A Process Operability App for Intensification and Modularization of Energy Systems

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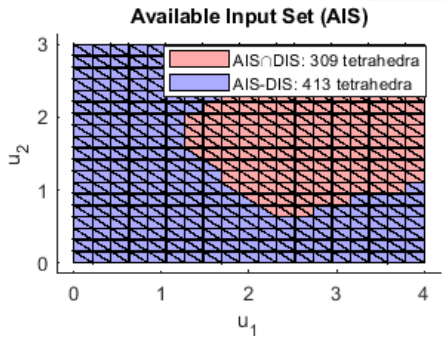

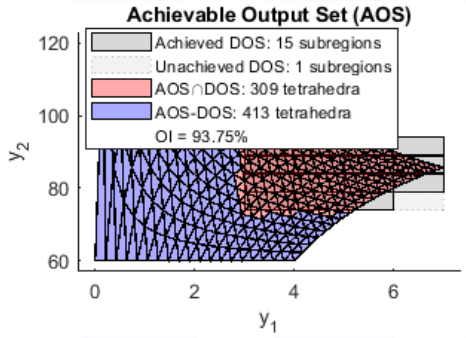

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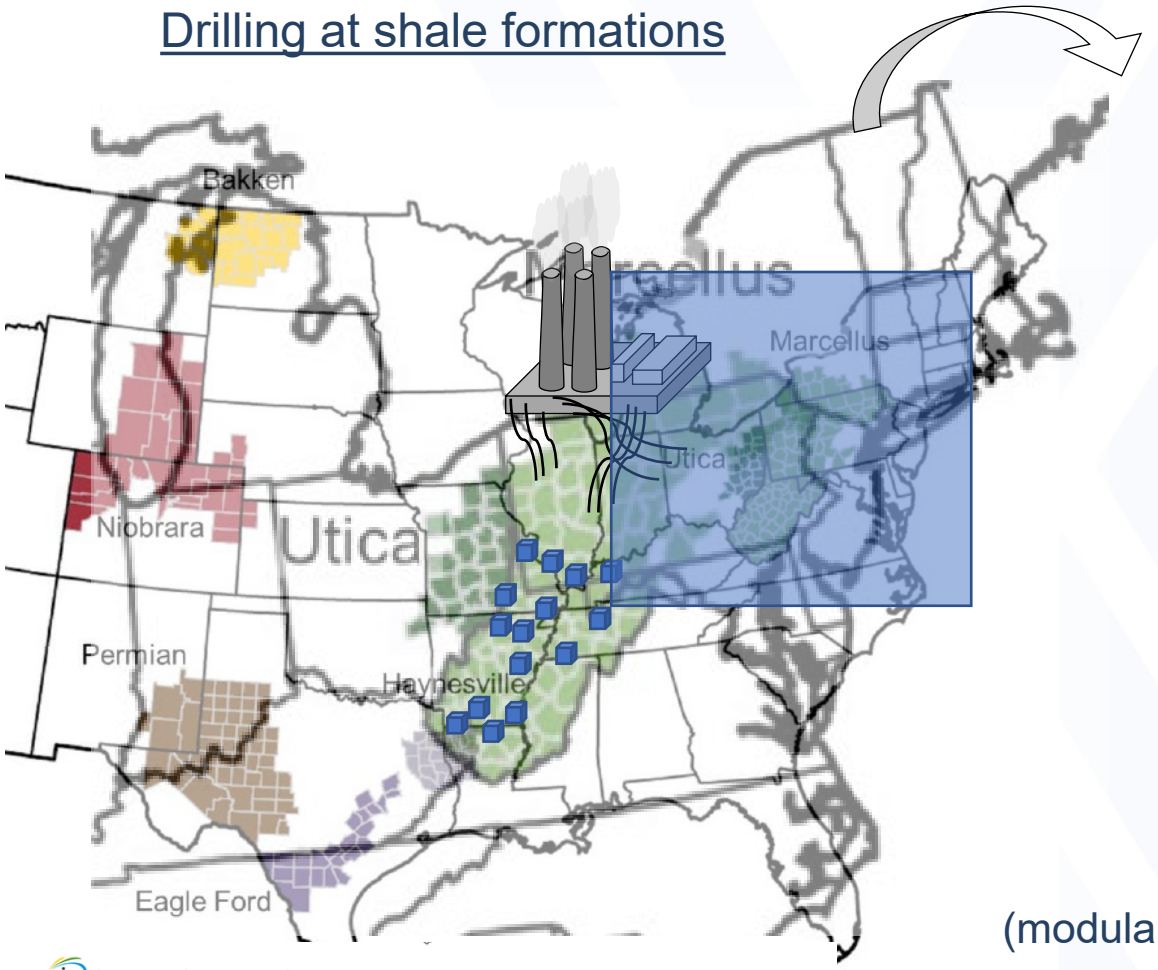
Outline

- Background
  - Modular energy systems
  - Process operability concepts
- Operability Framework
  - Multimodel operability approach
  - Nonlinear programming (NLP)-based methods
  - Process Operability App
- Applications
- Future Work

Modular Energy Systems

Drilling at shale formations



eia Source: U.S. Energy Information Administration

Geological formations, therefore, for each well:

- Specific production of gas
- Unique lifetime

Conventional natural gas utilization

×

Distributed natural gas utilization

(modular technologies for onsite utilization)

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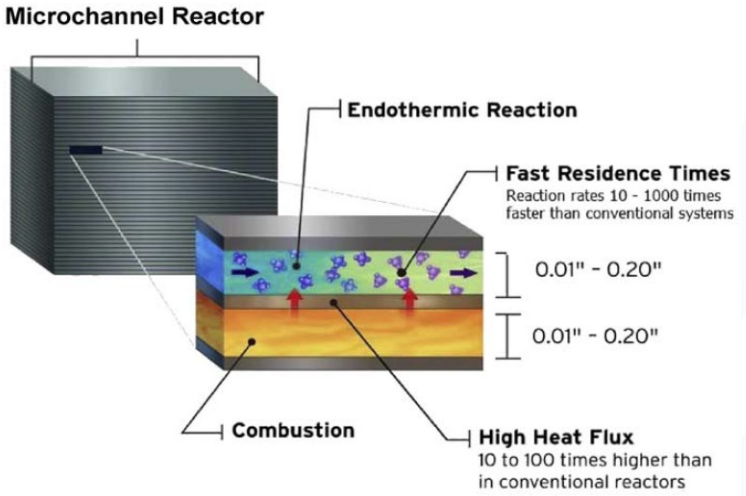
Modular Energy Systems

Modular energy systems

- System modularization (SM): physically small modular plants
- Possibly employ process intensification (PI) for process integration



Modular steam methane reforming (SMR) unit [1]

Process design challenges

- System nonlinearities, dimensionality and constraints
- High degree of process integration and customization
- Lack of guidelines and heuristics for operation

Process Design → Process Control

Integration of Design and Control (Operability Analysis)

[1] Lerou, J. J. et al., *Chemical Engineering Science*, 2010

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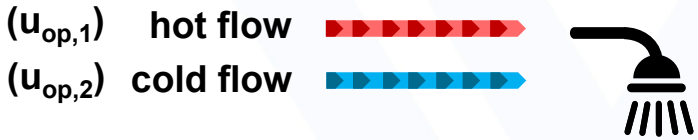
Process Operability Concepts

Operability Analysis[2,3]: Address operability challenges at the design phase

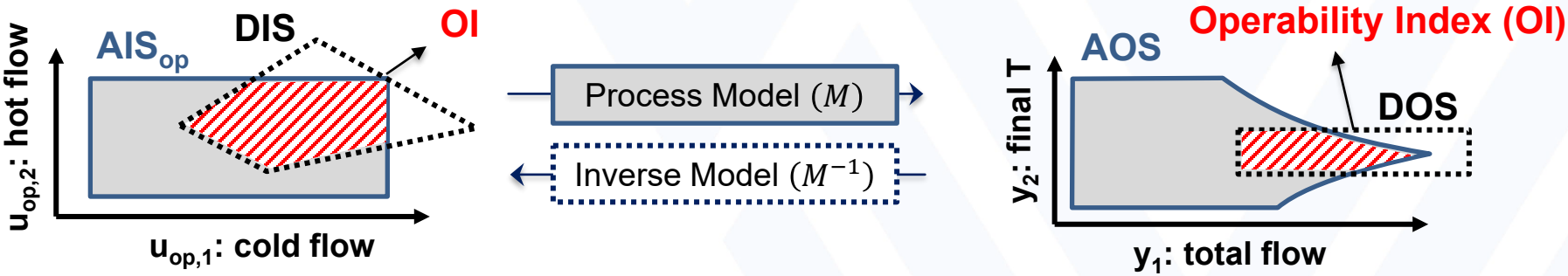


Available Input Set (AIS_{op})
Manipulated variables (MVs)

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

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

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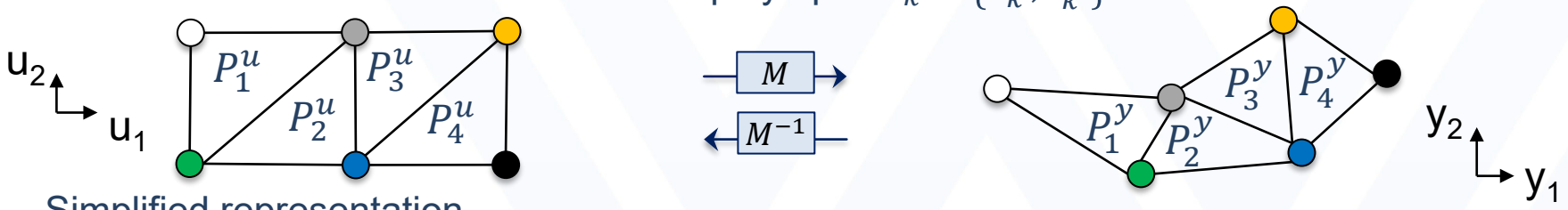
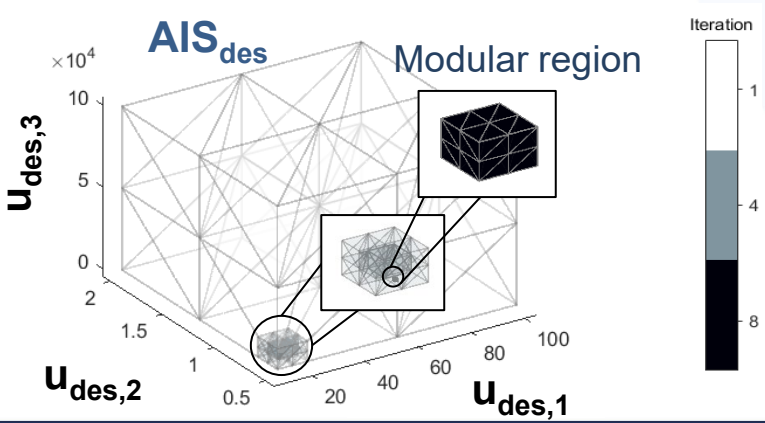
Multimodel Operability Approach

Multimodel operability representation[4]: Original nonlinear model substituted by paired polytopes $P_k = \{P_k^u, P_k^y\}$

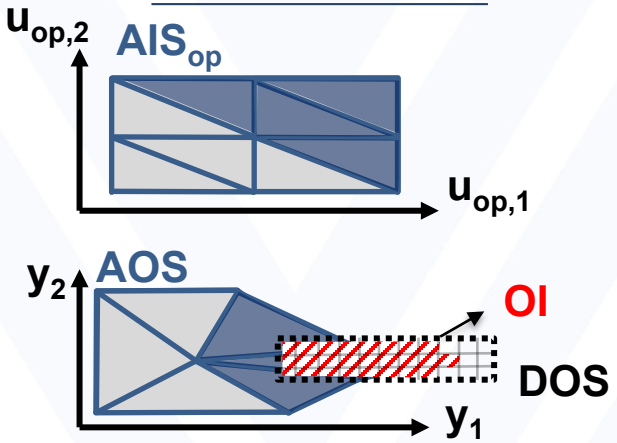


- Simplified representation
- Efficient quantification of operability regions
- Straightforward calculation of M^{-1}

Explore system modularization



Calculations of OI



[4] Gazzaneo V., Lima. F.V., *Ind. Eng. Chem. Res.*, 2019

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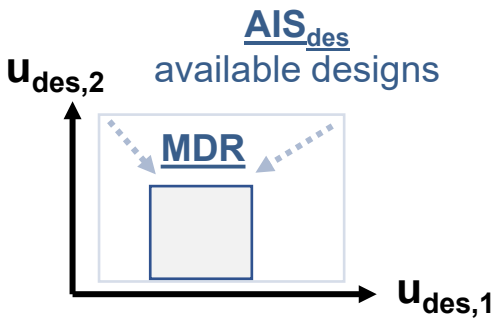
Multimodel Operability Approach

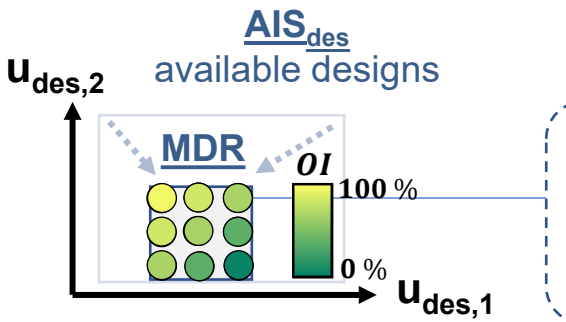
MULTILAYER OPERABILITY FRAMEWORK[3,4]

LAYER 1: MODULAR DESIGN PROBLEM

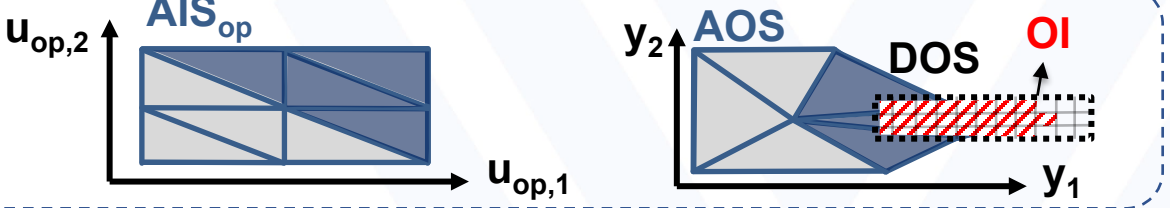


- Find the modular design region (MDR)
- Mixed integer linear programming (MILP)-based iterative algorithm[3,4]
- ↓ Process footprint (SM) – objective function
- ↑ Process efficiency (PI) – DOS limits

LAYER 2: INTENSIFIED OPERATION PROBLEM



- Evaluate intensified operation
- Rank competing modular designs with OI



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

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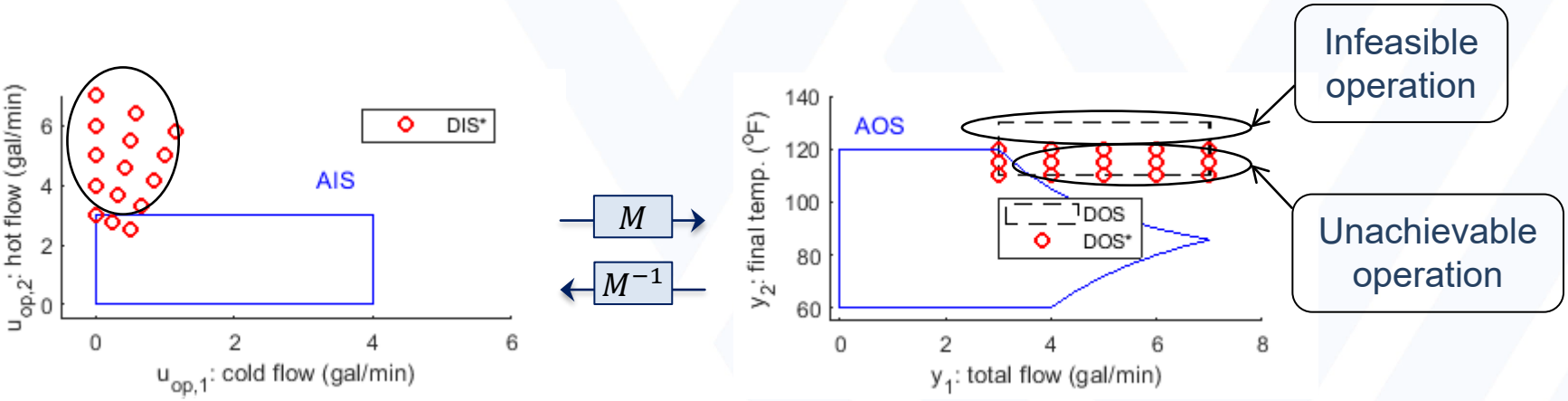
NLP-based methods

Nonlinear programming (NLP)-based operability method[5]

- Handles infeasible DOS with NLP-based model inversion
- Finds feasible spaces, feasible DOS (DOS*) and feasible Desired Input Set (DIS*)
- Insights for changes in the selected AIS



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

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Process Operability App Project

Process Operability App[3]

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

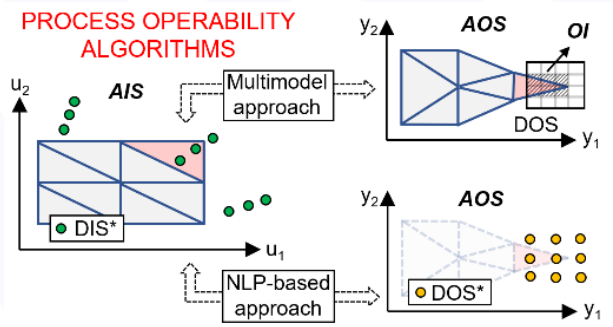
NLP-BASED APPROACH
- Feasibility of DOS
- NLP-based algorithm for DIS-DOS mappings

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



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

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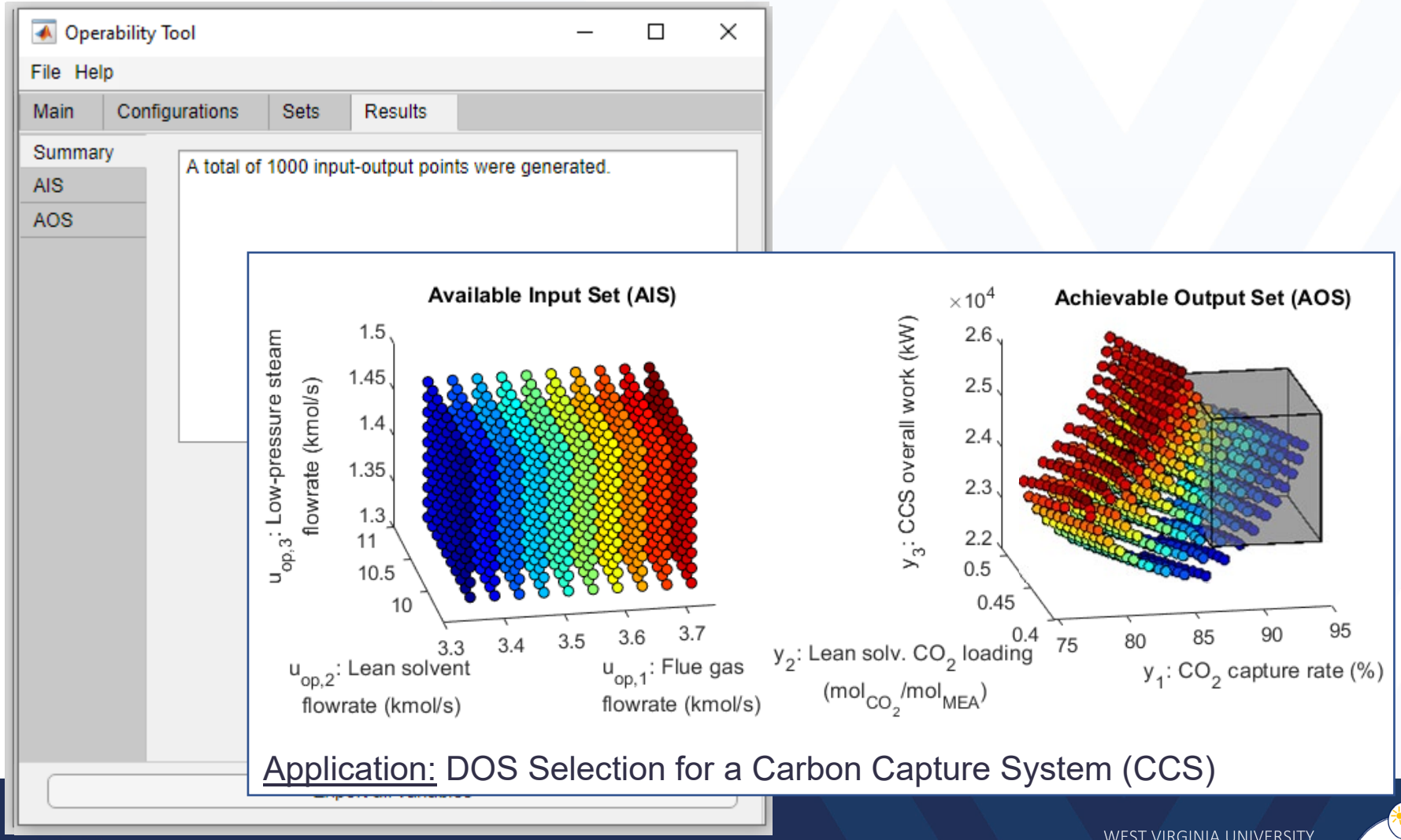
Process Operability App: Applications

Input-output mapping for selection of the DOS



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

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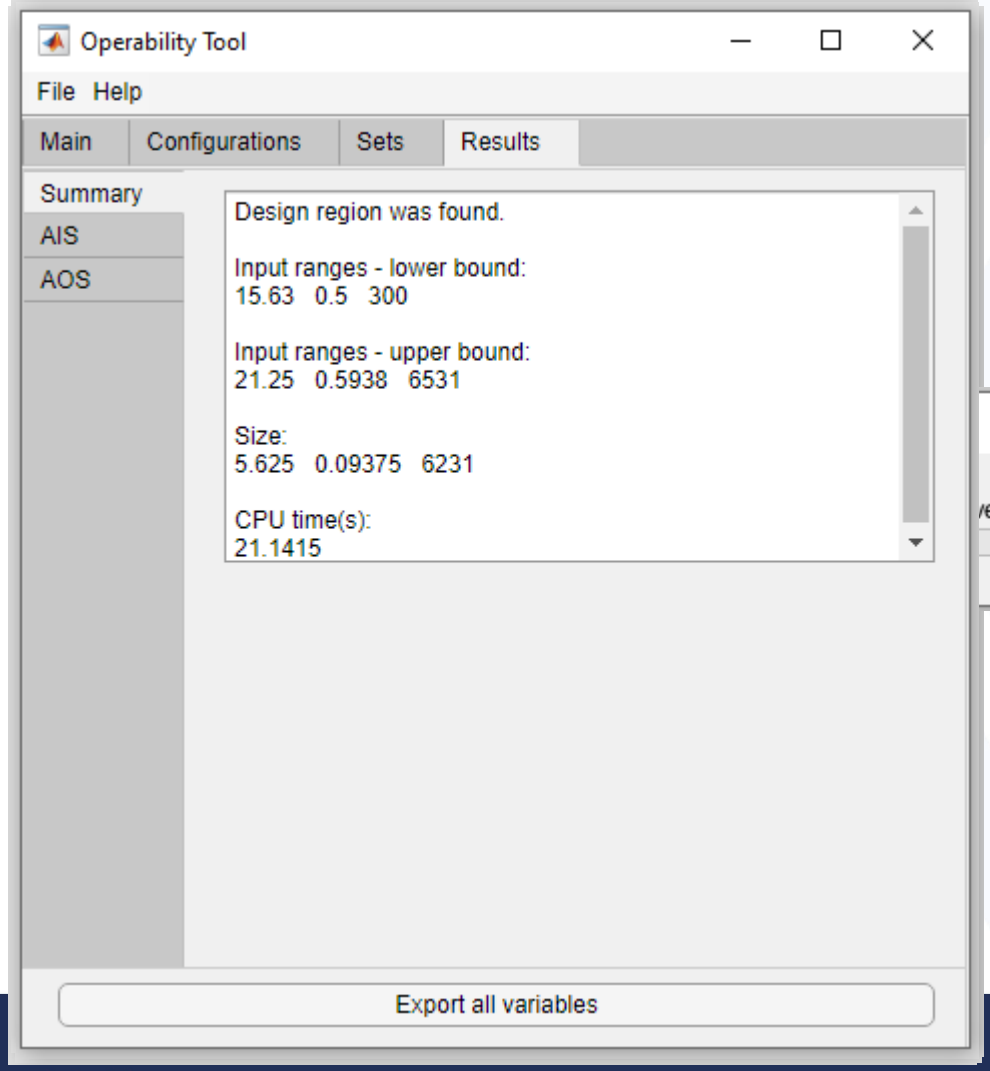
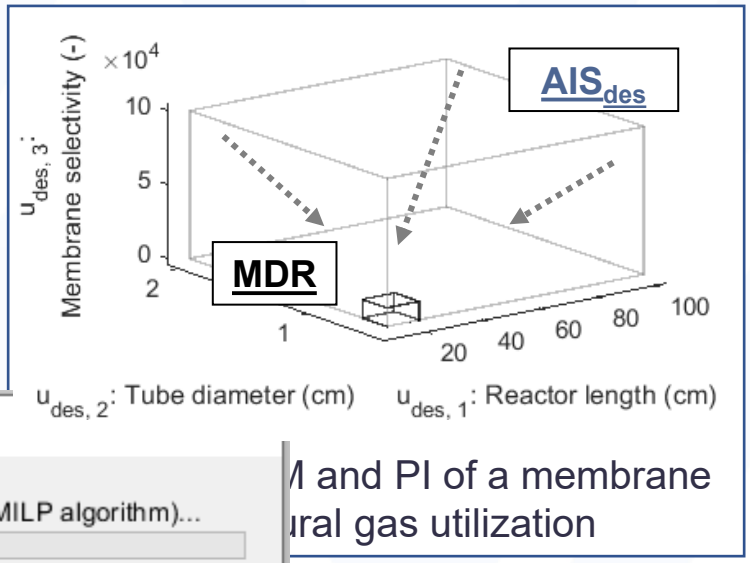
Process Operability App: Applications

Multimodel Operability Approach: LAYER 1: MODULAR DESIGN PROBLEM





...M and PI of a membrane
...ural gas utilization

...ve MILP algorithm)...

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Process Operability App: Applications

Multimodel Operability Approach:

LAYER 2: INTENSIFIED OPERATION PROBLEM

Operability Tool

File Help

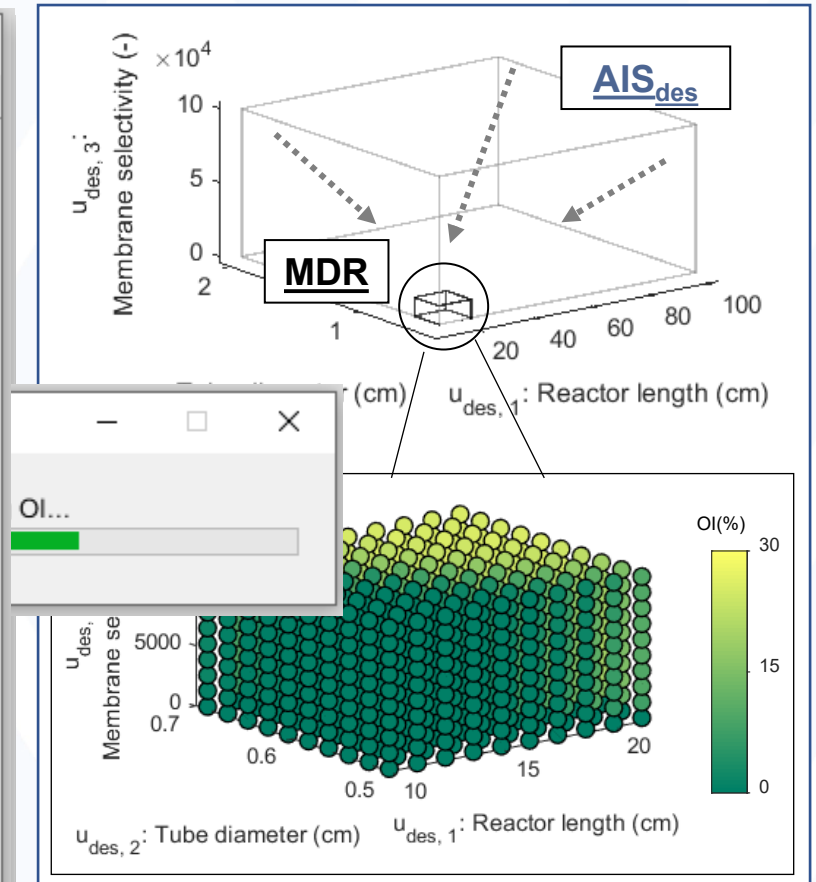
Main | Configurations | Sets | Results

Summary
AIS
AIS des
AIS op
AOS
DOS
OI

u des1	u des2	u des3	OI(AIS des)
16	0.5667	611.1111	1.5625
16	0.5667	722.2222	3.1250
16	0.5667	833.3333	3.1250
16	0.5667	944.4444	4.6875
16	0.5667	1.0556e+03	4.6875
16	0.5667	1.1667e+03	4.6875
16	0.5667	1.2778e+03	4.6875
16	0.5667	1.3889e+03	4.6875
16	0.5667	1500	4.6875
16	0.5778	500	3.1250
16	0.5778	611.1111	4.6875
16	0.5778	722.2222	6.2500
16	0.5778	833.3333	4.6875
16	0.5778	944.4444	4.6875
16	0.5778	1.0556e+03	4.6875
16	0.5778	1.1667e+03	6.2500
16	0.5778	1.2778e+03	6.2500
16	0.5778	1.3889e+03	6.2500
16	0.5778	1500	6.2500
16	0.5889	500	3.1250

Export all variables

OI...



Application: SM and PI of a membrane reactor for natural gas utilization

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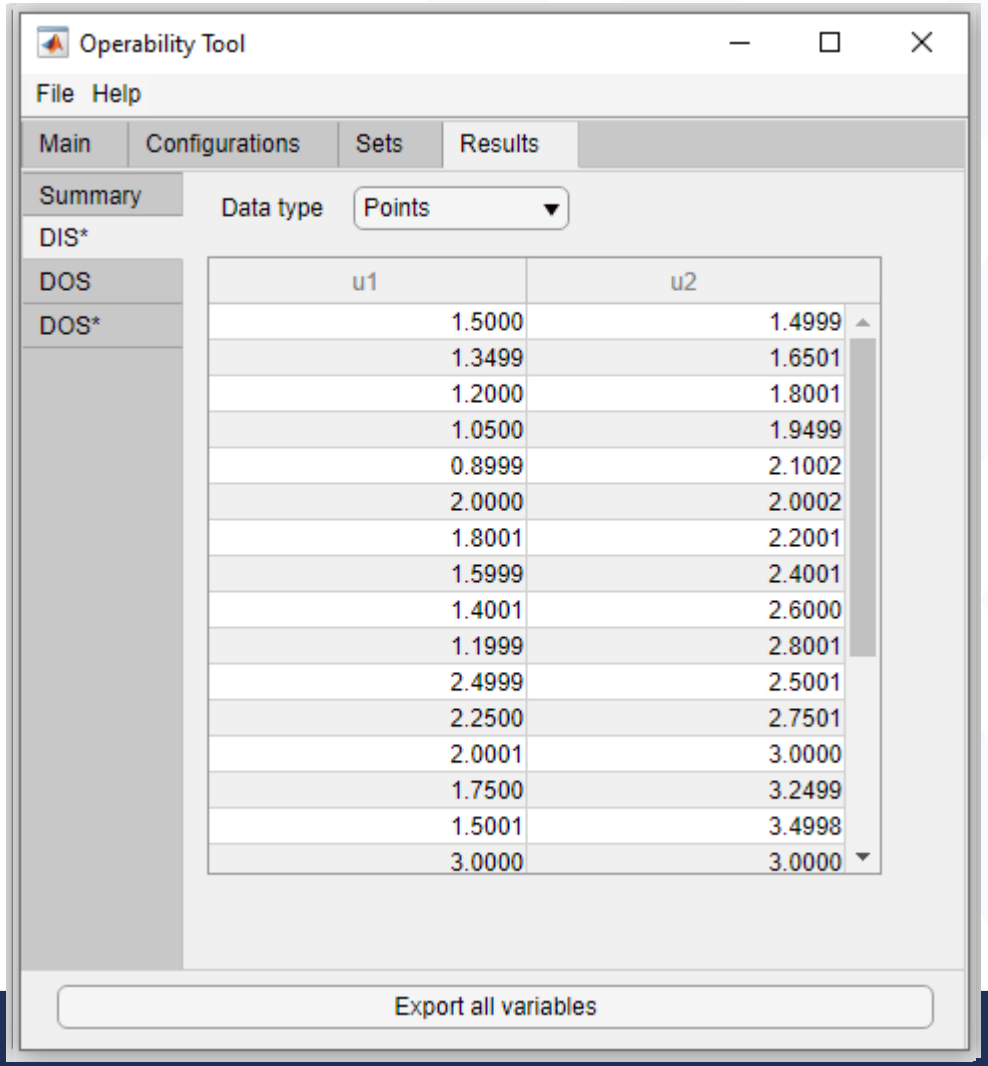
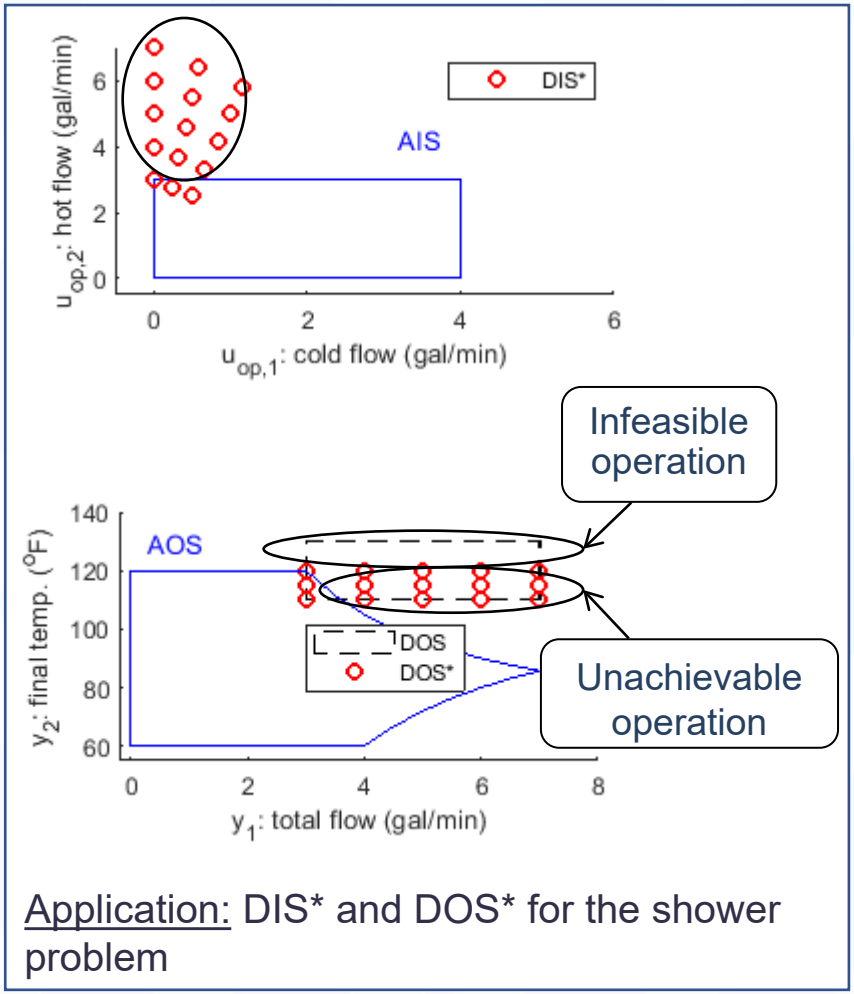
Process Operability App: Applications

NLP-based Approach: Feasible DIS and DOS





Application: DIS* and DOS* for the shower problem

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Conclusions and Future Work

Future work

- Improve OI with disturbance rejection (flexibility)
- Address app limitations (dimensionality)
- Include other input-output representations
- Explore connection with other software platforms (Aspen Plus, OSIsoft PI, etc.)

Acknowledgments

- Donors of the American Chemical Society Petroleum Research Fund for partial support of this research
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- Financial support from West Virginia University
- Dr. Lima's CODES research group

… QUESTIONS ?