

An MILP-based Operability Approach for Process Intensification and Design of Modular Energy Systems

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Abstract

A mixed-integer linear programming (MILP) operability approach is developed for the design of high-dimensional and nonlinear systems. For the approach formulation, classical operability concepts are extended to attain process intensification towards system modularity. Motivated by natural gas utilization processes, a catalytic membrane reactor for the direct methane aromatization (DMA-MR) conversion to hydrogen and benzene is chosen as case study. The DMA-MR is described by a system whose design is challenged by complexity, including nonlinearities and a highly-constrained environment. A DMA-MR subsystem is addressed, for which 80% reduction in membrane area and 78% reduction in reactor volume is obtained when compared to a base case with equivalent performance. The proposed approach presents a computational time reduction greater than 3 orders of magnitude compared with previously introduced nonlinear programming-based operability approaches. These results indicate that the proposed approach is computationally efficient and thus can be extended to address higher dimensional cases.

Keywords: Operability, Process Intensification, Modular Systems, Energy Systems, Optimization.

1. Introduction

Modular systems are promising technologies characterized by versatility. They provide an alternative for the traditional industry by considering small modules of higher efficiency. As these modules can be shipped and assembled, the exploitation of resources in remote and originally untapped areas becomes feasible. A DMA-MR for methane conversion to hydrogen and benzene can be considered as a potential candidate system for modular natural gas utilization that could be transported to stranded gas fields. In this case, the concept of process intensification characterized by the enhanced reaction and separation phenomena in the membrane reactor may enable high efficiency units for modular system applications. Additionally, a substantial decrease in cost and environmental footprint are key outcomes of system modularity that are also associated with process intensification. The design of a modular energy system, however, is challenged by its complexity, including nonlinearities, system dimensionality and a highly-constrained environment. An MILP-based operability approach is proposed here to overcome these challenges. Operability was first described as a mapping between inputs and outputs of a system that was established to measure the ability of a design to achieve specified desired operating states. The aim in the new formulation is to extend

classical operability concepts and tools to attain process intensification targets and ensure system modularity in a computationally efficient manner.

Process operability was initially used for the assessment of low-dimensional nonlinear systems. The expansion to high-dimensional nonlinear systems was successfully addressed by employing optimization algorithms based on nonlinear programming (NLP) [1,2]. However, previously proposed approaches were challenged by the system dimensionality in terms of high computational expense. The novelty in this work consists of the fully utilization of MILP tools to tackle systems of similar complexity, with the advantage of computational time reduction.

2. Process Operability Concepts

In traditional process operability concepts, inputs (u) and outputs (y) are respectively represented by the Available Input Set (AIS) and Achievable Output Set (AOS). The desired operating region for the outputs and the corresponding region for the inputs in order to achieve such outputs are called Desired Output Set (DOS) and Desired Input Set (DIS), respectively. For a given set of inputs, the calculation of the corresponding outputs is performed by direct mapping employing a first-principles process model, M . Conversely, the inverse model, M^{-1} , represents the pathway from the outputs to inputs. For an $m \times n$ dimensional input-output system, the operability sets are generically represented by:

$$AIS = \{u | u_i^{min} \leq u_i \leq u_i^{max}; 1 \leq i \leq m\}; \quad DIS = \{u | u = M^{-1}(y); y \in DOS\};$$

$$AOS = \{y | y = M(u); u \in AIS\}; \quad DOS = \{y | y_i^{min} \leq y_i \leq y_i^{max}; 1 \leq i \leq n\};$$

Nonlinear systems require a nonlinear model M . The derivation of M^{-1} may be complex and sometimes not straightforward. One contribution of this work is the numerical computation of M^{-1} employing computational geometry tools, overcoming the challenges associated with the analytical calculation of M^{-1} . The description of such computation can be found in section 3 below, along with the proposed approach.

3. MILP-Based Operability Approach

In the developed framework, the operability mapping accounts for design variables (physical dimensions, feed and operating conditions) as inputs and measures of production (production rates and efficiency) as outputs. Such mapping is established by dividing the original nonlinear space into several linear subspaces described by linearized models. This task is performed with the utilization of computational geometry techniques such as Delaunay-triangulation. The properties of the obtained subsets are then analyzed to find the minimum number of divisions that is needed to adequately represent the original system. Using such divisions, an optimization algorithm based on MILP concepts is formulated, considering all process constraints and specific targets associated with process intensification. The steps of the developed framework can be summarized as follows:

- 1) The nonlinear system is simulated, generating input-output data points. First-principles models for the application of interest are considered for this task.
- 2) Using a computational geometry-based technique, e.g., Delaunay-triangulation, sets of triangles are obtained. Each triangle in the AIS has a counterpart in the AOS. This step can be repeated, with gradual reduction in number of considered data points,

until the triangulation is still possible for the minimum number of points. Once executed, this gradual reduction results in the minimum number of triangles needed to adequately represent the original nonlinear system. Alternatively, if needed, this step can be performed using only the points of the operating envelope, i.e., points of the boundary of AIS and AOS.

- 3) The DOS is selected and its intersection with the AOS is calculated by employing computational geometry tools. The input counterpart of the calculated region is the feasible DIS. This pathway from outputs to inputs is the inverse model calculation performed using linearized models represented by triangles.
- 4) An MILP minimization problem is formulated to reduce footprint in terms of physical size and ensure the compliance of process constraints and intensification targets. Here, the MILP formulation considers the regions of input/output delimited by the DIS/DOS in step 3. This formulation is mathematically defined as:

$$\Phi = \underset{u}{\text{minimize}} (footprint)$$

Subject to: $u \in DIS, y \in DOS$
 Linearized process model and constraints
 Process intensification targets

The mixed-integer nature is necessary due to the existence of the discrete regions represented by triangles. For each triangle, a binary value is assigned and the sum of all assigned values have to be 1. Interpolations are allowed by using weights related to the vertices of existing triangles. The outcome of the optimization is an optimal design inside a unique triangle.

4. Results: DMA-MR Case Study

In this section, each step of the framework described above is applied to a 2x2 DMA-MR subsystem, in which each step is in a separate subsection.

4.1. Simulation of the DMA-MR System

The feed for the shell and tube MR configuration considered is natural gas (methane) in the tube side, and a sweep gas (a laboratory inert gas, e.g., helium) in the shell side. The methane is converted into benzene and hydrogen following a two-step reaction mechanism. Hydrogen is selectively permeated through the membrane, yielding a hydrogen-rich permeate and a benzene-rich retentate. Figure 1 shows the adopted configuration along with reactions.

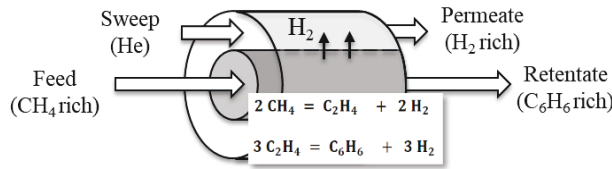


Figure 1. DMA-MR cocurrent configuration scheme.

For the performed operability analysis, the inputs are the reactor dimensions (length and diameter) and the outputs are benzene production and methane conversion. Other variables such as reactor temperature, pressure, feed, etc., are assumed

constant/controlled for this analysis. A nonlinear model is developed, which is characterized by a set of ordinary differential equations (ODEs) obtained from molar balances inside tube and shell (refer to [2] for model details and assumptions). An initial simulation is carried out considering 10,000 combinations of reactor dimensions, with the reactor length range from 10 to 100 cm and tube diameter range from 0.5 to 2.0 cm. Such simulation is performed in MATLAB, employing a stiff ODE solver, “ode15s”, due to the nature of the ODE system.

4.2. Triangulation of AIS and AOS

The obtained data points from the input-output simulation are used for the triangulation task. The AIS is constrained to the given rectangular mesh and the AOS is constrained to its original hull. Figures 2 and 3 show the initial triangulation and the one obtained with minimum number of triangles, respectively.

For an evenly spaced AIS grid, the configuration with the minimum number of triangles employing the approach described above is a 38 x 38 grid. To produce a system representation with an even lower number of triangles, an alternative triangulation using only the outside operating envelope has to be performed. In such case, an unconstrained Delaunay-triangulation is applied to the AOS envelope points, resulting in a set of triangles that connect the edges of the original shape. As a lower number of triangles is used to represent the system, an error increase is expected in such representation. The trade-off between computational time and relative error is further addressed in section 5.

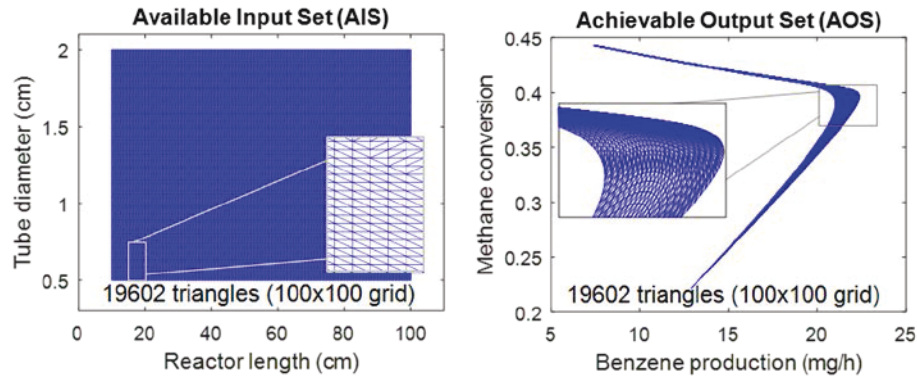


Figure 2. Constrained triangulation of AIS and AOS for initial case.

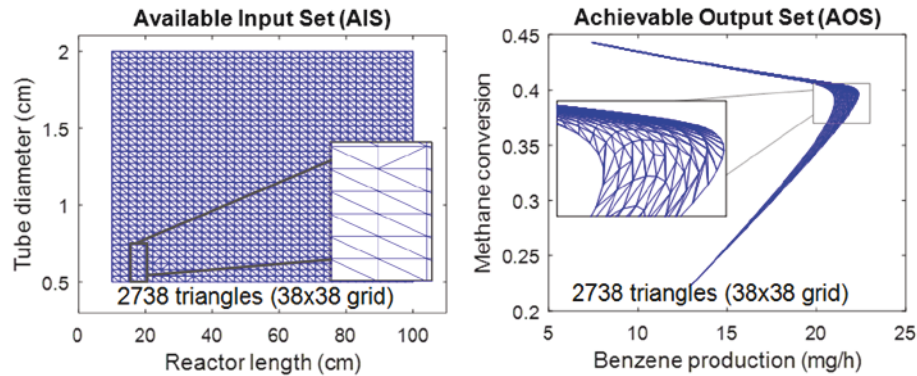


Figure 3. Constrained triangulation of AIS and AOS for case with minimum number of triangles.

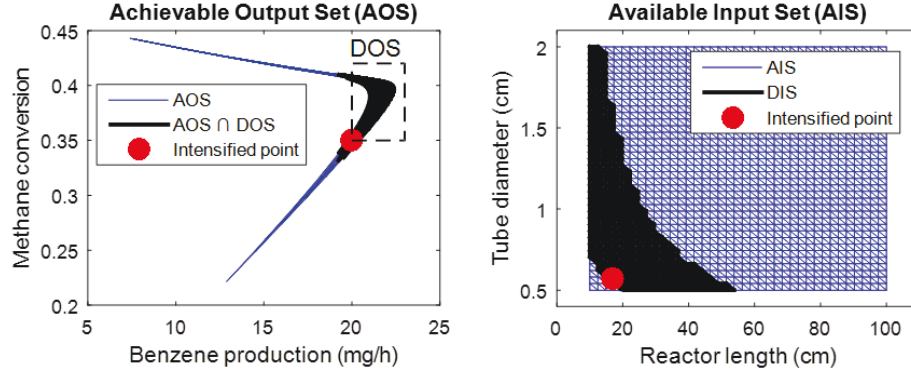


Figure 4. DOS selection, DIS calculation and MILP solution for minimum number of triangles.

4.3. Quantification of Linearized Spaces and DOS Selection

For this application, the DOS region is defined as benzene production ranging from 20 to 23 mg/h and methane conversion from 0.35 to 0.42 as shown in Figure 4. The intersection of this region with the AOS is calculated using the function “isOverlapping” in the MPT toolbox ^[3] in MATLAB. The inverse mapping step employing the triangles results in the region of desired inputs, the DIS. Figure 4 also illustrates the DIS calculation for the case with minimum number of triangles.

4.4. MILP Formulation and Optimal Design

The reduction of the MR footprint is defined as the MILP objective function. The model for the optimization task corresponds to a set of linearized multi-models. As constraints, the ratio $L/D \geq 30$ is considered here for plug flow, where L is the reactor length and D the tube diameter. An additional performance target is set for a benzene production of at least 20 mg/h. The MATLAB subroutine “intlinprog” is used for this task.

Figure 4 shows the intensified point given by $(L, D) = (17.0, 0.57)$ cm, obtained using the proposed MILP formulation. A comparison with a base case from literature ^[2] is established, where $(L, D) = (100, 0.50)$ cm. The obtained design shows equivalent reactor performance for an 80% reduction in membrane area and 78% reduction in reactor volume.

5. Computational Results

The developed approach is executed for a different number of initial points and the trade-off between computational cost and relative error is analyzed. For such activity, NLP-based approaches ^[2,4] are also run for similar number of initial points. The NLP result for the case with the largest number of initial points is considered as the benchmark result, given the detailed exploration of the input-output spaces performed in this case using the nonlinear model. Table 1 summarizes the obtained comparison.

From the results in Table 1, note that the proposed approach performs faster in all scenarios for the same number of initial points. When compared to the NLP-based approach benchmark case considering the same number of initial points, it shows a computational time improvement greater than 3 orders of magnitude with a relative error less than 2%. Such improvement indicates the computational efficiency of the developed approach and thus its feasibility to address high-dimensional calculations.

Table 1. Trade-off performed between computational time and relative error for proposed approach when compared to NLP-approaches.

Approach	CPU Time (hr:min:sec)	# Initial Points	Reactor Length (cm)	Tube Diameter (cm)	Relative Error (w.r.t. membrane area) (%)	Gain in CPU Speed (times) **
NLP-based Approach [2,4]	00: 06: 30.60	25	18.00	0.600	10.23	-
	00: 25: 21.15	100	17.38	0.577	2.31	-
	06: 11: 04.35	1444	17.26	0.570	0.50	-
	10: 35: 50.21	2500	17.14	0.571	0	-
Proposed MILP- based Approach	00: 00: 00.03*	24	18.02	0.601	10.50	12,844
	00: 00: 00.03*	100	17.63	0.588	5.74	44,773
	00: 00: 07.29	1444	17.03	0.568	1.28	3,051
	00: 00: 32.00	2500	17.00	0.567	1.66	1,191

*Rounded values; ** for the same number of initial points

6. Conclusions

The developed MILP-based operability approach was successfully applied to attain process intensification towards footprint reduction and system modularity. When compared to NLP-based operability approaches, it performed faster at any scenario with minimal errors, especially for a higher number of initial points. As computational cost was not a tractability barrier for the developed approach, this approach will be extended next to address higher dimensional cases.

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