Radically Engineered Modular Air Separation System with Tailored Oxygen Sorbents

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Project Partners: Thermosolv LLC and West Virginia University

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Outline

- Project Description and Objectives
- Project Update
- Preparing Project for Next Steps
- Concluding Remarks

Project Objectives

- Develop radically engineered modular air separation system (REM-ASU) for small-scale coal gasifiers (1-5 MW)
- Achieve air separation under a cyclic redox scheme using advanced mixed-oxide based oxygen sorbents (OS)
- Reduce 30% energy consumption for air separation using REM-ASU compared to state-of-the-art cryogenic air separation process
- Demonstrate the modular air separation technology to achieve the DOE goal to support the oxidant feed of an oxygen-blown REMS gasifier scaled to a range of 1 to 5 MW

Technology benchmarking

| | Cryogenic | Chemical Looping (Ideal) | REMS Process Model |
|---|-----------|-----------------------------|-----------------------|
| Status | mature | developing | Developing |
| Economic range (sTPD) | >20 | Undetermined | Undetermined |
| Energy consumption (MJ/kg O ₂) | 0.791 | ~0.2* | <0.54 |
| Thermodynamic efficiency (%) | 25% | >75% | >36% |
| Oxygen purity (%) | 99+ | 99+ | 99+ |
| By product capability | Excellent | Poor | Poor |

Chemical looping air separation has the potential to be highly energy efficient

^{*} Process analysis with idealized assumptions by Moghtaderi, et al. Energy Fuels, 2010, 24, 190–198.

Status of Project

Status at beginning of project:

- Developed (high temperature) oxygen sorbents (OSs) with high oxygen capacity and reaction kinetics, tested in a thermogravimetric analyzer (TGA)
- Preliminary process analysis.

Current status of project:

- Developed and demonstrated both "high temperature" (>750 °C) and "low temperature" OSs (400 – 600 °C).
- Scalable production of oxygen sorbents: produced five, 1 kg/batch OS. Performed extensive sorbent testing.
- Performed computational screening for sorbent optimization.
- Developed a preliminary REM-ASU design with energy consumption of 0.23-0.54
 MJ/kg O₂, 32-70% less comparing to benchmark cryogenic air separation.
- 10,000 cycles with <3% degradation, optimized operating conditions for >95% oxygen purity, developed a high-fidelity ASU model for system optimization.

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- Concluding Remarks

Journal Publications

- Wang, Xijun, et al. "Net Electronic Charge as an Effective Electronic Descriptor for Oxygen Release and Transport Properties of SrFeO₃-Based Oxygen Sorbents." Chemistry of Materials, 2021, 33, 7, 2446–2456.
- Jian Dou, Emily Krzystowczyk, Xijun Wang, Thomas Robbins, Liang Ma, Xingbo Liu, and Fanxing Li. A and B-site Co-Doped SrFeO₃ Oxygen Sorbents for Enhanced Chemical Looping Air Separation ChemSusChem 2020, 13, 385-393.
- Emily Krzystowczyk, Xijun Wang, Jian Dou, Vasudev Haribal, Fanxing Li. Substituted SrFeO₃ as Robust Oxygen Sorbents for Thermochemical Air Separation: Correlating redox performance with compositional and structural properties. Physical Chemistry Chemical Physics 2020, 22, 8924-8932.
- Jian Dou, Emily Krzystowczyk, Xijun Wang, Anthony R Richard, Thomas Robbins, and Fanxing Li. Sr_{1-x}Ca_xFe_{1-y}Co_yO_{3-δ} as facile and tunable oxygen sorbents for Chemical Looping Air Separation Journal of Physics: Energy 2020, 2, 025007.
- Jian Dou, Emily Krzystowczyk, Amit Mishra, Xingbo Liu, Fanxing Li*. Perovskite promoted mixed cobalt-iron oxides for enhanced chemical looping air separation. ACS Sustainable Chem. Eng. 2018, 6, 15528-15540.
- Amit Mishra, Tianyang Li, Fanxing Li*, and Erik Santiso*. Oxygen Vacancy Creation Energy in Mn-Containing Perovskites: An Effective Indicator for Chemical Looping with Oxygen Uncoupling. Chemistry of Materials, 2018, 31, 689-698.

Conference Presentations

- Emily Krzystowczyk, Jian Dou, Xijun Wang, and Fanxing Li. Perovskite Oxygen Sorbents for "Low Temperature" Thermochemical Air Separation: Correlating Compositions with Redox Performance AIChE Annual Meeting, Orlando, 2019.
- Jian Dou, Emily Krzystowczyk, Amit Mishra, and Fanxing Li*. Radically Engineered Modular Air Separation System with Tailored Oxygen Sorbents. DOE meeting, Washington DC, 2018
- Jian Dou, Emily Krzystowczyk, Amit Mishra, Xingbo Liu, and Fanxing Li*. Perovskite Promoted Mixed Co-Fe Oxides for Enhanced Chemical Looping Air Separation. ACS meeting, Orlando, 2019

Gantt Chart

| Task | Milestone | Milestone Ø (Expected completion date) (Ø Go/No Go) | Start Date | End Date | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | Q9 | Q10 | Q11 | Q12 |
|------|-----------|---|------------|------------|----|----|----|----|----|----|----|----|----|-----|-----|-----|
| 1 | | | 1/1/2018 | 2/15/2018 | | | | | | | | | | | | |
| | 1.1 | Modify PMP (2/15/2018) | | | ٥ | | | | | | | | | | | |
| | 1.2 | Kickoff meeting (2/15/2018) | | | ٥ | | | | | | | | | | | |
| 2 | | | 1/1/2018 | 9/30/2018 | | | | | | | | | | | | |
| | 2.1 | Oxygen sorbent synthesis and testing (6/30/2018) | | | | ٥ | | | | | | | | | | |
| | 2.2 | Oxygen sorbent characterization (9/30/2018) | | | | | 9 | | | | | | | | | |
| 3 | | | 4/1/2018 | 12/31/2018 | | | | | | | | | | | | |
| | 3.1 | Dopant effect quantification (12/31/2018) | | | | | | 0 | | | | | | | | |
| | 3.2 | Composite effect quantification (12/31/2018) | | | | | | 0 | | | | | | | | |
| 4 | | | 7/1/2018 | 3/31/2019 | | | | Γ | | | | | | | | |
| | 4.1 | Oxygen sorbent activity screening (12/31/2018) (Go/No Go) | | | | | | 0 | | | | | | | | |
| | 4.2 | Oxygen sorbent stability screening (3/31/2018) | | | | | | | 0 | | | | | | | |
| 5 | | | 1/1/2019 | 9/30/2019 | | | | | | | | | | | | |
| | 5.1 | Oxygen sorbent stability demonstration (6/30/2019) | | | | | | | | 0 | | | | | | |
| | 5.2 | Oxygen sorbent fixed bed characterization (9/30/2019) | | | | | | | | | 2 | | | | | |
| 6 | 6.1 | Preliminary REM-ASU design (12/31/2019) (Go/No Go) | 4/1/2019 | 12/31/2019 | | | | | | | | 2. | | | | |
| 7 | 7.1 | Synthesis scale up (3/31/2020) | 10/1/2019 | 3/31/2020 | | | | | | | | | 40 | | | |
| 8 | 8.1 | Pilot Scale REM-ASU demonstration (9/30/2020) (Deliverable) | 10/1/2019 | 9/30/2020 | | | | | | | | | | | 20 | |
| 9 | | | 4/1/2020 | 12/31/2020 | | | | | | | | | | | | |
| | 9.1 | Construct techno-economic model (9/30/2020) | | | | | | | | | | | | | 0 | |
| | 9.2 | Techno-economic report (12/31/2020) | | | | | | | | | | | | | | ٥ |

NC STATE UNIVERSITY

Oxygen Sorbent Development: Challenges and Opportunities



Mixed oxides are necessary in order to match P_{O2} of oxygen carriers with air separation conditions. Year 1 and Year 2 have resulted in promising mixed oxide sorbents suitable for different temperature ranges.

Milestone 7.1 (Q9) Scale-up Synthesis of OS

M3.1: Synthesize two 25 kg batch OS



- Sol-gel synthesis performed in-house by Thermosolv in 1 kg batches
- Multi-batch approach to produce 25 kg sorbents
- Five different compositions were prepared/tested.

THERMOSOLV LLC

Milestone 8.1 (Q11) Sorbent Stability

M3.2 Produce >95% pure O₂ over 2000 cycles with less than 10% decrease in oxygen capacity



SCFC8246 is stable for 10,000 cycles oxygen production at 25 psig and 600 °C with cycle structure of 90s/5s/60s/1s

Effect of Flow Rate on Oxygen Productivity



Oxygen purity increased to >95% with 3 SLPM air flow rate at 25 psi and 600 °C for SCFC8291 OS



Effect of Oxygen Recycle



Recycle of oxygen for purging increases purity >95% at 25 psi, 600 °C and 1 SLPM for SCFC8291 sorbent



Effect of flow rate and oxygen recycle



Oxygen with >95% purity obtained with 2 SLPM air flow rate and 5 s cycle of oxygen stream at 25 psi and 600 °C for SCFC8291



Breakthrough curve of SCFC8291 and data fitting



Best fitting of breakthrough curve for SCFC8291 at 20 psi and 600°C with Péclet number of 400

Detailed One Dimensional Absorber Modeling

• Spatial temporal distribution of O₂



• 4-step configuration:

Pressurization (4s); Adsorption (90s); Depressurization (5s); Desorption (30s)

Detailed One Dimensional Absorber Modeling



Model validation

- O_2 productivity: 80% data within $\pm 15\%$ error; 100% data within $\pm 25\%$ error
- O_2 purity: 90% data within $\pm 5\%$ error; 100% data within $\pm 10\%$ error

Detailed One Dimensional Absorber Modeling



• Modeling results

- t_{de} =60s, Q_{air} =2SLM, m_{steam}=0.1 mol/s:
- O₂ productivity and Power consumption: a peak value;
- Purity increases and recovery decreases
- Optimal cycle structure

Detailed One Dimensional Absorber Modeling



• Modeling results

- t_{ad} =150s, Q_{air} =2SLM, m_{steam}=0.1 mol/s:
- O₂ productivity and Power consumption: a peak value;
- Purity and recovery increase with desorption time
- Optimal cycle structure

Detailed One Dimensional Absorber Modeling



• Optimization

- Power-productivity Pareto front
- Pump compression is highly energy consuming, but preferable for high productivity

Detailed One Dimensional Absorber Modeling



• Optimization

- Higher purity requires higher power consumption
- Minimum power consumption for 95% purity: 150 kW·h/ ton O_2
- Reduce the dead volume will lead to higher purity with low energy consumption

Optimization of Oxygen Sorbent

Theoretical understanding of dopant effects for SrFeO₃ based sorbents



In most cases,

- > n-type doping (larger Δe) \rightarrow Up-shifting of $E_F \rightarrow$ More negative $\varepsilon_p \rightarrow$ O anion less active \rightarrow Higher ΔH (ΔG)
- P-type doping (smaller Δe) → Down-shifting of E_F → More positive ε_p → O anion more active → Lower ΔH (ΔG)

Optimization of Oxygen Sorbent

DFT based high-throughput screening of SrFeO₃-based oxygen



Sr

Sr





The Gibbs free energies of vacancy formation of 2401 Sr_xA1_ _xFe_yB_{1-y}O₃ (A=<u>Sr, Ca, K, Y, Ba, La, Sm</u>; B=<u>Fe, Co, Cu, Mn, Mg, Ni, Ti</u>) candidates were computed, and the ones with suitable ΔG were screened for experimental verification.

| Overlap (T=400 and 700°C) | | $\Delta G (T = 40)$ | 0 °C) | | $\Delta G (T = 70)$ | 0 °C) | Overlap (T=400 and 700°C) | | $\Delta G (T = 40)$ | 0 °C) | | $\Delta G (T = 70)$ | 0°C) |
|----------------------------------|------------|---------------------|---------------|------------|---------------------|---------------|-----------------------------------|------------|---------------------|---------------|------------|---------------------|--------------|
| δ | 0.25-0.375 | 0.375-0.5 | 0.3125-0.4375 | 0.25-0.375 | 0.375-0.5 | 0.3125-0.4375 | õ | 0.25-0.375 | 0.375-0.5 | 0.3125-0.4375 | 0.25-0.375 | 0.375-0.5 | 0.3125-0.437 |
| BaFeCo-1-0.875-0.125 | 0.48271 | 0.33693 | 0.40982 | -0.03574 | 0.28383 | 0.12405 | SrCaFeMn-0.875-0.125-0.25-0.75 | 0.35706 | 0.52131 | 0.43919 | 0.03505 | 0.27756 | 0.15631 |
| BaFeTi-1-0.875-0.125 | 0.5933 | 0.36382 | 0.47856 | 0.49613 | 0.08819 | 0.29216 | SrCaFeMn-0.875-0.125-0.375-0.625 | 0.2352 | 0.56394 | 0.39957 | -0.01947 | 0.34458 | 0.16255 |
| CaFeCo-1-0.5-0.5 | 0.08972 | 0.56377 | 0.32674 | -0.03696 | 0.33952 | 0.15128 | SrCaFeNi-0.125-0.875-0.25-0.75 | 0.06578 | 0.18893 | 0.12736 | -0.05503 | -0.21339 | -0.13421 |
| CaFeMn-1-0.625-0.375 | 0.50979 | 0.4605 | 0.48514 | 0.30081 | 0.15275 | 0.22678 | SrCaFeNi-0.25-0.75-0.75-0.25 | -0.01217 | 0.10001 | 0.04392 | -0.10069 | -0.15425 | -0.12747 |
| LaCu-1-1 | 0.58164 | 0.3715 | 0.47657 | 0.07186 | 0.07078 | 0.07132 | SrCaFeNi-0.625-0.375-0.625-0.375 | 0.11689 | 0.2378 | 0.17734 | -0.04446 | -0.19482 | -0.11964 |
| SrBaFe-0.125-0.875-1 | 0.53478 | 0.10298 | 0.31888 | 0.28772 | -0.17794 | 0.05489 | SrCaMn-0.5-0.5-1 | 0.24631 | 0.17118 | 0.20874 | -0.04433 | -0.1354 | -0.08987 |
| SrBaFeCo-0.125-0.875-0.375-0.625 | 0.14835 | 0.0959 | 0.12213 | -0.19153 | -0.17867 | -0.1851 | SrCaMn-0.875-0.125-1 | 0.26709 | 0.12885 | 0.19797 | -0.11171 | -0.16091 | -0.13631 |
| SrBaFeCo-0.25-0.75-0.625-0.375 | 0.38635 | 0.32112 | 0.35373 | 0.23514 | 0.00333 | 0.11923 | SrFeCo-1-0.375-0.625 | 0.12955 | 0.41986 | 0.27471 | -0.11361 | 0.15769 | 0.02204 |
| SrBaFeCo-0.5-0.5-0.5-0.5 | 0.30449 | 0.59474 | 0.44961 | 0.09269 | 0.2085 | 0.15059 | SrFeCo-1-0.625-0.375 | 0.19303 | 0.41837 | 0.3057 | 0.07862 | 0.114 | 0.09631 |
| SrBaFeCo-0.625-0.375-0.5-0.5 | 0.03721 | 0.13755 | 0.08738 | -0.18969 | -0.17432 | -0.182 | SrFeCu-1-0.75-0.25 | 0.30731 | 0.41729 | 0.3623 | 0.07264 | 0.10923 | 0.09093 |
| SrBaFeCo-0.75-0.25-0.5-0.5 | 0.23642 | 0.27035 | 0.25339 | 0.02808 | -0.11008 | -0.041 | SrFeMn-1-0.25-0.75 | 0.13157 | 0.28482 | 0.2082 | -0.16554 | 0.03328 | -0.06613 |
| SrBaFeCo-0.75-0.25-0.75-0.25* | 0.28408 | 0.16514 | 0.22461 | 0.05287 | -0.16683 | -0.05698 | SrFeMn-1-0.375-0.625 | 0.00106 | 0.05198 | 0.02652 | -0.20494 | -0.21165 | -0.20829 |
| SrBaFeCo-0.875-0.125-0.375-0.625 | 0.16511 | 0.52432 | 0.34472 | -0.05709 | 0.26353 | 0.10322 | SrFeMn-1-0.5-0.5 | 0.52152 | 0.21742 | 0.36947 | 0.29186 | -0.02942 | 0.13122 |
| SrBaFeCo-0.875-0.125-0.5-0.5 | 0.05355 | 0.12663 | 0.09009 | -0.21381 | -0.00867 | -0.11124 | SrFeMn-1-0.625-0.375 | 0.51378 | 0.15933 | 0.33655 | 0.35306 | -0.04384 | 0.15461 |
| SrBaFeCu-0.5-0.5-0.75-0.25 | 0.11351 | 0.19492 | 0.15422 | -0.17456 | -0.10925 | -0.1419 | SrKCo-0.875-0.125-1 | 0.32613 | 0.09959 | 0.21286 | 0.10637 | -0.14991 | -0.02177 |
| SrBaFeMg-0.375-0.625-0.5-0.5 | -0.01091 | 0.34401 | 0.16655 | -0.10427 | 0.11638 | 0.00606 | SrKFe-0.625-0.375-1 | 0.27688 | 0.12352 | 0.2002 | 0.01242 | -0.15055 | -0.06906 |
| SrBaFeMg-0.375-0.625-0.875-0.125 | 0.16771 | 0.07822 | 0.12296 | -0.05453 | -0.11482 | -0.08467 | SrKFe-0.875-0.125-1 | 0.4351 | 0.57842 | 0.50676 | 0.17555 | 0.22575 | 0.20065 |
| SrBaFeMg-0.75-0.25-0.75-0.25 | -0.09957 | 0.45867 | 0.17955 | -0.13136 | 0.19618 | 0.03241 | SrKFeCo-0.875-0.125-0.75-0.25* | 0.44088 | 0.46146 | 0.45117 | 0.20654 | 0.14667 | 0.17661 |
| SrBaFeMg-0.875-0.125-0.75-0.25 | 0.18231 | -0.06099 | 0.06066 | -0.10135 | -0.20737 | -0.15436 | SrKFeMg-0.875-0.125-0.625-0.375 | 0.0851 | -0.0433 | 0.0209 | -0.20243 | -0.21451 | -0.20847 |
| SrBaFeMn-0.125-0.875-0.75-0.25 | 0.21511 | 0.52965 | 0.37238 | -0.00363 | 0.24004 | 0.11821 | SrKFeMn-0.875-0.125-0.375-0.625 | 0.10576 | 0.35482 | 0.23029 | -0.10413 | 0.09299 | -0.00557 |
| SrBaFeMn-0.25-0.75-0.5-0.5 | 0.37246 | 0.3374 | 0.35493 | 0.18143 | 0.08588 | 0.13366 | SrKFeMn-0.875-0.125-0.75-0.25 | 0.2193 | 0.27336 | 0.24633 | -0.10859 | -0.02782 | -0.0682 |
| SrBaFeMn-0.375-0.625-0.25-0.75 | 0.01613 | 0.25094 | 0.13354 | -0.20936 | -0.06259 | -0.13598 | SrLaCo-0.75-0.25-1 | 0.56372 | 0.49102 | 0.52737 | 0.31562 | 0.36582 | 0.34072 |
| SrBaFeMn-0.5-0.5-0.75-0.25 | 0.17028 | 0.2868 | 0.22854 | -0.07792 | 0.12363 | 0.02285 | SrLaCu-0.625-0.375-1 | 0.05413 | 0.24897 | 0.15155 | -0.22745 | -0.08991 | -0.15868 |
| SrBaFeMn-0.625-0.375-0.5-0.5 | 0.0704 | 0.24001 | 0.15521 | -0.20419 | 0.05717 | -0.07351 | SrLaFeCo-0.875-0.125-0.125-0.875* | 0.42866 | 0.48005 | 0.45436 | 0.10681 | 0.24468 | 0.17575 |
| SrBaFeMn-0.75-0.25-0.25-0.75 | 0.22292 | 0.58233 | 0.40263 | 0.01588 | 0.18357 | 0.09972 | SrLaFeCo-0.875-0.125-0.25-0.75 | 0.17304 | 0.49265 | 0.33284 | -0.10557 | 0.09846 | -0.00355 |
| SrBaFeMn-0.75-0.25-0.75-0.25 | 0.57074 | 0.49875 | 0.53474 | 0.405 | 0.22733 | 0.31616 | SrLaFeCo-0.875-0.125-0.5-0.5 | 0.56692 | 0.54863 | 0.55777 | 0.34608 | 0.09996 | 0.22302 |
| SrBaFeMn-0.875-0.125-0.125-0.875 | 0.34797 | 0.17679 | 0.26238 | 0.08093 | -0.06899 | 0.00597 | SrLaFeCu-0.5-0.5-0.25-0.75 | 0.31725 | 0.12518 | 0.22122 | 0.02344 | -0.17733 | -0.07695 |
| SrBaFeMn-0.875-0.125-0.375-0.625 | 0.17094 | 0.40018 | 0.28556 | -0.05548 | 0.15608 | 0.0503 | SrLaFeCu-0.625-0.375-0.625-0.375 | 0.56318 | 0.15869 | 0.36094 | 0.28582 | -0.07373 | 0.10604 |
| SrBaFeMn-0.875-0.125-0.5-0.5 | 0.0472 | 0.38986 | 0.21853 | -0.21607 | 0.16122 | -0.02743 | SrLaFeCu-0.75-0.25-0.625-0.375 | 0.40215 | 0.32947 | 0.36581 | 0.18322 | -0.03735 | 0.07293 |
| SrBaFeNi-0.125-0.875-0.875-0.125 | -0.0962 | 0.19215 | 0.04798 | -0.22659 | -0.0426 | -0.1346 | SrLaFeCu-0.875-0.125-0.75-0.25 | 0.38722 | 0.25224 | 0.31973 | 0.12097 | -0.07601 | 0.02248 |
| SrBaFeNi-0.375-0.625-0.625-0.375 | 0.16963 | 0.35434 | 0.26199 | -0.09042 | 0.18209 | 0.04584 | SrLaFeMg-0.25-0.75-0.375-0.625 | 0.11726 | 0.56336 | 0.34031 | -0.091 | 0.26861 | 0.08881 |
| SrBaFeNi-0.5-0.5-0.75-0.25 | 0.08683 | 0.05129 | 0.06906 | -0.18171 | -0.2099 | -0.19581 | SrLaFeMg-0.875-0.125-0.75-0.25 | 0.08061 | 0.52183 | 0.30122 | -0.13506 | 0.25454 | 0.05974 |
| SrBaFeNi-0.875-0.125-0.75-0.25 | 0.28202 | 0.35396 | 0.31799 | 0.00711 | 0.1003 | 0.0537 | SrLaFeMg-0.875-0.125-0.875-0.125 | 0.39941 | 0.58209 | 0.49075 | 0.15359 | 0.29215 | 0.22287 |
| SrCaCo-0.75-0.25-1 | 0.19103 | 0.40577 | 0.2984 | -6.57E-04 | -0.00444 | -0.00255 | SrLaFeMn-0.875-0.125-0.125-0.875 | 0.62728 | 0.58765 | 0.60747 | 0.31092 | 0.20223 | 0.25657 |
| SrCaFe-0.875-0.125-1 | 0.57668 | 0.57066 | 0.57367 | 0.33086 | 0.34956 | 0.34021 | SrLaFeNi-0.375-0.625-0.125-0.875 | 0.61531 | 0.34358 | 0.47944 | 0.36103 | -0.08201 | 0.13951 |
| C+C+C+C+ 0.125 0.075 0.25 0.75 | 0.05631 | 0 59.42 | 0.22026 | 0.00000 | 0.00000 | 0.00040 | 01 5 M 05 05 0405 0075 | 0.40044 | 0.00004 | 0.05460 | 0.00/00 | 0.44470 | 0.00005 |

113 promising compositions are proposed for further experimental verifications.

High Throughput Study: Materials Tested



Visual representation of the materials tested and how they compare

Milestone 9.2 (Q11) Confirm REM-ASU Design

 M9.2 (Q12) Confirm REM-ASU system with >30% reduction in energy consumption compared to cryogenic ASU



Milestone 9.2 (Q11) Confirm REM-ASU Design

$$W_{loss} = K_{EC}Q\left(\frac{T_{heat\ source} - 313}{T_{heat\ source}}\right)$$



- Total work for CLAS is estimated to be ~0.63 MJ/kg O₂
- With "free" low grade process heat, energy consumption can be lowered to 0.1 MJ/kg
- REM-ASU can reduce energy consumption by 30-70% comparing to cryogenic air separation

CLAS Aspen Simulation: Reactor Sizing

- Basis: a plant with a 5 MW operating capacity
- Kinetics of SCFC 8246 at 600 C, a reduction time of 90 seconds, an oxidation time of 60 seconds, an oxygen capacity of 0.5 wt%
- Oxygen sorbent requirement is 3.88 tons or 2.59 m³
- Bundled tubes configuration and 7 tubes in a packed formation, the tubes would have a diameter of 18 in and a height to diameter ratio of 5 to 1, the height is 90 in



Steam Effects



Steam vaporization takes up the most energy and accounts for the most lost work

Effect of Driving Force



Changing the driving force, P_{O2} difference in the reactor, leads to lower energy costs but higher bed size factors

Sensitivity Analysis



Changing these factors indicates that the Efficiency coefficient has the highest impact on total energy

REM-ASU Design and **TEA**



| Equipment Designation | Recommended | Cost Estimate and | Energy | | |
|--------------------------|-----------------|-----------------------|-------------|--|--|
| and Description | Vendor(s) | Method: | Requirement | | |
| B101 main process air | | | | | |
| blower and associated | URAI or | | | | |
| filtration | Howden | \$45,000 | 40 kW | | |
| HX 102. Final process | SPX, Xylem, | | | | |
| heat exchanger. | Harsco | \$215,000 - \$575,000 | 1,600 kW | | |
| | Emerson | | | | |
| | Vanessa Valves | | | | |
| BFV 100 and 200 series | (10" air side, | \$19,000/\$34,000 | | | |
| (qty 8) Butterfly Valves | 16" steam side) | respectively ea | N/A | | |
| Main Sorption/Desorption | Custom | | | | |
| Reactors (2) | fabrication | \$800,000 <u>ea</u> | N/A | | |
| HX 201. Condensation | SPX, Xylem, | | | | |
| Unit | Harsco | \$500,000 | 4,150 kW | | |
| HX 202. Process heat | Custom | | | | |
| exchanger | fabrication | \$230,000 | 2,000 kW | | |
| C-301. Oxygen | Rix Industries, | | | | |
| Compressor | Gardner Denver | \$75,000 | 75 kW | | |
| ST-301 Product Storage | Custom | | | | |
| Tank | fabrication | \$55,000 | N/A | | |
| | | 4"CS \$18/foot. 8"CS | | | |
| | | \$50/foot. 10"SS | | | |
| | | 400/foot. 16"SS | | | |
| Process piping | Shelf Materials | \$750/foot. | N/A | | |
| Controls, Data | ABB, | | | | |
| Acquisition, | Yokogawa, | | 5 1-337 | | |
| Human/Machine Interface, | Rockwell, and | | JKW | | |
| Sensors | Honeywell | \$275,000 | | | |

THERMOSOLY LLC

Outline

- Project Description and Objectives
- Project Update
- Preparing Project for Next Steps
- Concluding Remarks

Future work

- DFT based high throughput screening on sorbent develop has screened out a few thousand sorbent compositions, experimental preparation/characterization is currently under way;
- We discovered interesting dopant effect, showing that even 0.03 at.% dopant can significantly impact sorbent performance. This phenomena is being further investigated in detail, including Neutron Diffraction studies;
- Novel double perovskite sorbents offer high oxygen capacity and opportunity for integrated O₂ compression have been investigated. It can be particularly suitable for gasification applications;
- Refinement of the reactor model for optimized REM-ASU system design.

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Market Benefits/Assessment and Tech to Market

- REM-ASU produces low-cost oxygen compatible with modular coal gasification
- REM-ASU can lead to 30% reduction in energy consumption comparing to cryogenic method for air separation
- REM-ASU integrates with gasification system for low-grade heat utilization and O₂ cost reduction
- REM-ASU has lower capital cost and is easy to scale up



Conclusions

- REM-ASU has the potential to produce low-cost oxygen via pressure swing with oxygen sorbent materials
- REM-ASU is tailored to be compatible with 1-5 MW coal gasifier, with the potential for >30% reduction in energy consumption for air separation
- Low-cost oxygen reduces cost for coal gasifier deployment, leading to cost effective CO₂ capture and utilization
- Future work include TEA analysis, additional stability test, and evaluation of oxygen sorbents selected by high throughput DFT method.

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