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Project Title: Novel Operability-Based Approach for the Efficient Design and Intensification of Energy Systems

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Objectives: The goal in this project is to extend classical operability concepts to attain process intensification (PI) towards system modularity (SM) of natural gas utilization processes. Applications include the membrane reactor for the direct methane aromatization (DMA-MR) conversion to hydrogen and benzene and the natural gas combined cycle (NGCC) for power generation.

Aims and Results

Specific aim #1: Establish a Multi-Model Operability Approach for High-Dimensional Nonlinear Systems

(i) Obtain Linearized Versions of the Process Model at Different Operating Regions

The mathematical relationships between triangles and linearized models were investigated in order to reduce the number of models that adequately represent a nonlinear system. The input-output mapping using triangulation turned out to be extensive and thus an iterative method that only increases the number of models/triangles in regions of interest was explored. Details of the developed algorithm are further explained in item (ii) below.

The inclusion of process disturbances was performed and applied to the DMA-MR system. For a given design, the disturbance mapping was done considering a 3 x 3 (input x output) case. The expected disturbance set (EDS) was constructed considering changes of ±10% from nominal operation to the variables of methane inlet flow, temperature and sweep gas inlet flow. The achievable output set (AOS) was built using benzene production, hydrogen production and methane conversion as outputs. The desired output set (DOS) was also characterized by these three outputs, within the ranges of 20 to 25 mg/h, 3 to 6 mg/h and 0.3 to 0.45, respectively. Figure 1 depicts the obtained EDS-AOS mapping for a flexible design, represented by the achievable DOS in which the system never leaves the desired operating region despite of the occurrence of disturbances. A detailed discussion on how this flexible design was obtained is included below in specific aim #2, item (i).

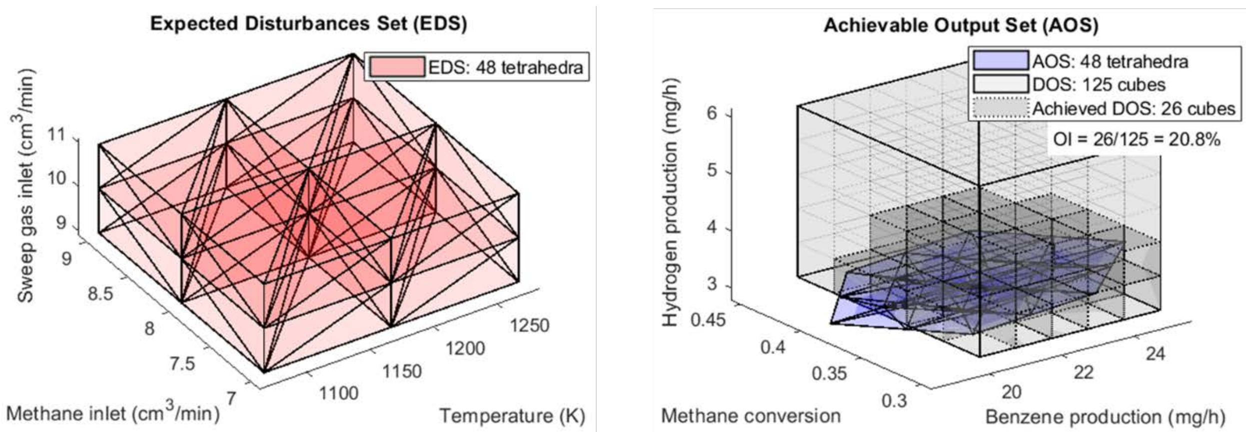

Figure 1. EDS-AOS mapping and intersection of AOS with DOS.

(ii) Quantify the Operability Spaces for the Linearized Models using a Multi-Model Operability Approach

The previously reported algorithm was improved to eliminate the need of extensive simulations. Similar computational geometry tools and calculations were employed, but instead of generating a detailed model representation of the entire available input set (AIS) and AOS, an iterative algorithm was developed so that the number of models locally increase as the program approaches the optimal design region. Figure 2 shows a schematic representation of the developed algorithm.

In each iteration, a solution is obtained for the optimal design and this solution is compared to the previous one in terms of a relative error, E_{rel}. If this error is smaller than a predefined threshold or tolerance, E_{tol}, the algorithm converged, and the final solution is obtained. Otherwise, new variable bounds are redefined based on the polytope of the solution and another iteration takes place. The algorithm was developed to accommodate a generic number of dimensions n.

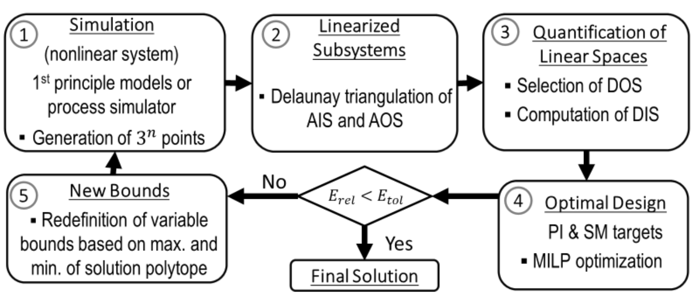

Figure 2. Steps of the multi-model operability approach.

For the DMA-MR system, scenarios of dimensionality 2 x 2 and 3 x 3 were evaluated. In both cases, the algorithm successfully found the optimal solution, taking 7 s and 28 s, respectively. These results show that the algorithm is capable of finding an optimal design, without the need of extensive simulations. Although there was some increase in computational time, the total computational time was still on the order of seconds, showing the promising capabilities of the developed algorithm for expansion to high-dimensional cases. Another conclusion from comparing the two scenarios is that changing more input variables provides higher number of degrees of freedom, enabling modular systems even smaller, while keeping the PI targets.

The developed framework can accommodate n-dimensional systems. For 2-D and 3-D cases, it was verified that this can be done either by employing constrained Delaunay triangulations or even unconstrained Delaunay triangulations when the AIS is evenly spaced. For 4-D and higher-dimensional cases, due to the lack of constrained triangulation tools available in the literature, the verification of the unconstrained n-dimensional Delaunay triangulations with an evenly spaced AIS is under further testing.

Specific aim #2: Develop a Fully Nonlinear Method for High-Dimensional Systems

(i) Introduce an Iterative Algorithm for the Analysis of High-Dimensional Nonlinear Systems in the Output Space

The developed iterative algorithm was systematically applied for the evaluation of designs described by the AIS of the DMA-MR example. This evaluation consisted of an analysis in the output space for each disturbance scenario. The complete mapping of the output space with respect to the specified EDS was accomplished as shown in Figure 1.

Then, the achievability of system objectives was quantified by an operability index (OI), computed by measuring the number of sub-regions of the DOS that can be achieved under the presence of disturbances. A sub-region of the DOS is assumed to be achievable when it contains at least one point of the AOS in its interior. The designs in which the AOS was contained in the desired operating region, the DOS, considering every disturbance scenario, were considered flexible designs. For these designs, every perturbation scenario can be handled without moving the operation away from the desired region.

Based on the optimal design point from the 3 x 3 case above, a box of designs was built around this point, considering feasible construction values. Figure 3 shows the obtained achievability for each of these designs, represented by the OI. It also shows the selected flexible designs and the design of maximum achievability.

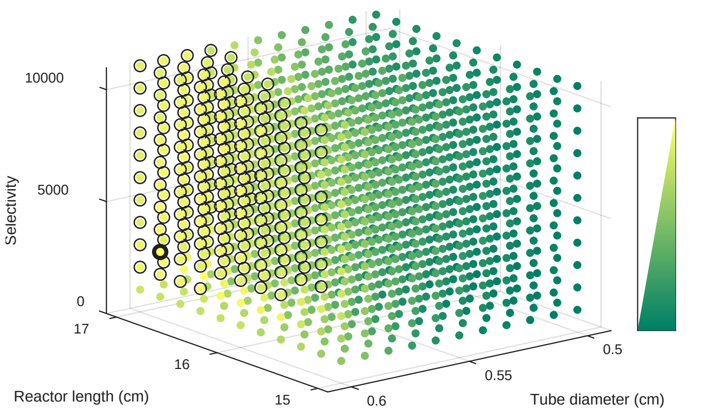

Figure 3. Analysis of achievability and flexibility of considered designs.

The design of maximum achievability is the flexible design in which most sub-regions of the DOS were achieved. This design is depicted in Figure 1, with a measured OI of 20.8%.

The same EDS-AOS analysis was performed to the previously obtained optimal design point. An OI of 6.4% was calculated which indicates that even though the iterative algorithm can find an optimum, it does not necessarily take into account the system operability features.

Thus, the additional EDS-AOS analysis shows that a more operable design can be obtained with a small deviation from the original optimal design that was computed for footprint reduction.

(ii) Develop a Nonlinear Optimization-based Approach for Computationally Efficient Operability Computations

A bilevel optimization and parallel computing-based operability framework was developed and compared to the mixed-integer linear programming (MILP) based approach described above. The results of this framework when applied to high-dimensional NGCC processes (up to 8-D) were published as part of an AIChE Journal paper that has been reported in the list of publications.

Specific aim #3: Apply the developed approaches to natural gas utilization processes

The developments in this aim have been reported as part of the application systems (DMA-MR and NGCC) for the operability tools developed in aims #1 and #2.

Research Impact and Products

In addition to the scientific contribution, this research project has provided students with training in a wide range of process systems and computational tools, including the participation in conferences (AIChE and PSE) and publications (see reported published articles acknowledging ACS-PRF).