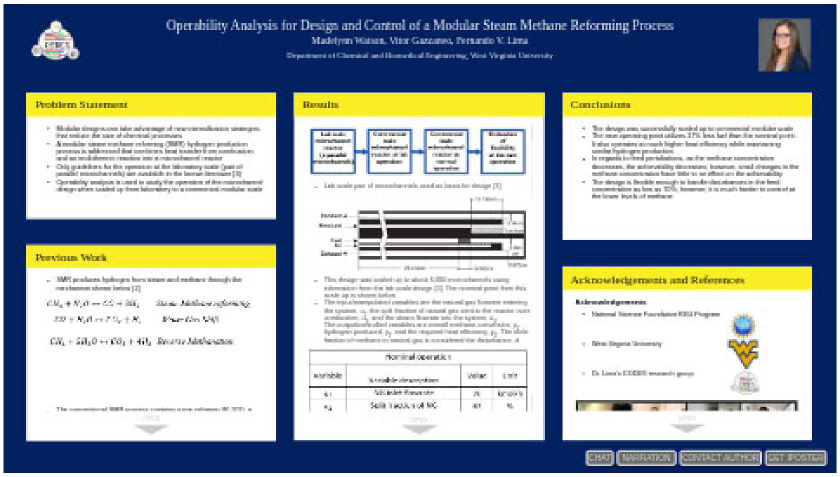
Operability Analysis for Design and Control of a Modular Steam Methane Reforming Process



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PROBLEM STATEMENT

- Modular designs can take advantage of new intensification strategies that reduce the size of chemical processes
- A modular steam methane reforming (SMR) hydrogen production process is addressed that combines heat transfer from combustion and an endothermic reaction into a microchannel reactor
- Only guidelines for the operation at the laboratory scale (pair of parallel microchannels) are available in the known literature [3]
- Operability analysis is used to study the operation of the microchannel design when scaled up from laboratory to a commercial modular scale
- The operability analysis also accounts for perturbations in the natural gas composition and checks the disturbance ranges that the design is capable of handling

PREVIOUS WORK

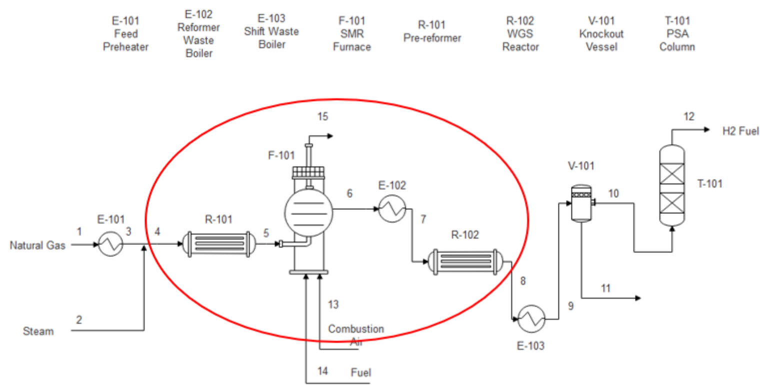
- SMR produces hydrogen from steam and methane through the mechanism shown below [2]

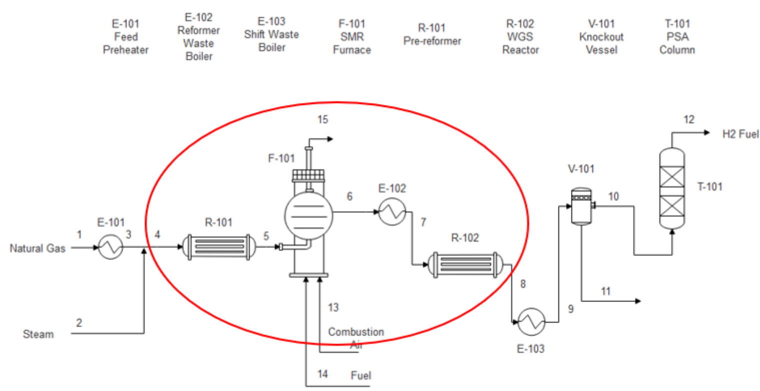
$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad \textit{Steam Methane reforming}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad \textit{Water Gas Shift}$$

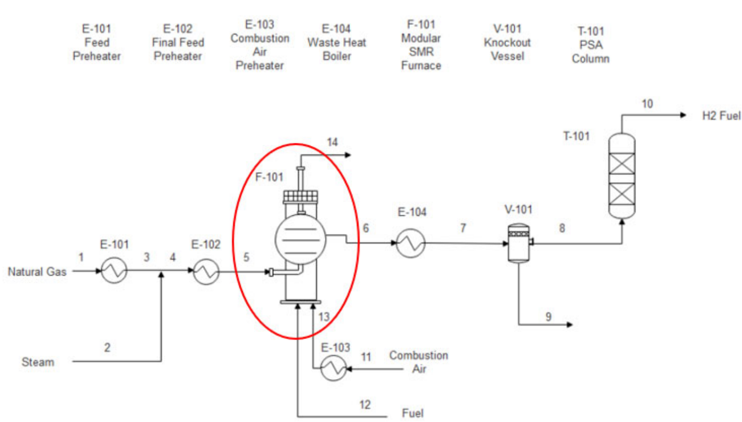
$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \quad \textit{Reverse Methanation}$$

- The conventional SMR process contains a pre-reformer (R-101), a SMR furnace (F-101), and a water gas shift reactor (R-102) [2]



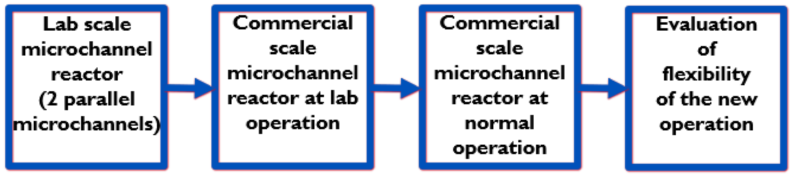


- The Modular SMR process combines R-101, F-101, and R-102 into one microchannel reactor F-101 [2]. The combined process was modeled in Aspen Plus

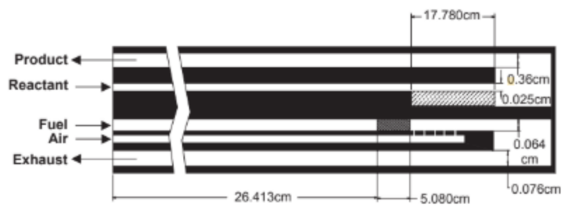


- The elements of operability analysis are AIS, DOS, AOS, and EDS. The available input set (AIS) can be operational inputs (manipulated variables) or design inputs. The desired output set (DOS) represents the desired output region (controlled variables). The achievable output set (AOS) is the set of all controlled variables the system can achieve from all of the AIS and EDS. The EDS is the set of expected disturbances for the system [1]

RESULTS



- Lab scale pair of microchannels used as basis for design [3]



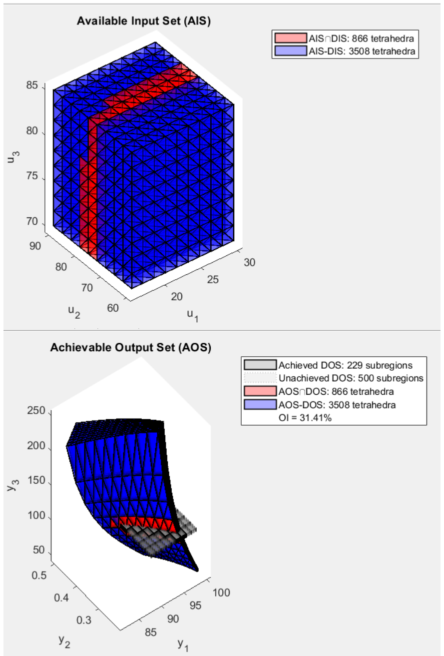
- This design was scaled up to about 6,000 microchannels using information from the lab scale design [3]. The nominal point from this scale up is shown below
- The input/manipulated variables are the natural gas flowrate entering the system, u_1, the split fraction of natural gas sent to the reactor over combustion, u_2, and the steam flowrate into the system, u_3. The output/controlled variables are overall methane conversion, y_1, hydrogen produced, y_2, and the required heat efficiency, y_3. The mole fraction of methane in natural gas is considered the disturbance, d

Nominal operation			
Variable	Variable description	Value	Unit
u_1	NG inlet flowrate	26	kmol/h
u_2	Split fraction of NG	63	%
u_3	Steam inlet flowrate	79	kmol/h
y_1	Overall methane conversion	95.31	%
y_2	Hydrogen production	0.35	Sm^3/s
y_3	Required heat efficiency	57.35	%
d	Molar fraction of methane	100.00	%

- Operability analysis was then used to see how to operate this scaled up design
- The AIS was selected by expanding the nominal inlet values
- The DOS was selected using the expectation that heat efficiences would increase to between 95% to 100% while maintaining high methane conversion and similar hydrogen production

Selected Sets					
Sets	Variable	Variable description	Lower Bound	Upper Bound	Unit
AIS (Manipulated Variables)	u_1	NG inlet flowrate	16	30	kmol/h
	u_2	Split fraction of NG	60	90	%
	u_3	Steam inlet flowrate	70	85	kmol/h
DOS (Controlled Variables)	y_1	Overall methane conversion	90	100	%
	y_2	Hydrogen production	0.25	0.5	Sm^3/s
	y_3	Required heat efficiency	95	100	%

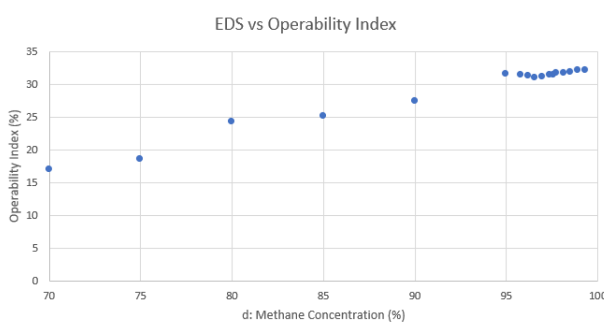
- Using the above sets, the input-output mapping was generated in the Operability App in MATLAB [1] connected to Aspen Plus

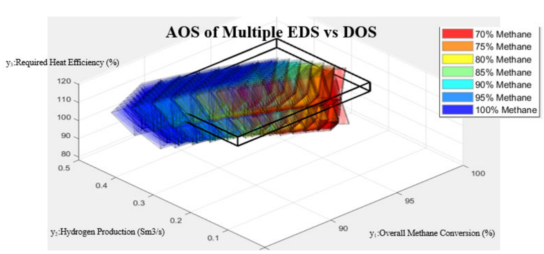


- Using this mapping, the operating regions were selected for each input variable as follows: natural gas inlet flow rate (kmol/h) [19.11 25.33], split fraction of natural gas (%) [73.33 80], and steam inlet flow rate (kmol/h) [70 85]
- The new operating point was determined to be in the middle of this region and is shown below

New Operation			
Variable	Variable description	Value	Unit
u_1	NG inlet flowrate	22.2	kmol/h
u_2	Split fraction of NG	76.665	%
u_3	Steam inlet flowrate	77.5	kmol/h
y_1	Overall methane conversion	94.1325	%
y_2	Hydrogen production	0.3459	Sm^3/s
y_3	Required heat efficiency	98.1004	%

- This new operating point was then tested to see how it handles disturbances in the methane composition in the feed. The operability index represents the achievability of each disturbance case





CONCLUSIONS

- The design was successfully scaled up to commercial modular scale
- The new operating point utilizes 37% less fuel than the nominal point. It also operates at much higher heat efficiency while maintaining similar hydrogen production
- In regards to feed pertubations, as the methane concentration decreases, the achievability decreases; however, small changes in the methane concentration have little to no effect on the achievability
- The design is flexible enough to handle disturbances in the feed concentration as low as 70%; however, it is much harder to control at the lower levels of methane

ACKNOWLEDGEMENTS AND REFERENCES

Acknowledgements

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References

[1] Gazzaneo, V., Carrasco, J.C., Vinson, D.R., Lima, F.V. "Process Operability Algorithms: Past, Present and Future Developments." Ind. Eng. Chem. Res., vol. 59, no. 6, 2020, pp. 2457-2470.

[2] Ramsayer, C. B., Gazzaneo, V., Lima, F. V. (2020). Techno-Economic Analysis of a Modular Steam-Methane Reforming Process. Technical Report. Department of Chemical and Biomedical Engineering, West Virginia University.

[3] Tonkovich, A.Y., Perry, S., Wang, Y., Qiu, D., LaPlante, T., Rogers, W.A. "Microchannel Process Technology for Compact Methane Steam Reforming." Chemical Engineering Science, vol. 59, 2004, pp. 4819-4824.