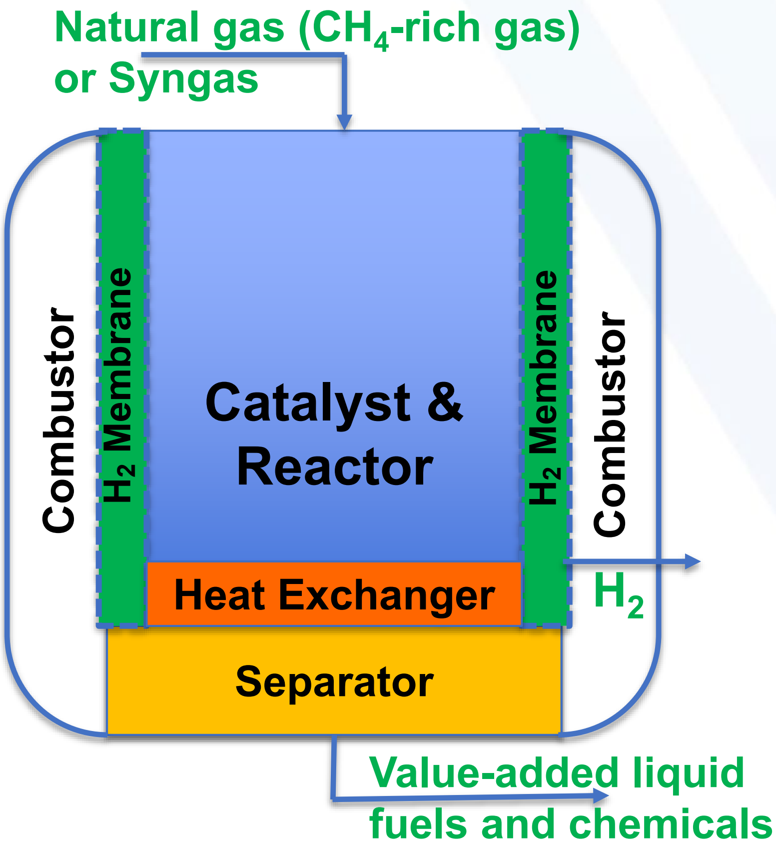
- Extend operability concepts to address new directions on
  - ✓ design of high-dimensional nonlinear systems
  - ✓ process intensification towards modularity
  - ✓ dynamic operability for feasible modular operation under uncertainties

- Introduce bilevel optimization, parallel computing and machine learning-based approaches

- Apply developed approaches to modular system candidates
  - ✓ catalytic membrane reactor
  - ✓ natural gas combined cycle (NGCC)

Modular Natural/Shale Gas System

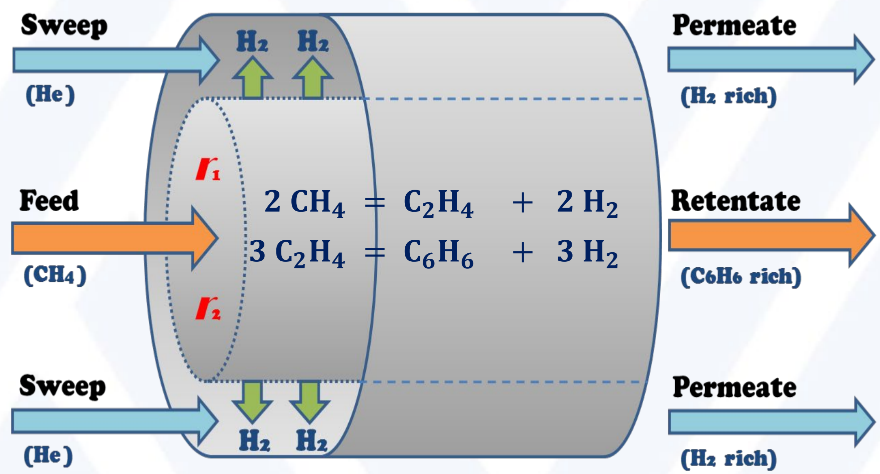
Research Concept



Catalytic Process Intensification for a Modular System

Direct Methane Aromatization Conversion in a Modular System

Catalytic Membrane Reactor Application



Endothermic reaction and Equilibrium controlled

Membrane Reactor Model

<u>*Molar balances:*</u>

$$\frac{dF_{t,CH_4}}{dz} = r_1 A_t - \frac{Q}{\propto_{H_2/CH_4}}\left(P_{t,CH_4}^{1/4} - P_{s,CH_4}^{1/4}\right)\pi\, d_t$$

$$\frac{dF_{t,C_2H_4}}{dz} = -\frac{r_1}{2} A_t + r_2 A_t - \frac{Q}{\propto_{H_2/C_2H_4}}\left(P_{t,C_2H_4}^{1/4} - P_{s,C_2H_4}^{1/4}\right)\pi\, d_t$$

$$\frac{dF_{t,H_2}}{dz} = -r_1 A_t - r_2 A_t - Q\left(P_{t,H_2}^{1/4} - P_{s,H_2}^{1/4}\right)\pi\, d_t$$

$$\frac{dF_{t,C_6H_6}}{dz} = -\frac{r_2}{3} A_t - \frac{Q}{\propto_{H_2/C_6H_6}}\left(P_{t,C_6H_6}^{1/4} - P_{s,C_6H_6}^{1/4}\right)\pi\, d_t$$

- First-principles model based on molar balances
- Laboratory scale
- Initial value problem, subroutine "ode15s" (MATLAB)

- Simulation validated with experimental data*

Reaction mechanism **

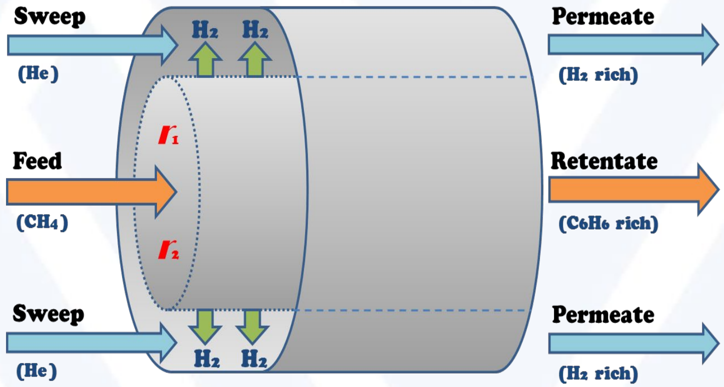
Step 1:

$$r_1 = k_1\, C_{CH_4}\left(1 - \frac{k_1'\, C_{C_2H_4}\, C_{H_2}^2}{k_1\, C_{CH_4}^2}\right)$$

Step 2:

$$r_2 = k_2\, C_{C_2H_4}\left(1 - \frac{k_2'\, C_{C_6H_6}\, C_{H_2}^3}{k_2 C_{C_2H_4}^3}\right)$$

C_i: Concentration of species "i"
r_1 and r_2: reaction rates of steps 1 and 2
k_1 , k_1' , k_2 , and k_2': reaction rate constants

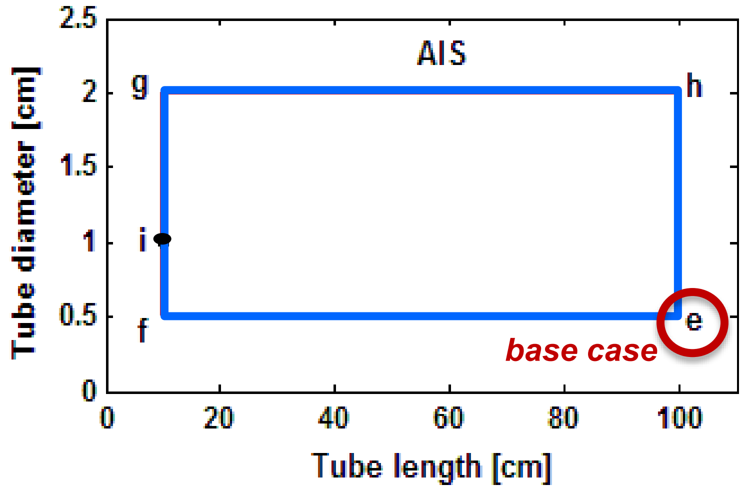


- Input variables: L and d_t
- Outputs: CH_4 conversion, C_6H_6 production

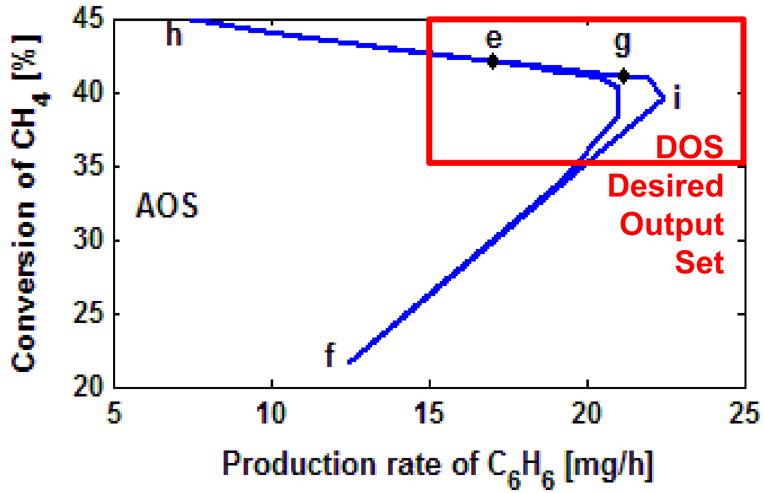
*Iliuta et al. *Ind. Eng. Chem. Res.*, 2003
**Li et al., *Chem. Eng. Sci.*, 2002

MR Operability Analysis

Available Input Set (AIS): reactor length and diameter



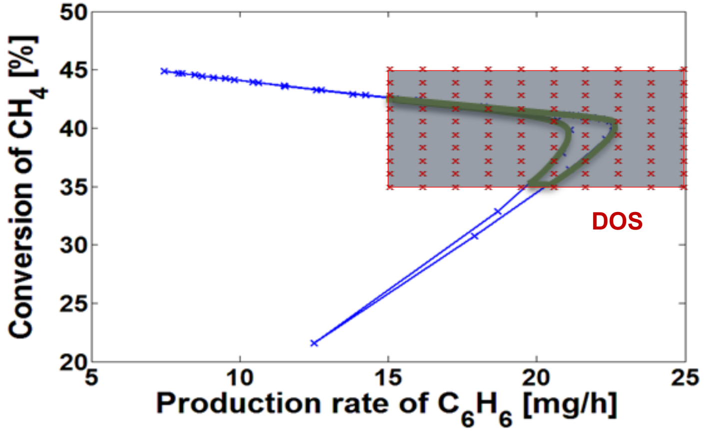
Achievable Output Set (AOS): methane conversion and benzene production



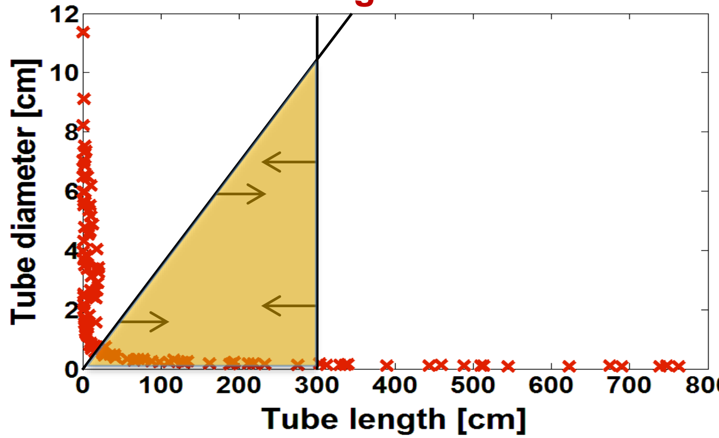
- **High conversion does not translate to high benzene production**
- **The point "i" presents the best production of benzene**
- **Segment "g-h" shows the critical effect of *length* on production rate of benzene**

MR Optimization-based Operability

AOS & DOS: methane conversion and benzene production



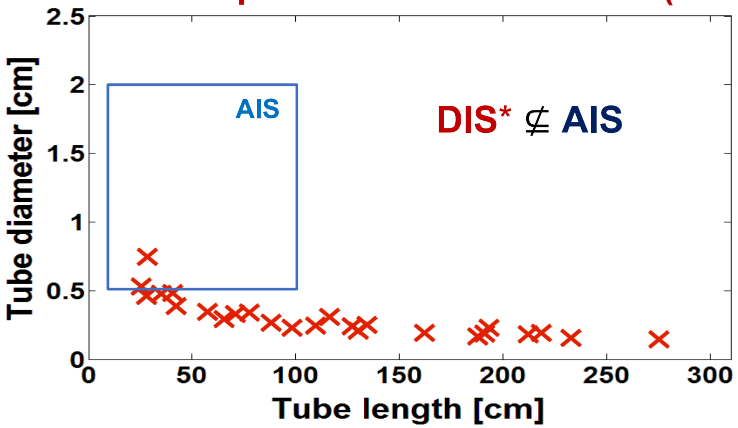
Desired Input Set (DIS): reactor length and diameter



- **Reactor diameter (d_t) and length (L) show a large dispersion**
- **Design constraints: $L \leq 300$ [cm] and $L / d_t \geq 30$* (for PFR)**

*Rawlings, J. B. and Ekerdt, J. G. Chemical Reactor Analysis and Design Fundamentals; Nob Hill: Madison, WI, USA, 2002

Desired Input Set with Constrains (DIS*)

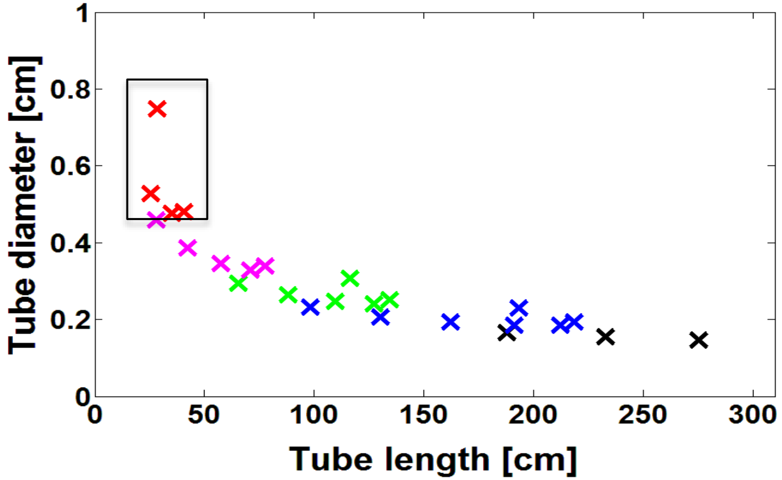


Proposed framework is flexible as allows the computation of DIS from any DOS

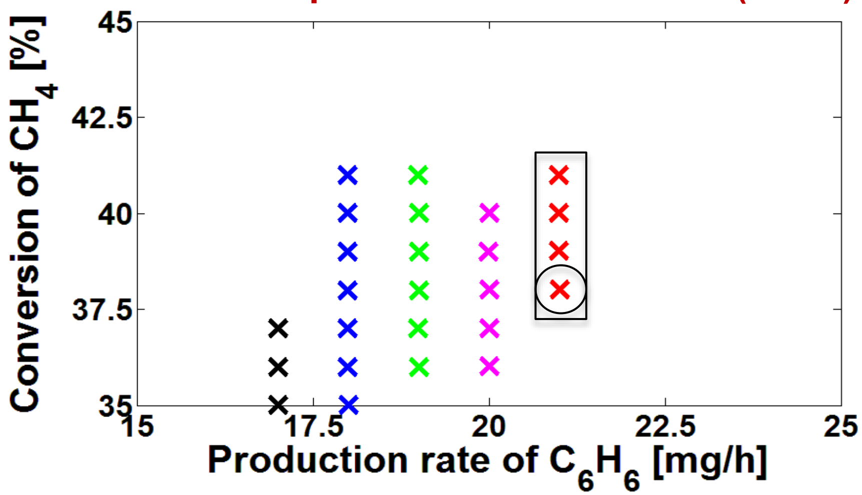
WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

MR Process Intensification

Desired Input Set with Constrains (DIS*)



Desired Output Set with Constrains (DOS*)



- Desired level of performance can be specified
- Reduction of DMA-MR footprint (reactor volume and membrane surface area)

- When compared to *base case* point "e"
- MR design can be intensified by 77% volume reduction and 80% membrane area reduction
- Bilevel optimization problem may be formulated as tool for process intensification

Integrated Bilevel *Operability* Framework For Process Design and *Intensification*

$$\mathbf{AIS} = \{\mathbf{u} \mid \mathbf{u}_i^{min} \leq \mathbf{u}_i \leq \mathbf{u}_i^{max}\ ; 1 \leq i \leq m\}$$

$$\mathbf{AOS} = \{\mathbf{y} \mid \mathbf{y} = \mathbf{M}(\mathbf{u}, \mathbf{d});\ \mathbf{u} \in \mathbf{AIS}, \mathbf{d} \text{ is fixed}\}$$

Bilevel Optimization

P1: $$\emptyset_k = \min_{\mathbf{u}_k^*} \sum_{j=1}^{n} \left((y_{j,k} - y_{j,k}^*)/y_{j,k} \right)^2$$

P2: $$\Omega = \min_{\mathbf{u}_{PI}^*} \mathrm{PI}_{target}$$

Define:
- ✓ DOS
- ✓ Constraints
- ✓ Performance
- ✓ Intensification

$$\mathbf{DOS}^* = \{\mathbf{y}^* = \mathbf{M}(\mathbf{u}^*)\}$$

$$\mathbf{DIS}^* = \{\mathbf{u}^* = (\mathbf{u}_1^*, \mathbf{u}_2^*, \mathbf{u}_3^*, \ldots, \mathbf{u}_p^*)\}$$

$$(\mathbf{u}_{PI}^*, \mathbf{y}_{PI}^*)$$

P3: $$\Psi = \min_{u \in \mathbb{U}} [\mathrm{PI}_{target}]$$

Subject to: $$u_k^* \in \underset{u_k^* \in \mathbb{U}_k}{\mathrm{argmin}} \left\{ \sum_{j=1}^{n} \left(\frac{(y_{j,k} - y_{j,k}^*)}{y_{j,k}} \right)^2 \right\}$$

$$y_k \in \mathrm{DOS}$$

$$\mathbf{c}_1 (u_k^*) \leq \mathbf{0}$$

$k = 1,2,3 \ldots p$

Define: $\mathrm{DOS} = \{\mathbf{y} = (y_1, y_2, y_3 \ldots y_p)\}$

PI_{target}: volume, area, or others

$u_{1,o}^*$: initial guess for input point

(u_{PI}^*, y_{PI}^*): intensified input and output values

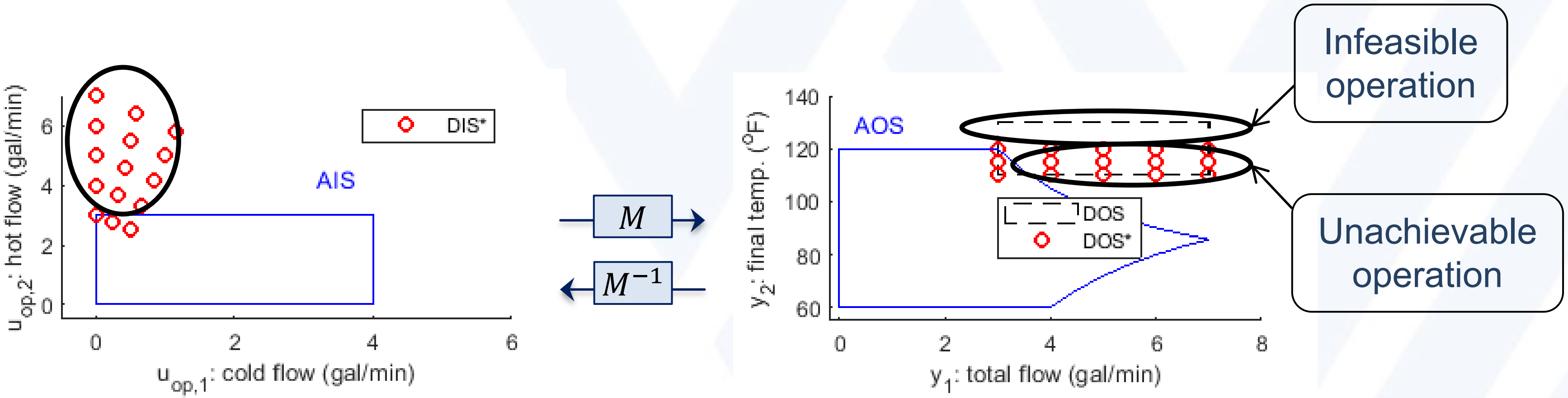
Carrasco J.C. and Lima F.V. *AIChE Journal*, 2017
Carrasco J.C. and Lima F.V. *Comput. Chem. Eng.*, 2017

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

NLP-based Method

Nonlinear programming (NLP)-based operability method

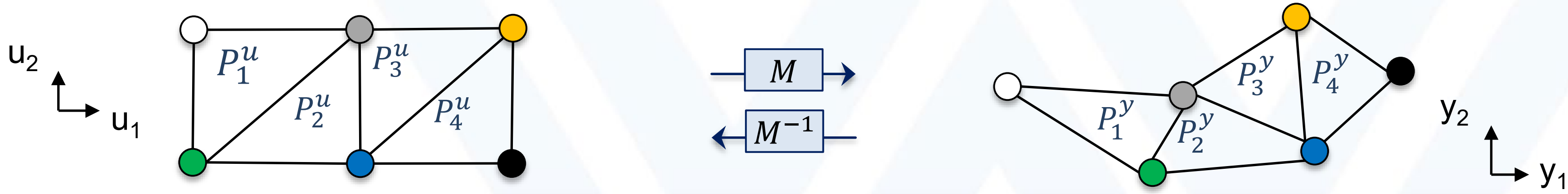
- Handles infeasible DOS with NLP-based model inversion
- Finds feasible spaces, feasible DOS (DOS*) and feasible Desired Input Set (DIS*)
- Feasible points can be used in other optimization layers
- Provides insights for changes in the selected AIS



Carrasco J. C. and Lima F.V., *Comput. Chem. Eng.*, 2017

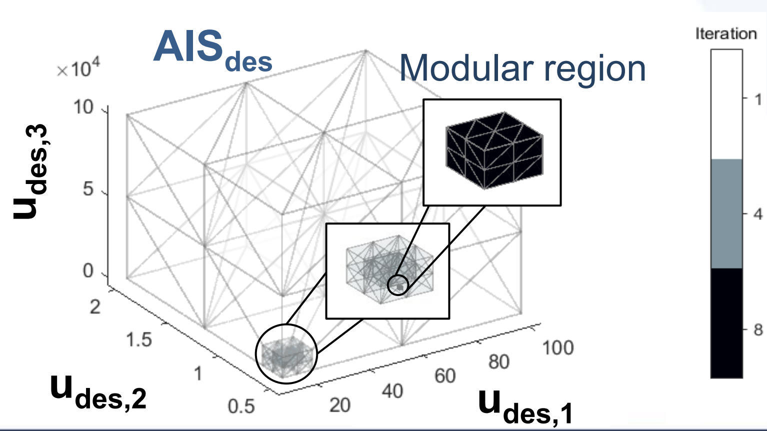
Multimodel Operability Approach

Multimodel operability representation: Original nonlinear model paired polytopes $P_k = \{P_k^u, P_k^y\}$

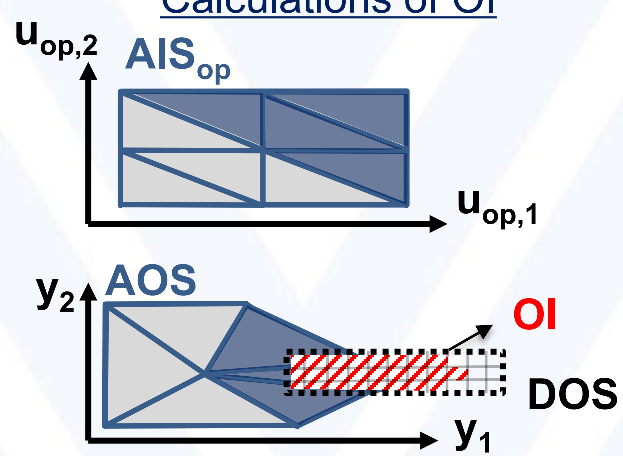


- Simplified representation
- Efficient quantification of operability regions
- Straightforward calculation of M^{-1}

Explore system modularization



Calculations of OI



Gazzaneo V., Lima. F.V., *Ind. Eng. Chem. Res.*, 2019
Gazzaneo V., Carrasco J.C., Vinson D. R., Lima F. V., *Ind. Eng. Chem. Res.*, 2020

Process Operability App Project

Process Operability App*

MULTIMODEL APPROACH
- Multimodel representation
- MILP-based algorithms
- OI Calculations

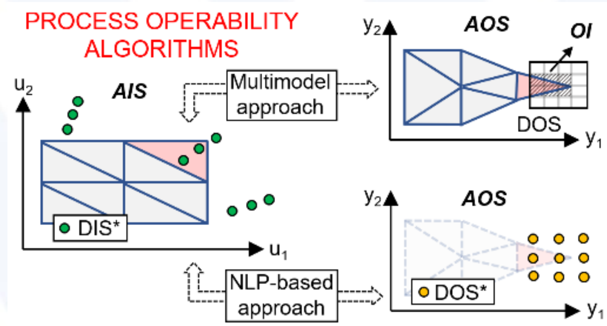
NLP-BASED APPROACH
- Feasibility of DOS
- NLP-based algorithm for DIS-DOS mappings

OTHER TOOLS
- Input-output mappings

Generalization in dimensionality and process model

Process Operability App
- Open-source MATLAB app with user-friendly interface
- Dissemination and improvement of algorithms

https://fernandolima.faculty.wvu.edu/operability-app

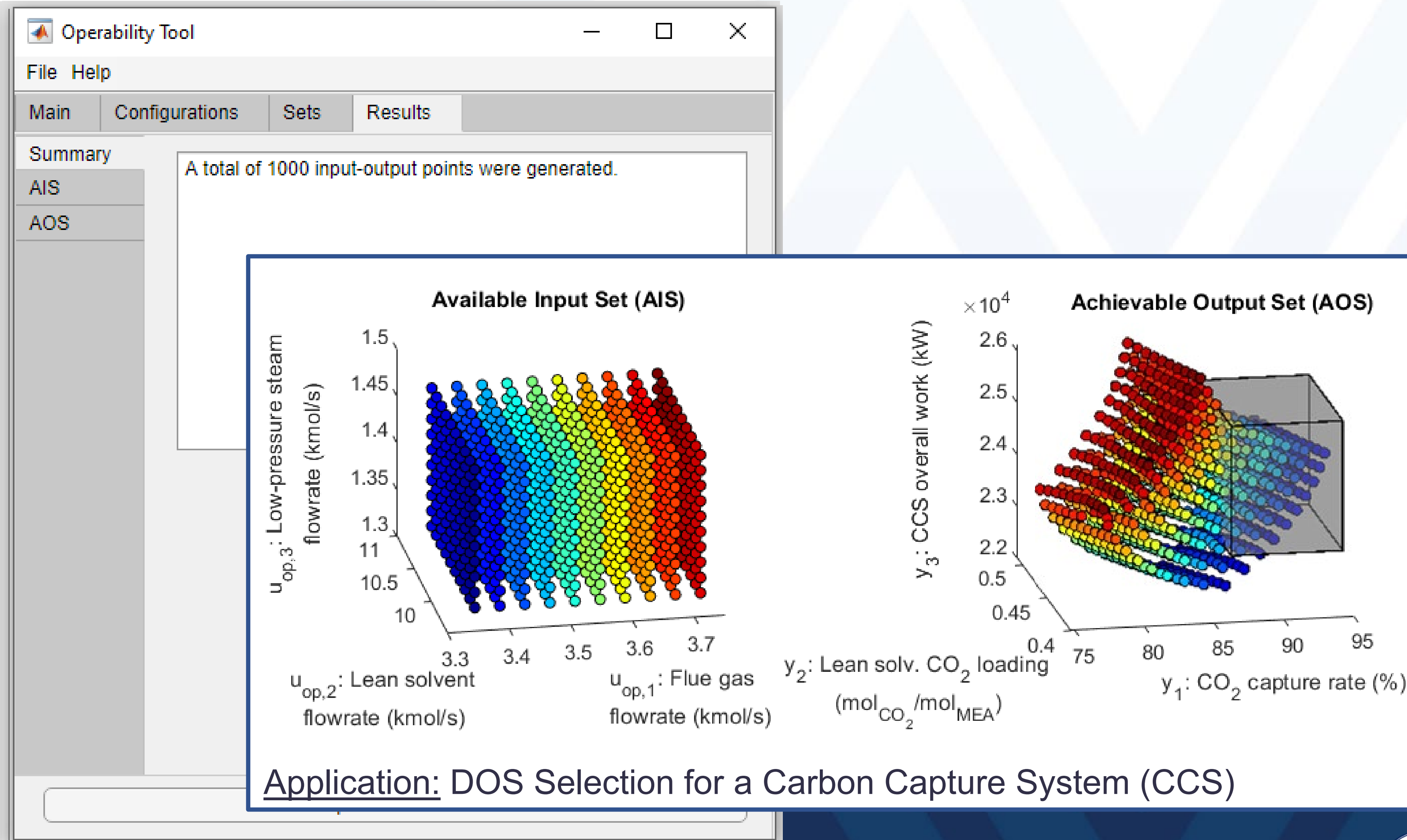


*Gazzaneo V., Carrasco J.C., Vinson D. R., Lima F. V., *Ind. Eng. Chem. Res.*, 2020

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Process Operability App: Applications

Input-output mapping for selection of the DOS

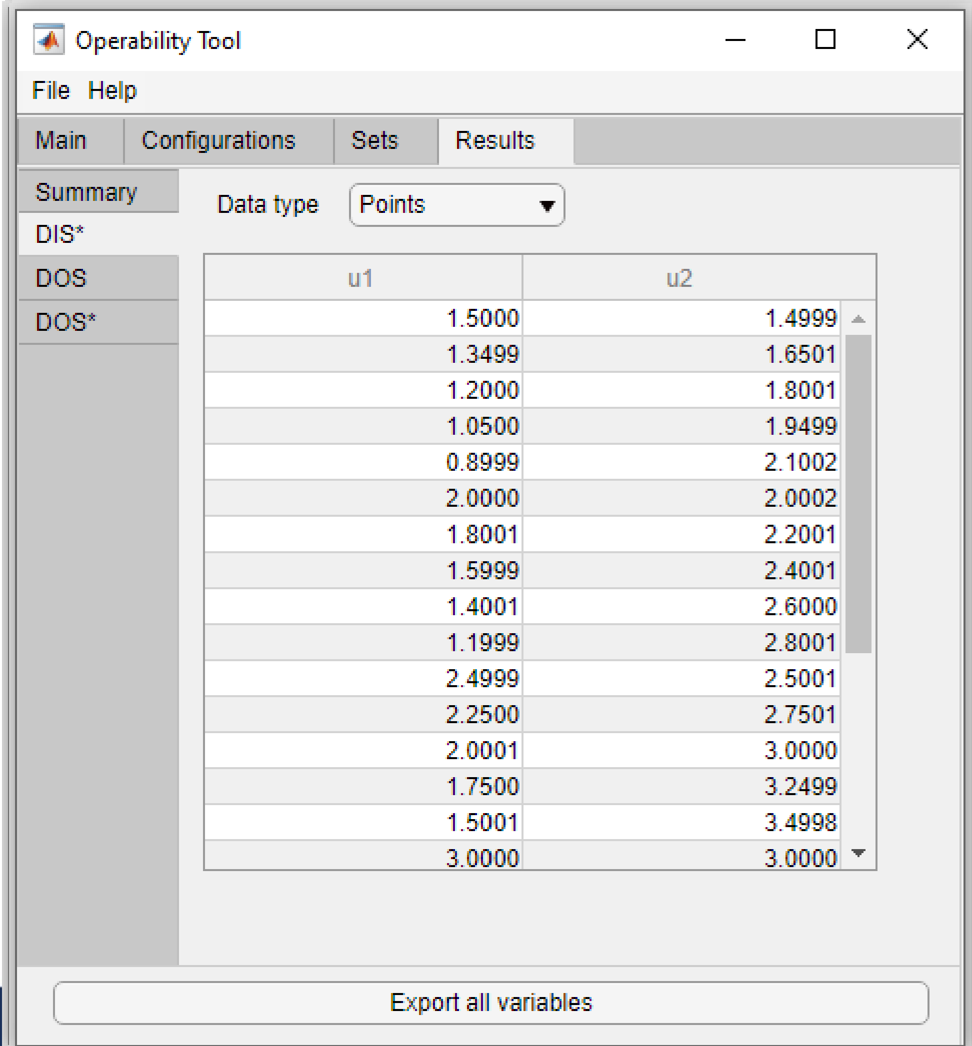


Application: DOS Selection for a Carbon Capture System (CCS)

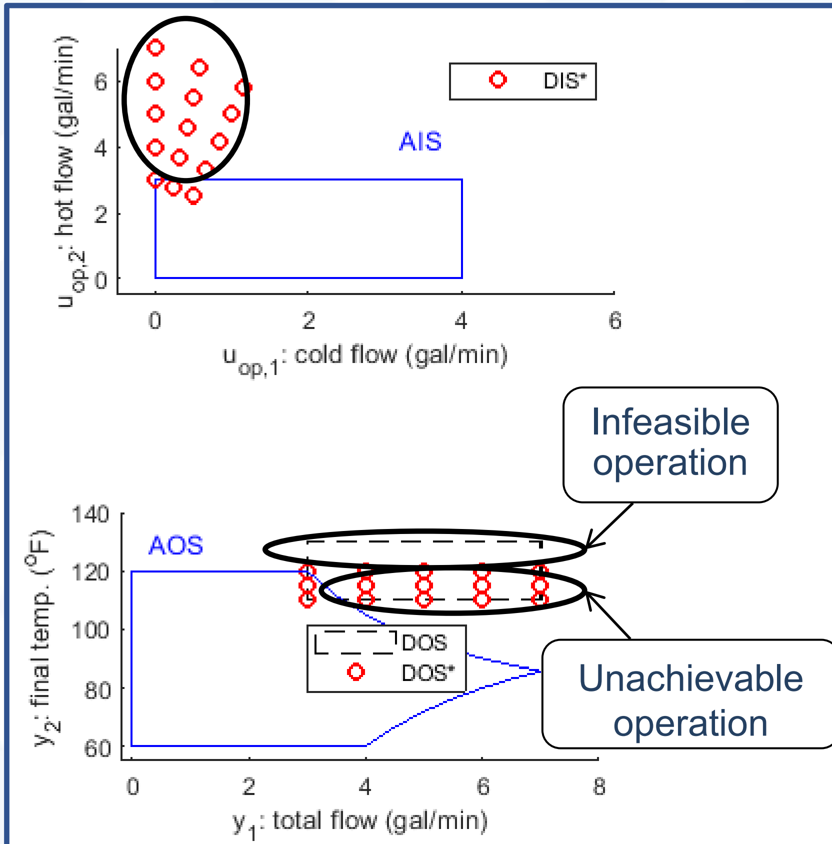
West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Process Operability App: Applications

NLP-based Approach: Feasible DIS and DOS



u1	u2
1.5000	1.4999
1.3499	1.6501
1.2000	1.8001
1.0500	1.9499
0.8999	2.1002
2.0000	2.0002
1.8001	2.2001
1.5999	2.4001
1.4001	2.6000
1.1999	2.8001
2.4999	2.5001
2.2500	2.7501
2.0001	3.0000
1.7500	3.2499
1.5001	3.4998
3.0000	3.0000

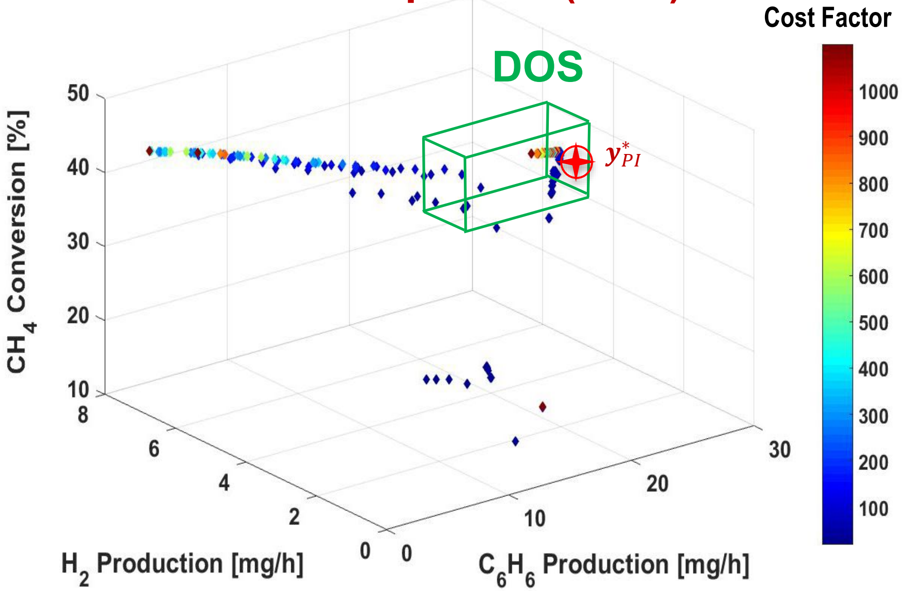


Application: DIS* and DOS* for the shower problem

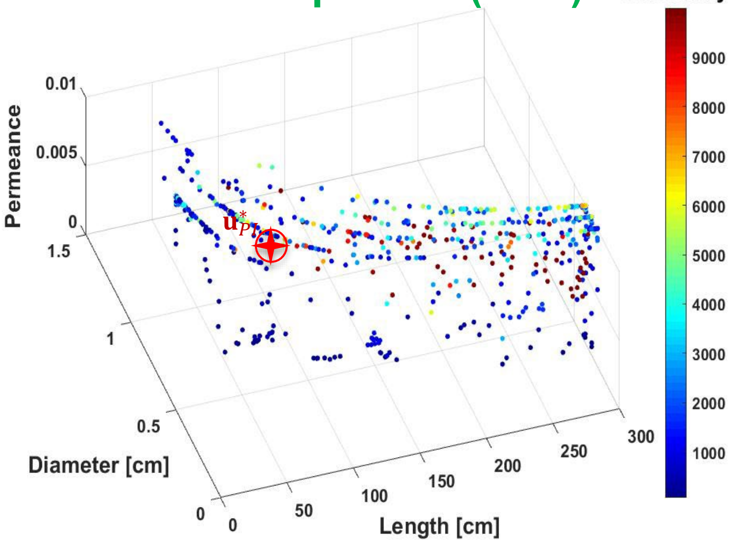
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

MR Bilevel Operability Analysis (4-D)

Achievable Output Set (AOS)



Desired Input Set (DIS*):



Computational Time**

AOS calculations (Control Problem)

System	Points	Time [min:sec]
2x2	25	00:03
3x3	125	00:18
4x4	625	01:42

DIS* calculations (Design Problem)

System	Points	Time [hr:min:sec]
2x2	25	00:06:15
3x3	125	01:25:02
4x4	625	13:08:08
Higher-D	---	???

**Intel Core i7 (Sandy bridge) 3.40 GHz processor

Carrasco J.C. and Lima F.V. *In Proceedings of the FOCAPO/CPC*, 2017

WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Strategies Towards Computational Time Reduction

- ✓ Parallel computing
- ✓ Machine learning (Gaussian Process) mapping

WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Novel Operability Framework Based on Parallel Computing

$$\mathbf{AIS} = \{\mathbf{u} \mid \mathbf{u}_i^{\min} \leq \mathbf{u}_i \leq \mathbf{u}_i^{\max} \; ; 1 \leq i \leq m\}$$

$$\mathbf{AOS} = \{\mathbf{y} \mid \mathbf{y} = \mathbf{M}(\mathbf{u}); \; \mathbf{u} \in \mathbf{AIS}\}$$

P4: $\Psi = \min_{\mathrm{u} \in \mathbb{U}} [\mathrm{PI}_{\ target}]$

Subject to:

$$\mathrm{u}^*_{k_{w=1}} \in \left[\underset{\substack{\mathrm{u}^*_{k_w} \in \mathbb{U}_{k_w} \\ y_{k_w} \in DOS}}{\mathrm{argmin}} \{\varphi_1\} \right]_{w=1}$$

$$\mathrm{u}^*_{k_{w=2}} \in \left[\underset{\substack{\mathrm{u}^*_{k_w} \in \mathbb{U}_{k_w} \\ y_{k_w} \in DOS}}{\mathrm{argmin}} \{\varphi_2\} \right]_{w=2}$$

⋮

$$\mathrm{u}^*_{k_{w=ws}} \in \left[\underset{\substack{\mathrm{u}^*_{k_w} \in \mathbb{U}_{k_w} \\ y_{k_w} \in DOS}}{\mathrm{argmin}} \{\varphi_{ws}\} \right]_{w=ws}$$

$$\mathbf{c}_1(\mathrm{u}^*_k) \leq \mathbf{0}$$

Define:

$\mathbf{DOS} = \{\mathbf{y} = (y_1, y_2, y_3 \dots y_p)\}$

ws: number of cores or workers

$\mathrm{PI}_{\ target}$: volume, area, or others

$\mathrm{u}^*_{1,o}$: initial guess for input point

$(\mathrm{u}^*_{PI}, y^*_{PI})$: intensified input and output values

$$\varphi_w = \sum_{j=1}^{n} \left| \frac{y_{j,k_w} - y^*_{j,k_w}}{y_{j,k_w}} \right| \qquad w = 1,2,3 \dots ws\,; \quad k = 1,2,3 \dots p$$

$$k_w = round\left[(w-1)\frac{p}{ws}\right] + 1, \dots, round\left[w\frac{p}{ws}\right]$$

Carrasco J.C. and Lima F.V. *AIChE Futures Issue*, 2018

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Computational Time Analysis for Parallelization

Computational time (Improvements after mathematical manipulation)

System	Points	Time [hr:min:sec]
2x2	25	00:02:55
3x3	125	00:31:02
4x4	625	05:14:04

Parallelization (2 workers)

System	Points	Time [hr:min:sec]
2x2	25	00:01:31
3x3	125	00:14:59
4x4	625	02:28:42

(3 workers)

System	Points	Time [hr:min:sec]
2x2	25	00:01:02
3x3	125	00:10:53
4x4	625	01:44:46

(4 workers)

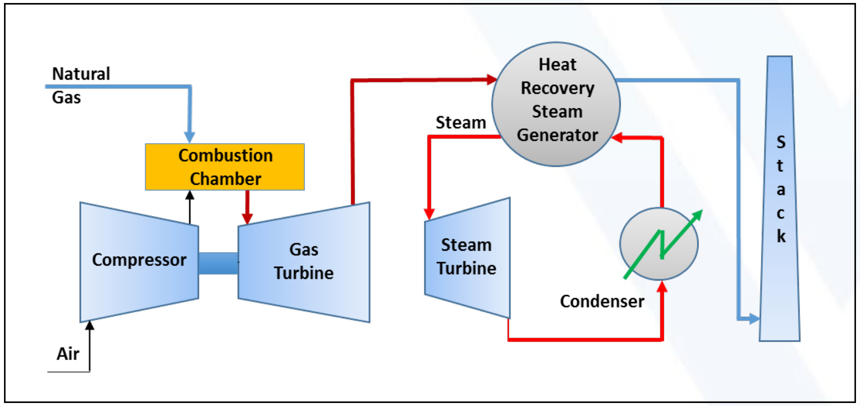
System	Points	Time [hr:min:sec]
2x2	25	00:00:54
3x3	125	00:07:51
4x4	625	01:16:49

4.09

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)
CODES

Natural Gas Combined Cycle (NGCC) High-D Application – 8x8

Simplified Schematic of NGCC Power Plant*



* DOE/NETL-341/061013 Technical report, 2013

Selected intensified 5 inputs	Inputs points
Natural gas feed [ton/h]	0.013
HRSG steam feed [ton/h]	0.157
Compressor outlet pressure [atm]	5.8
Air feed temperature [K]	329
Steam cycle pressure [atm]	140

- **Minimize size (power generation) of NGCC plant for intensification and modularity**
- **Maintain combined cycle efficiency**

Selected intensified 5 outputs	Output points
Net plant power [MW]	0.11
Net plant efficiency [%]	56.5
Capital cost* [$ millions]	0.5
Gas turbine power [MW]	0.09
Air compressor power [MW]	0.06

Capital Cost** [MM$] = 2.821 (NPP)$^{0.7991}$
NPP: Net plant power [MW]

U.S. EIA, 2013. Updated capital cost estimates for utility scale electricity generating plants
ESMAP Technical paper 122/09. Study of equipment prices in the power sector

Carrasco J.C. and Lima F.V. *AIChE Futures Issue,* 2018

WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

NGCC Computational Time Analysis

Subsystems	Points DOS	P3 Time [hr:min:sec]	P4 (63 cores) Time [hr:min:sec]	Reduction [times]
4x4	625	00:00:38	00:00:07	5.4
5x5	3125	00:05:06	00:00:19	16.1
7x7	78125	02:58:42	00:03:01	59.2
8x8	390625	16:56:26	00:14:24	70.6

NGCC plant computational time estimations:

- ✓ NGCC 10x10 system (63 cores) would require approx. 11,400 seconds
- ✓ If the NETL supercomputer (Joule*) was used:
  - ❖ 3 seconds would be estimated for 10x10 system
  - ❖ 3,600 seconds would be estimated for 22x22 system

***Joule is one of the top 100 supercomputers in the world, has 1512 nodes, each node has two 8-core 2.6 GHz Intel Sandy Bridge CPUs, with approx. 17,000 available cores**

Carrasco J.C. and Lima F.V. *AIChE Futures Issue,* 2018

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Machine Learning-based Operability

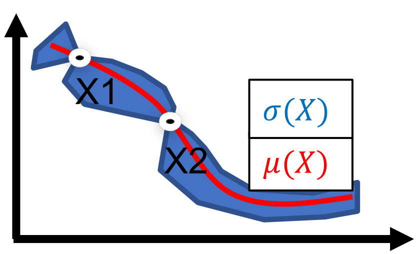
Proposed method: supervised machine learning to generate process model surrogates for the developed operability algorithms

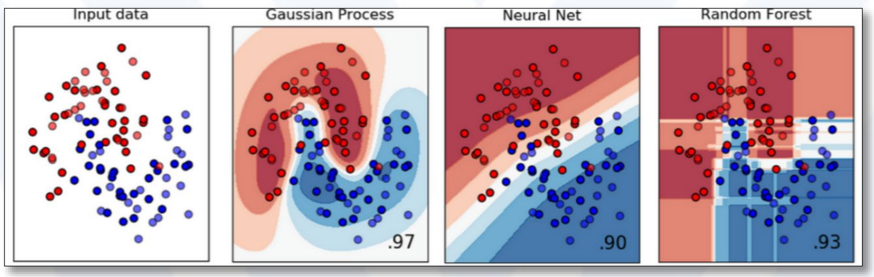
Surrogate models should be able to:

- decrease computational time
- represent nonlinearities, input-output multiplicities, etc.
- be compatible with previous process operability algorithms (NLP-based and multimodel approaches)

Gaussian Processes:
$\mathbb{GP} \stackrel{\text{def}}{=} \hat{Y}(X) = \mu(X) + K(X)$

This concept has been extended to applications such as: Computer Experiments*, Flowsheet Optimization**, Real-time Optimization***





Extracted from https://towardsdatascience.com

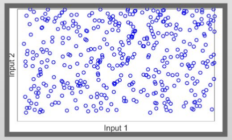
* A. Forrester, A. Sobester and A. Keane, *John Wiley & Sons*, 2008; J. Sacks et al., *Statistical Science*, 1989
** J. A. Caballero and I. E. Grossmann, *AIChE Journal*, 2008; *** M.V.C Gomes, PhD Thesis. *UFRJ*, 2007

Machine Learning-based Operability

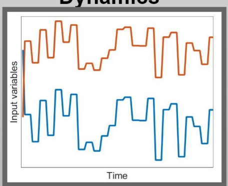
Sampling of Available inputs

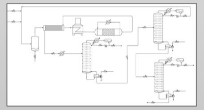
Use sampling techniques to generate input-output data efficiently

Sampling - Steady-state



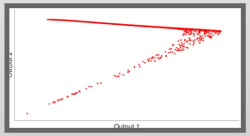
Sampling - Dynamics



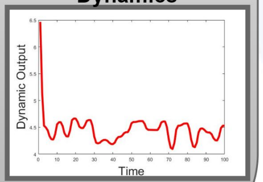


Process model (M)

Achievable outputs - Steady-state



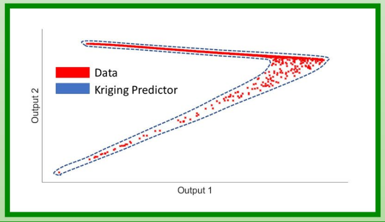
Achievable outputs - Dynamics



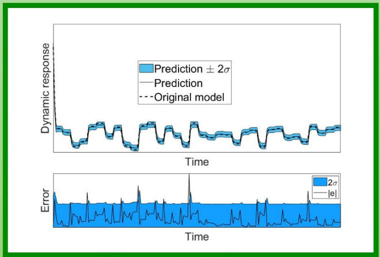
Machine Learning Model Training

Generate Kriging models of the desired system responses

Steady-state Kriging



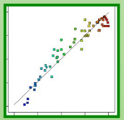
$$\mathbb{GP} \overset{\text{def}}{=} \hat{Y}(X) = \mu(X) + K(X)$$



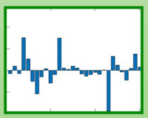
Dynamic Kriging

Performance assessment (Validation)

Ensure quality of machine learning models



Hold-out validation

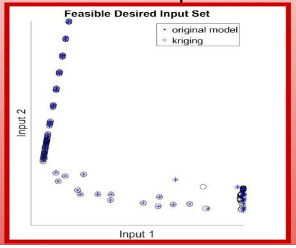


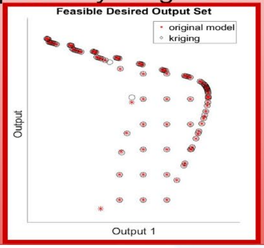
Cross-validation

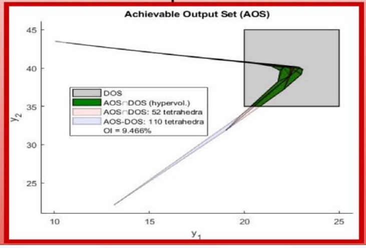
Operability Framework

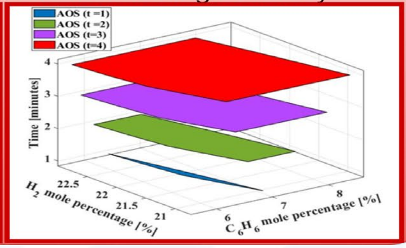
Use the generated machine learning models to obtain process operability insights with reduced computational time while maintaining accuracy

Process Operability algorithms:
Multimodel Approach
NLP-Based Approach
Operability Index (OI)
Dynamic Operability





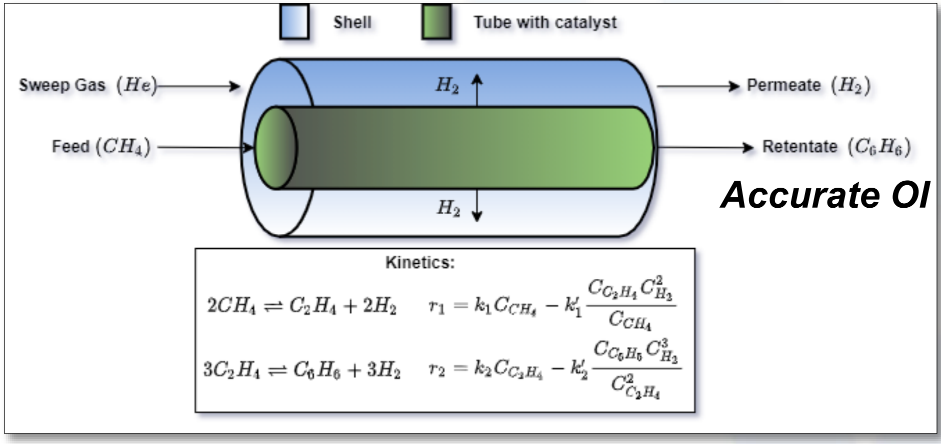




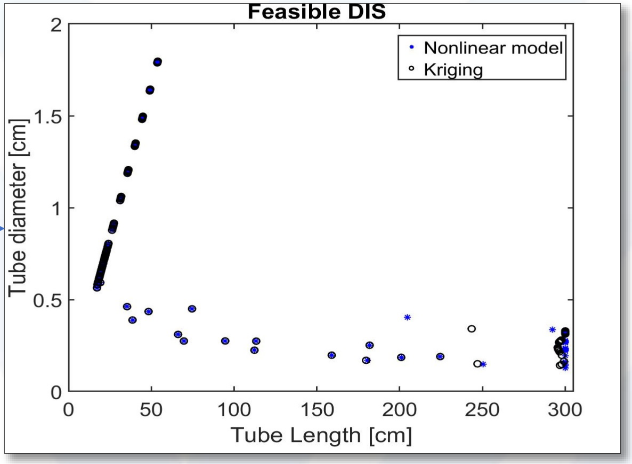
WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Surrogate Model-based Operability Calculations

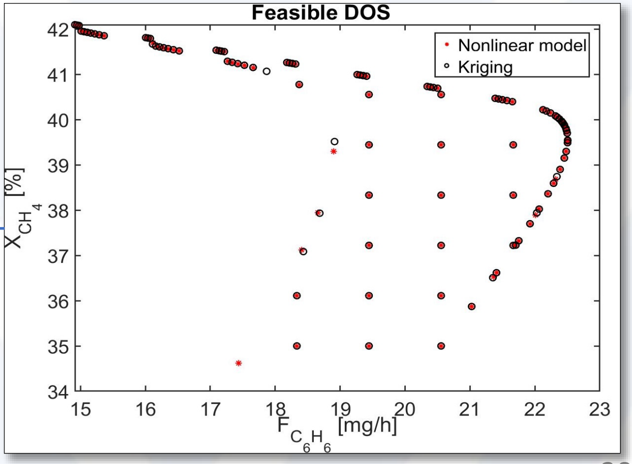
Case Study: Direct Methane Aromatization-Membrane Reactor (DMA-MR)



Accurate OI quantification



NLP-based approach (M^{-1})



Intensified design variable	Non-linear model	GP (Kriging)	Relative error [%]
Tube length [cm]	17.2283	17.2205	0.0454
Tube diameter [cm]	0.5634	0.5636	0.0388

Nonlinear model NLP Approach = 5 min 38s

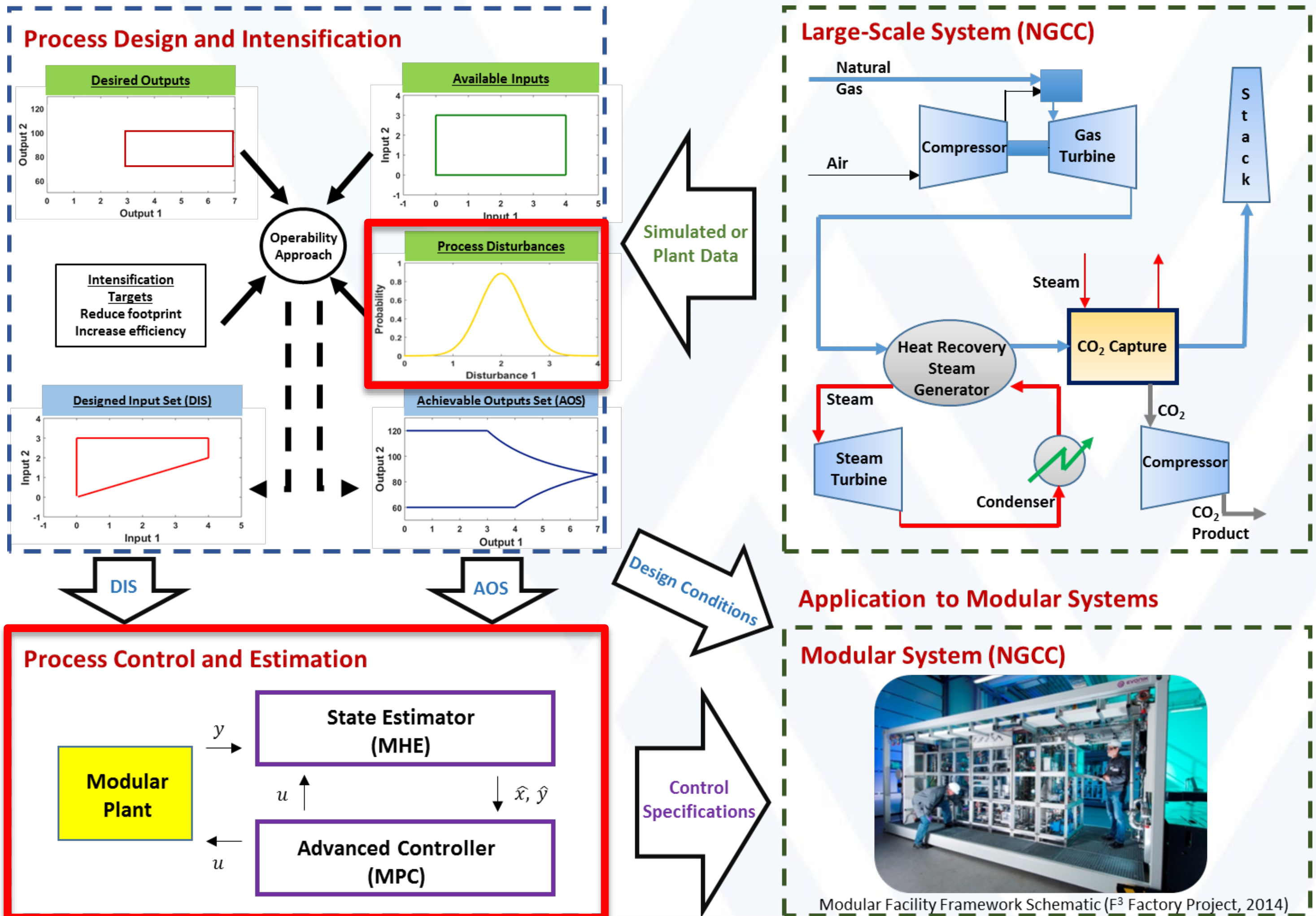
Generation of 2,000 points + create GP + validate + NLP = 58s

5.8 times decrease in computational time

NLP-based GP approach = 0.0477s, up to four orders of magnitude in computational time reduction

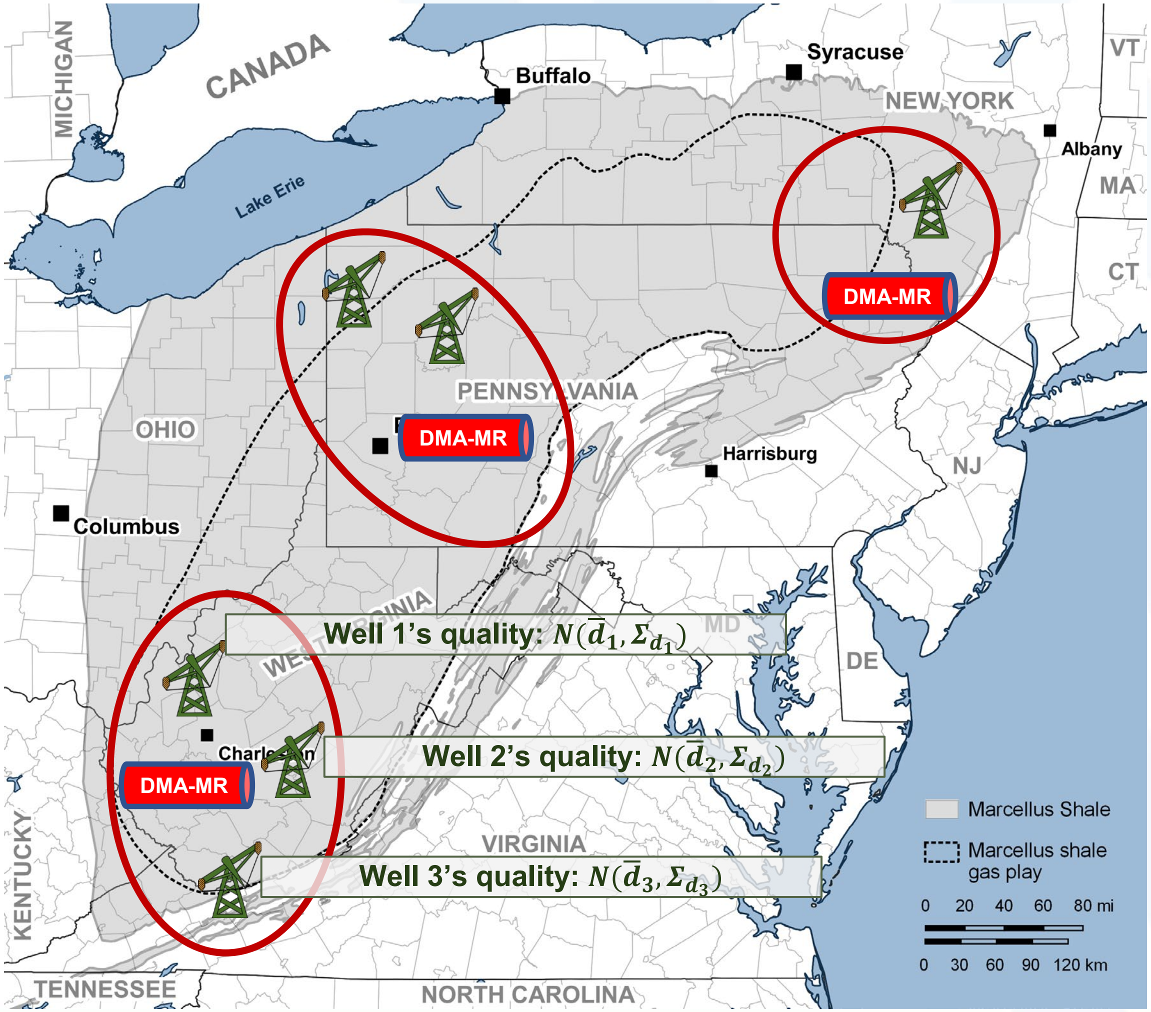
Alves V. , Gazzaneo V. and Lima F. V., *Submitted for Publication*, 2021

Operability for Control and Estimation



Modular Facility Framework Schematic (F[3] Factory Project, 2014)

Dynamic Operability: DMA-MR Motivation



Challenges

- Intensified and modular units are harder to control due to the loss of degrees of freedom
- Under large disturbances, the process may not be able to return to the desired operating regions

Dynamic Operability Objective

- Construct the **dynamically operable funnel**: the operating region within which the process can always be retained regardless of the disturbances
- Dynamically operable funnel can be expressed as output constraints for MPC applications

Source: Gretarsson, Mahlzeit. "Marcellus Shale Revised Map 2019", Wikipedia, 23 Aug. 2019, https://en.wikipedia.org/wiki/File:Marcellus_shale_revised_map_2019.png.

WestVirginiaUniversity.

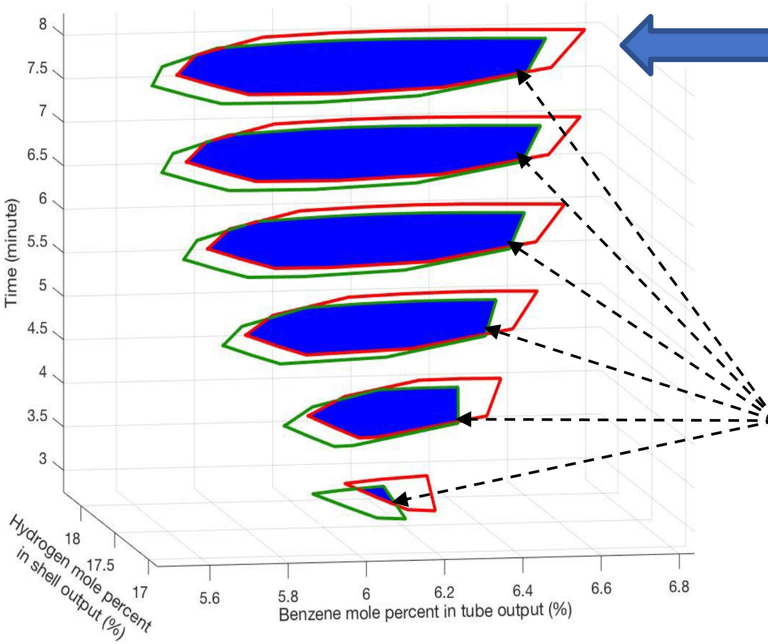
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Dynamic Operability: Formulation

A dynamic process is operable if it can achieve desired performance requirements from the given inputs regardless of the realization of the disturbances

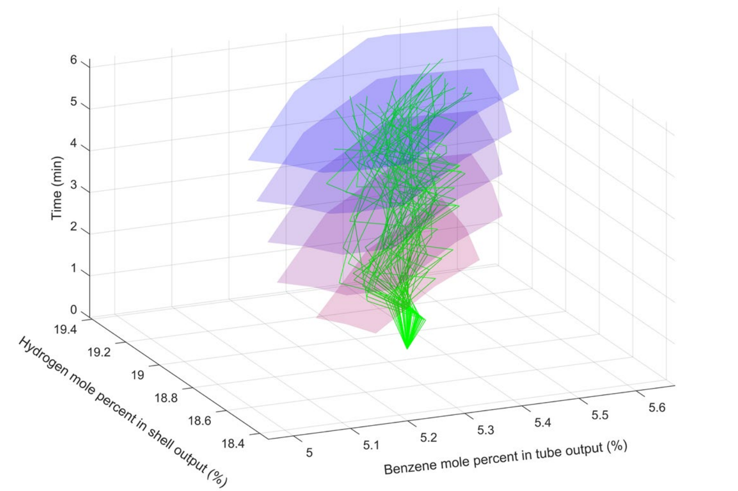
<u>Membrane reactor case study</u>: Disturbance is the methane concentration in the feed stream. If the dynamic disturbance only takes 2 values:

- Natural gas composition in the **first** well→ First set of dynamic AOS **(red)**
- Natural gas composition in the **second** well → Second set of dynamic AOS **(green)**



Time that both dynamic AOS sets converge to their invariant AOS

The intersection region **(blue)** of the 2 dynamic AOS sets represents the reachable outputs regardless of the values of the disturbance

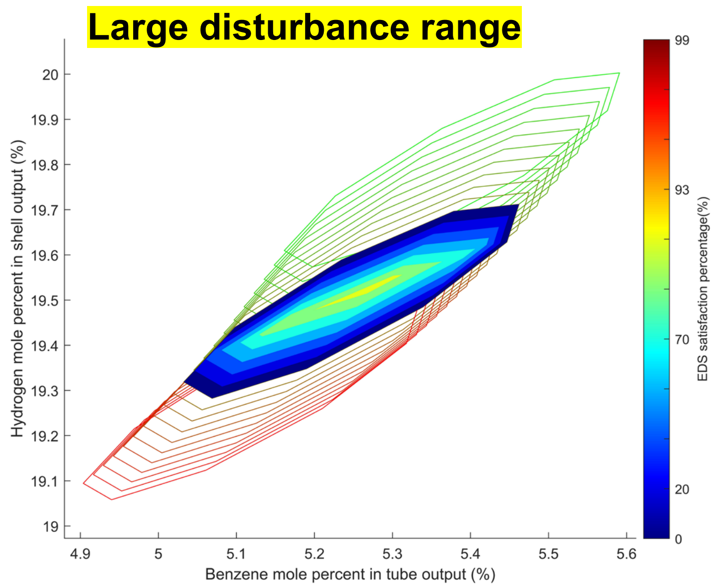


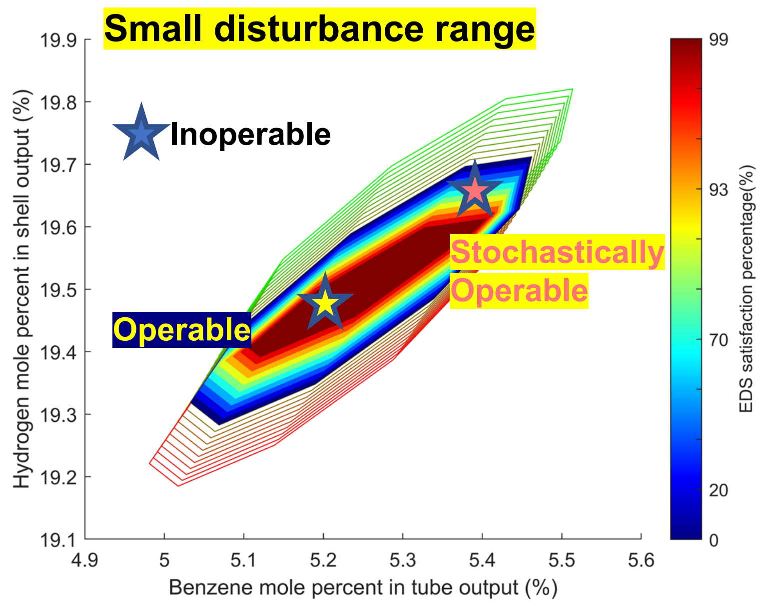
Dynamic AOS (**red**-**purple** polytopes) with Monte Carlo simulation (**green** trajectory) as verification

WestVirginiaUniversity
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Dynamic Operability: Results

For **all** time steps:



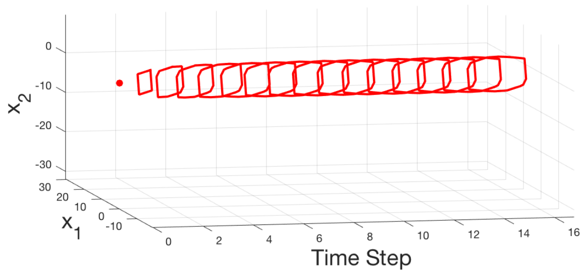


Inoperable because the control moves cannot compensate for all disturbance effects	(Stochastically) Operable if the setpoint is in the (stochastic) achievable region

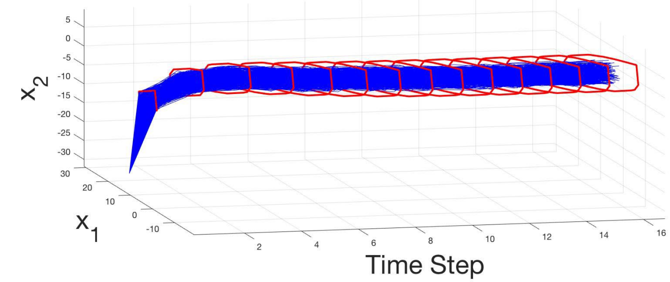
If the **operable region exists** for every time step (from initial to invariant region time) **and** the **set points are inside** the final invariant regions, then the given steady-state design is **operable**

Dynamic Operability Mapping

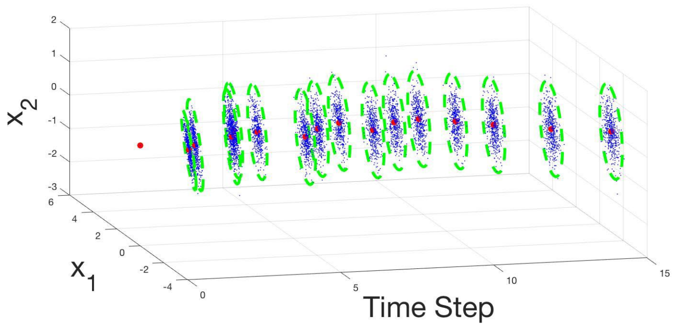
Offline Mapping of Achievable Funnel at Nominal State



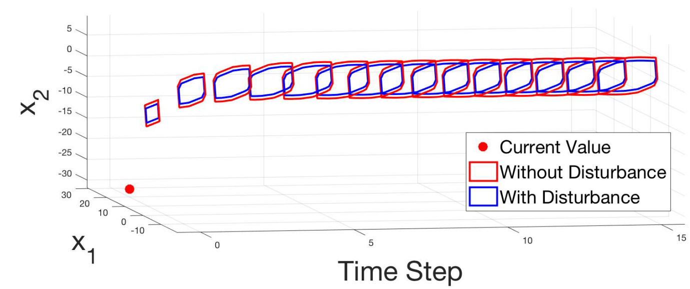
Online Update of Achievable Funnel at Each Time Step



Uncertainty Propagation



Dynamically Operable Funnel



Dinh S. and Lima F.V. Accepted in PSE 2021+, 2022

West Virginia University
WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Dynamic Operability Mapping Computation (Ongoing)

Dynamic funnel when the initial states are at the nominal values (Future idea: Branch and Bound)

→

Dynamic funnel update after the state measurements arrive, at nominal disturbance values (Sensitivity update/ Implicit Function Theorem)

↓

Disturbance effects on the dynamic funnel (Moment recovered approximation)

→

Dynamic funnel of all achievable outputs regardless of the disturbances:

- Transient output constraints for MPC feasibility
- Chance constraints

Dinh S. and Lima F.V. Accepted in PSE 2021+, 2022

WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)

Conclusions and Future Avenues

- Operability approaches provide **new directions** for **process intensification** of chemical and energy systems towards modularity
- Proposed bilevel **optimization-based** operability approaches using **parallel computing** and **machine learning** present themselves as alternatives to tackle computational time challenges
- Future avenues:
  - ✓ explore Gaussian Process methods for the dynamic mapping of operability
  - ✓ incorporate multiple objectives (e.g., economics, sustainability) into process operability
  - ✓ perform dynamic operability funnel updates using sensitivity calculations (with Larry Biegler)
  - ✓ develop operability open-source software in Python (with Carl Laird)
- Other research directions: www.statler.wvu.edu/~fernando.lima

Contact: Fernando.Lima@mail.wvu.edu; flima@andrew.cmu.edu

Acknowledgments

- **Lima CODES Research Group: Dr. Juan C. Carrasco (U de Concepción), Dr. Vitor Gazzaneo (Air Products), San Dinh and Victor Alves**
- **National Science Foundation CAREER Award**
- **ACS-PRF Doctoral New Investigator Award**

CODES Group Support

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

WEST VIRGINIA UNIVERSITY
DEPARTMENT OF CHEMICAL AND BIOMEDICAL ENGINEERING
LIMA RESEARCH GROUP
Control, Optimization and Design for Energy and Sustainability (CODES)