Mathematical Modeling and Optimization of Ion Transport Membrane for Oxygen Separation from Air

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Introduction and Background on Air Separation

- There is a growing demand for high purity oxygen (oxy-combustion) as a replacement for air in combustion and gasification processes.
- Energy-related emissions have been growing in importance recently due to them accounting for roughly 68 percent of greenhouse gas emissions.
- In comparison to Air-Combustion, Oxy-combustion processes have exhibited lower harmful CO2 and NOx emissions and higher overall combustion efficiency, due to a drop in heat loss (as a result of lower mass flow rates) out of the stack.
- The main air separation technologies used currently to produce high purity (99%>) oxygen are Cryogenic Air Separation, Pressure or Vacuum Swing Absorption (PSA or VSA respectively), as well as, membrane technologies.
- In comparison to cryogenic air separation, ITM technologies exhibit lower electricity costs attributed to the lack of a need for much (if any) external electrical loadings to drive the separation process.
- Approximately 1520 mol/s of oxygen is required for a 620 MWe IGCC power plant.

Ion Transport Membrane Modeling and Optimization

- An Ion Transport Membrane (ITM) consists of a shell and tube setup where surface ion exchange reaction/permeation occur simultaneously.

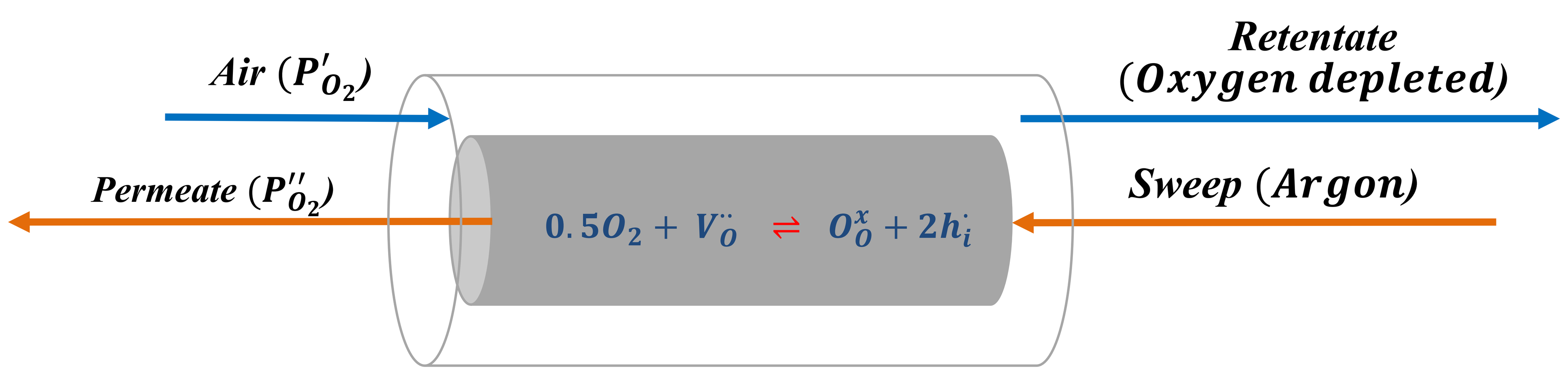

Figure 1: Ion Transport Membrane

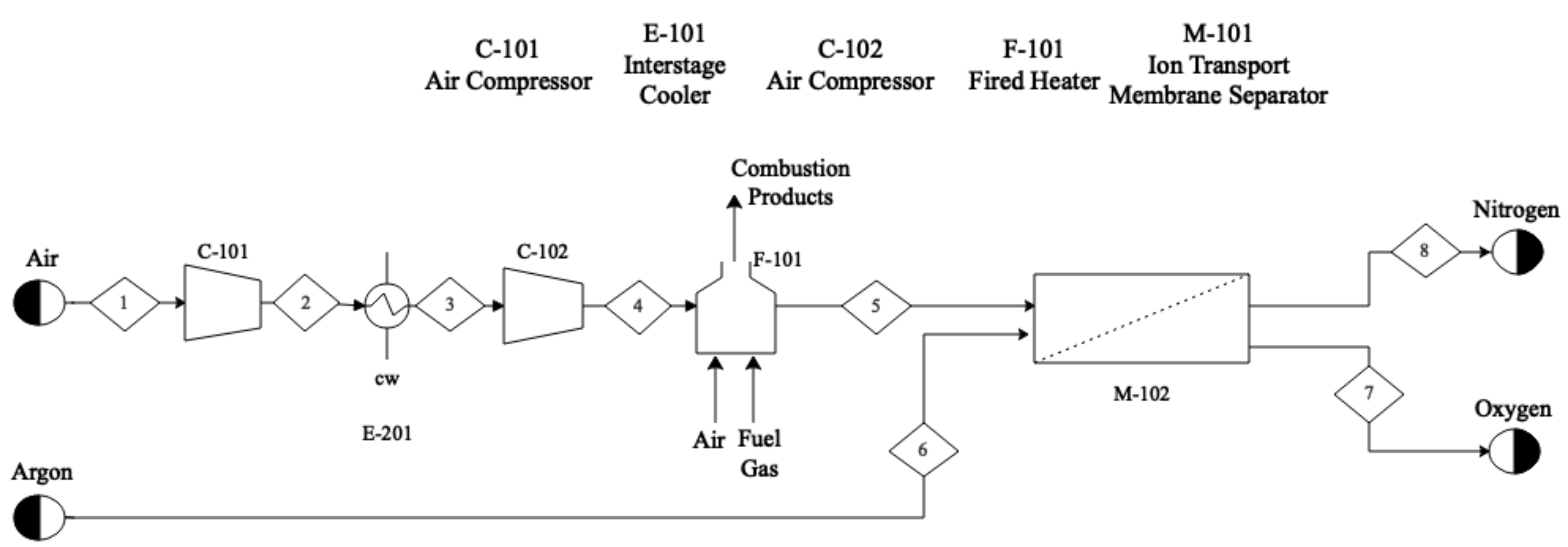

Figure 2: OITM based air separation unit

Table 1: Values for cost parameters objective function

$\$_{Ar}$($/Kmol)	8.92
$\$_{Air}$($/Kmol)	0.11
$\$_{O_2}$($/Kmol)	960
$\$_{NG}$($/GJ)	3.95
$\$_m$($/m^2)	1000
Op (hours)	7880

*Based on LHV of natural gas of 0.7935 GJ/mol ** Price at pressure of 3.3 barg

- Oxygen permeation rate equation for perovskite membrane material $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\alpha}$ (LSCF)*

$$\frac{\partial N_{O_2}}{\partial l} = \frac{k_r\left[\left(p'_{O_2}\right)^{0.5} - \left(p''_{O_2}\right)^{0.5}\right]}{\frac{(p''_{O_2})^{0.5}}{2\pi R_o} + \frac{k_f \ln\left(\frac{R_o}{R_i}\right)(p'_{O_2})^{0.5}(p''_{O_2})^{0.5}}{\pi D_v} + \frac{(p'_{O_2})^{0.5}}{2\pi R_{in}}}$$

Results

Optimization Results

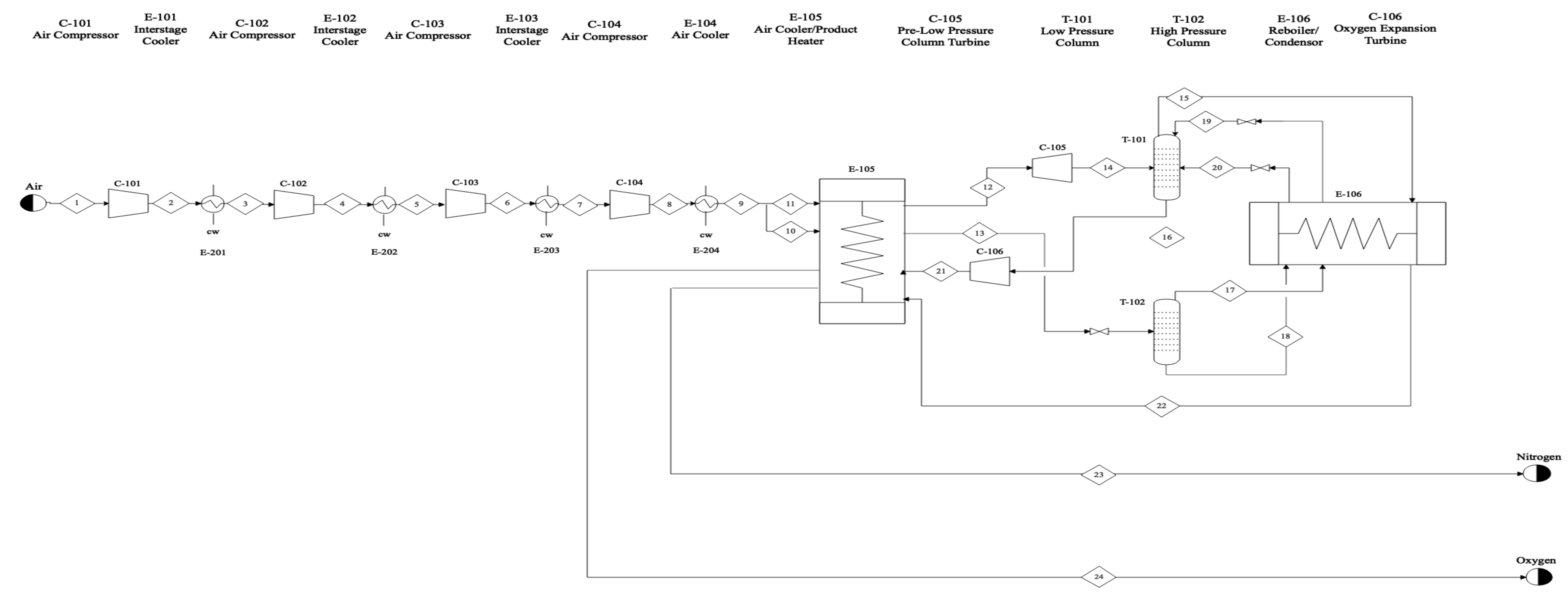

Figure 3: Cryogenic ASU unit PFD

Table 2: Base case economic evaluations

Unit Type	Capital Cost (Thousands of dollars)	Comparison with Literature (Thousands of dollars)**
Cryogenic ASU	125,900	113,000
OITM based ASU*	158,600	182,000

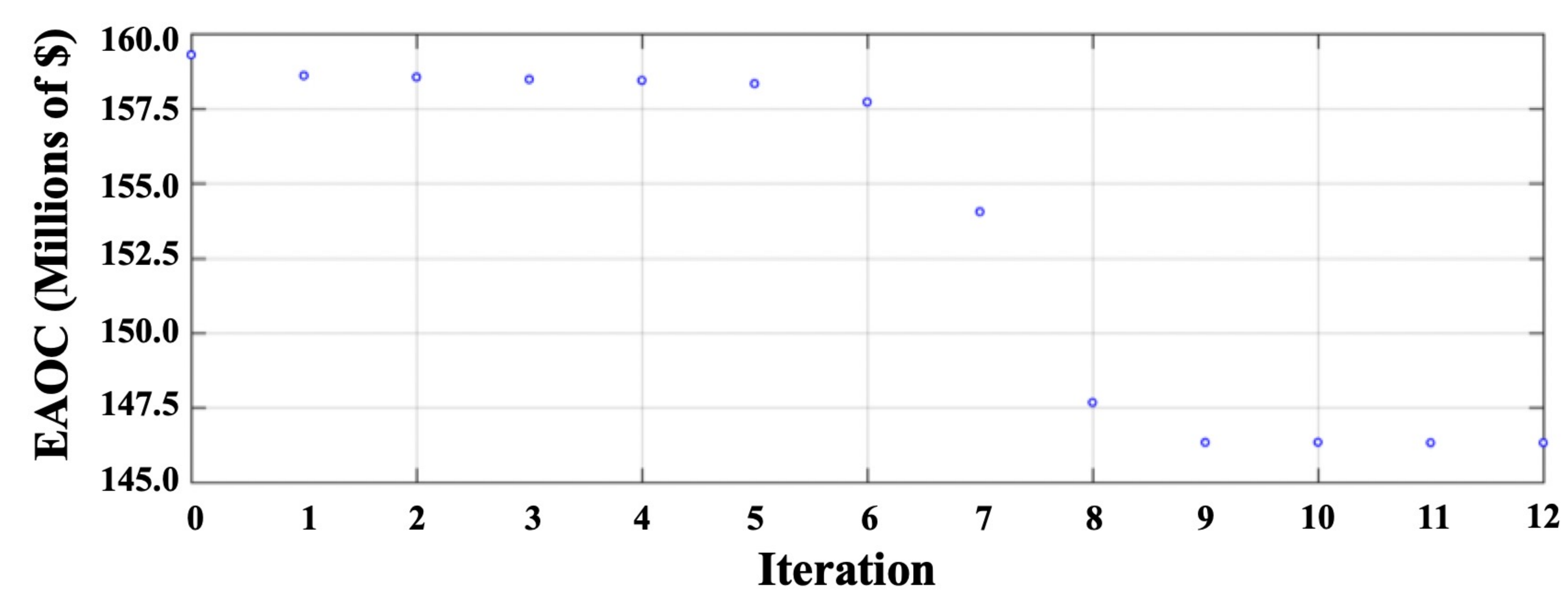

Figure 4: Preliminary optimization results for ITM ASU

Conclusion and Future Directions

- A membrane reactor model was developed and integrated into an ASU to be economically evaluated
- Constrained optimization problem was formulated, permitting the systematic selection of optimal reactor design through more efficient membrane utilization.
- A Cryogenic ASU simulation was economically evaluated and altered in order to match the IGCC specifications found in the literature***
- These models may be integrated into larger power plant simulations and evaluated for further research on the economic and environmental validity of OITM technology
- Future work will consider application to operability and process control studies.

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