Upscaling Thin-Film Aluminum Oxide Production via Atomic Layer Deposition

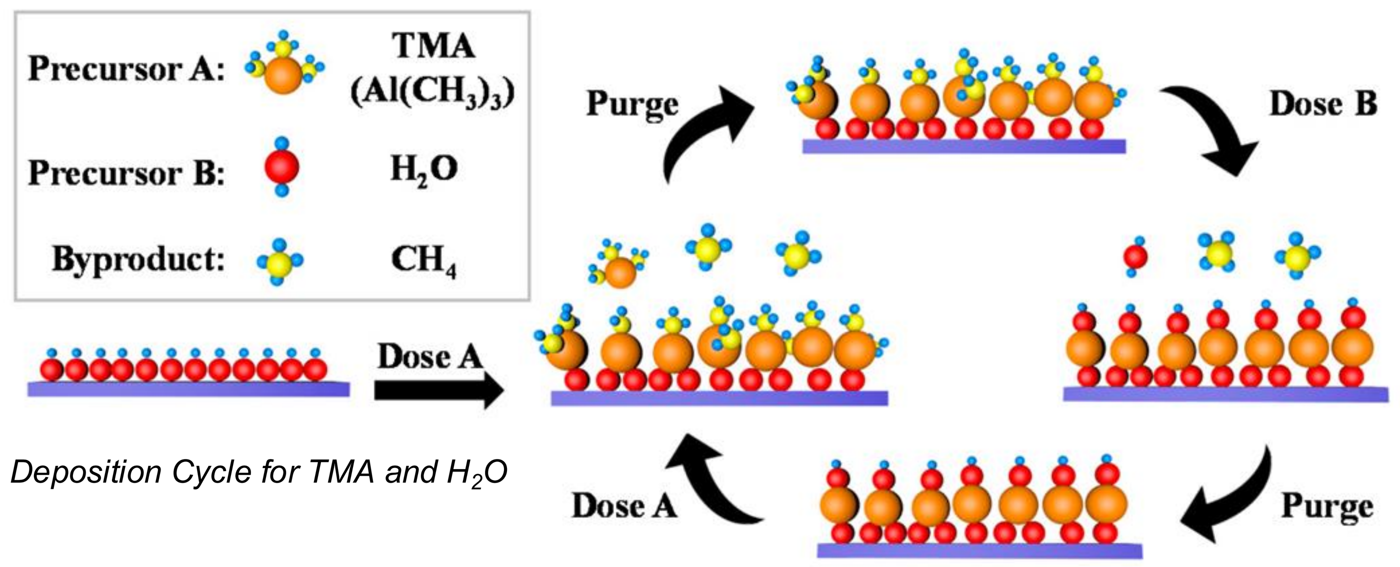
A. JAMES CLARK SCHOOL OF ENGINEERING

Ethan Bolinger, Gabriella D'Orto, Hayden Medlin, Bryan Sosa Morazan, Cassidy Sudell

DEPARTMENT OF CHEMICAL & BIOMOLECULAR ENGINEERING

Background

- Atomic Layer Deposition (ALD) is a coating process that follows a self-limiting, layer-by-layer deposition mechanism through sequential half reactions.
- Through cycles of purging and pulsing the reactor, a thin film with exceptional step coverage, conformity, and monolayer thickness control is grown.



Deposition Cycle for TMA and H_2O

- The most established ALD reaction is depositing trimethylaluminum (TMA) and H_2O on a silicon wafer to grow thin-film aluminum oxide (Al_2O_3).
- Al_2O_3 is valued for its use in microelectronics, energy storage, optics, LEDs/OLEDs, and biomedical applications.

TMA x H_2O Reaction

$$2Al(CH_3)_3\,(g) + 3H_2O\,(g) \rightarrow Al_2O_3\,(s) + 6CH_4\,(g)$$

Motivation

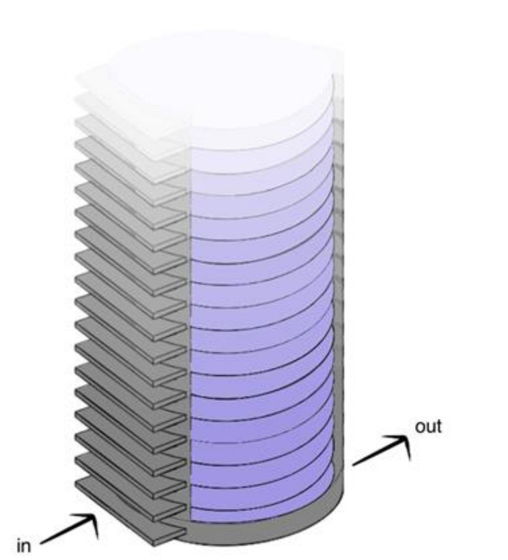
- Market demands for high quality, thin film Al_2O_3 increase yearly as relevant industries uses expand.
- There is currently no dominant, cost-effective, high-throughput ALD reactor on the market that can be used for thin film Al_2O_3 production.

Goals

Design a viable upscaled process for ALD grown Al_2O_3

a) **Customize a reactor design and model in COMSOL**
   - High-throughput and optimized geometry to maximize product and minimize cost and precursor waste

b) **Construct a downstream process with recycle stream using Aspen**
   - Extract TMA to recycle for further use and purify methane to sell

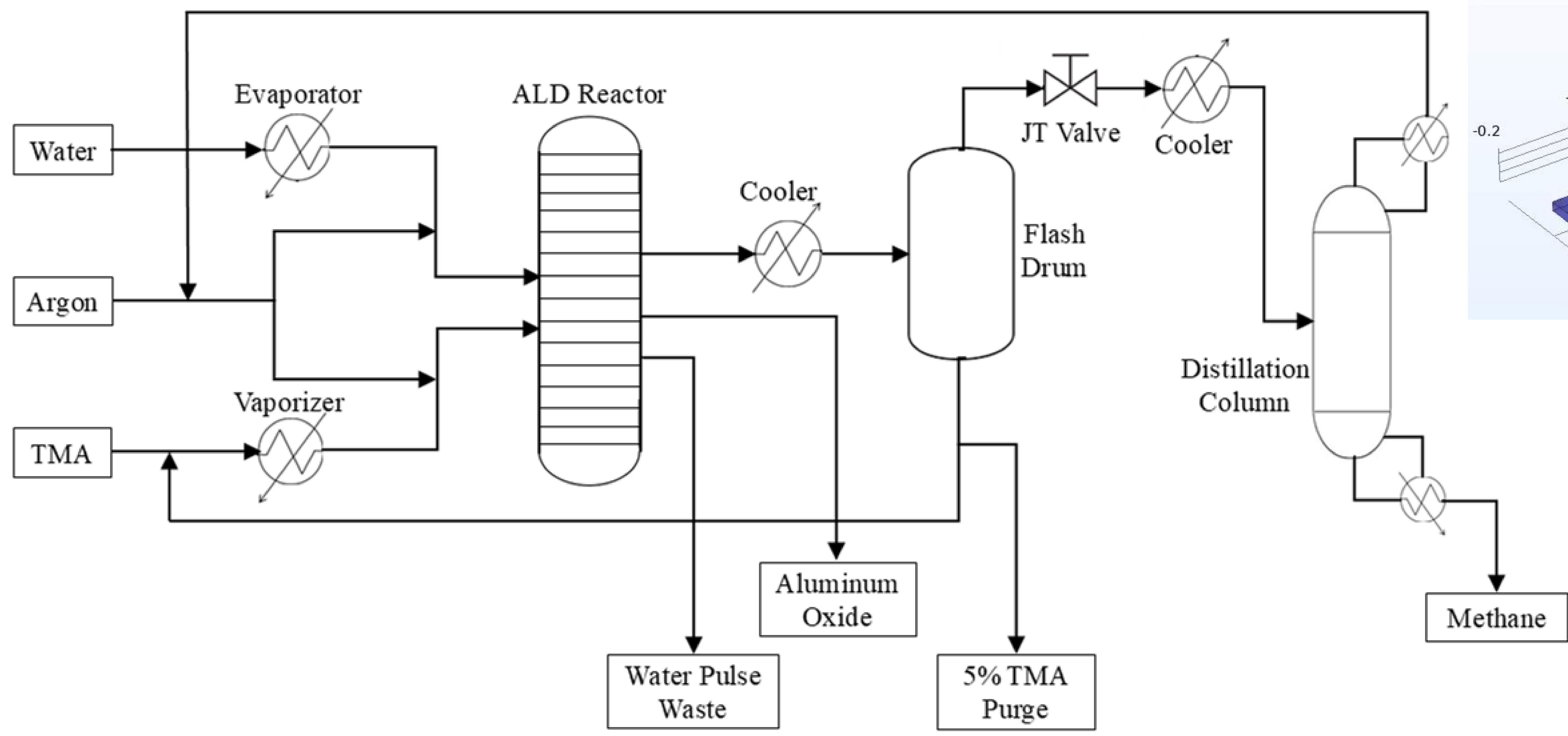


Reactor Mock-up

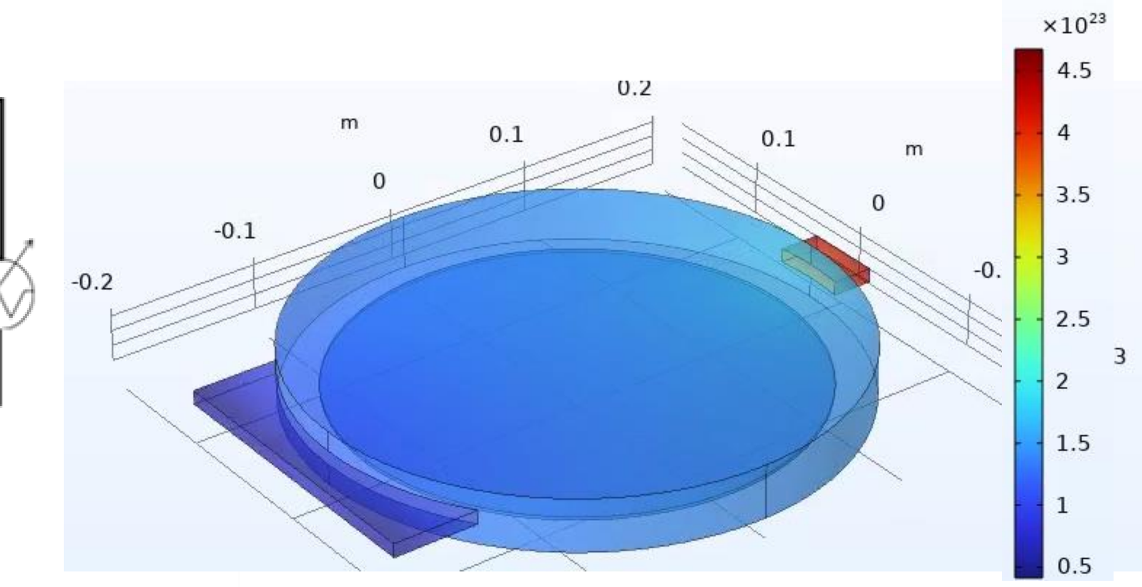
Environmental Impact & Safety

- TMA is a pyrophoric chemical so precautions following OSHA regulations & the EPA's Toxic Substance Control Act for storage, use, and necessary disposal are required.
- Methane byproduct is a greenhouse gas so it is purified and sold as to comply with The Clean Air Act.

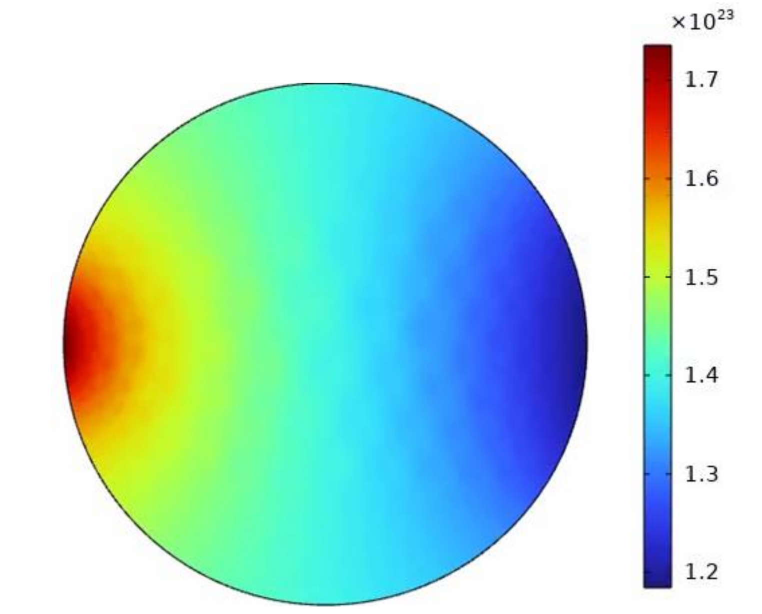
Process



Proposed Process Flow Diagram



*Incident molar flux through the reactor (1/(m²*s))*



*Incident molar flux over the deposition site(1/(m²*s))*

Justification

- Upstream heaters optimize precursor temperature feeding into the reactor.
- Minimized reactor internal surface area limits material waste and cycle time.
- TMA is a high cost precursor and thus the cost benefit of recycling greatly outweighs flash drum utility costs.
- Purification and sale of methane prevents environmental impacts of burning methane and allows for argon recycle.
- 5% TMA purge is necessary to mitigate pressure build up
- Temperature PI controllers are necessary to prevent production losses and decreased productivity

Conclusion

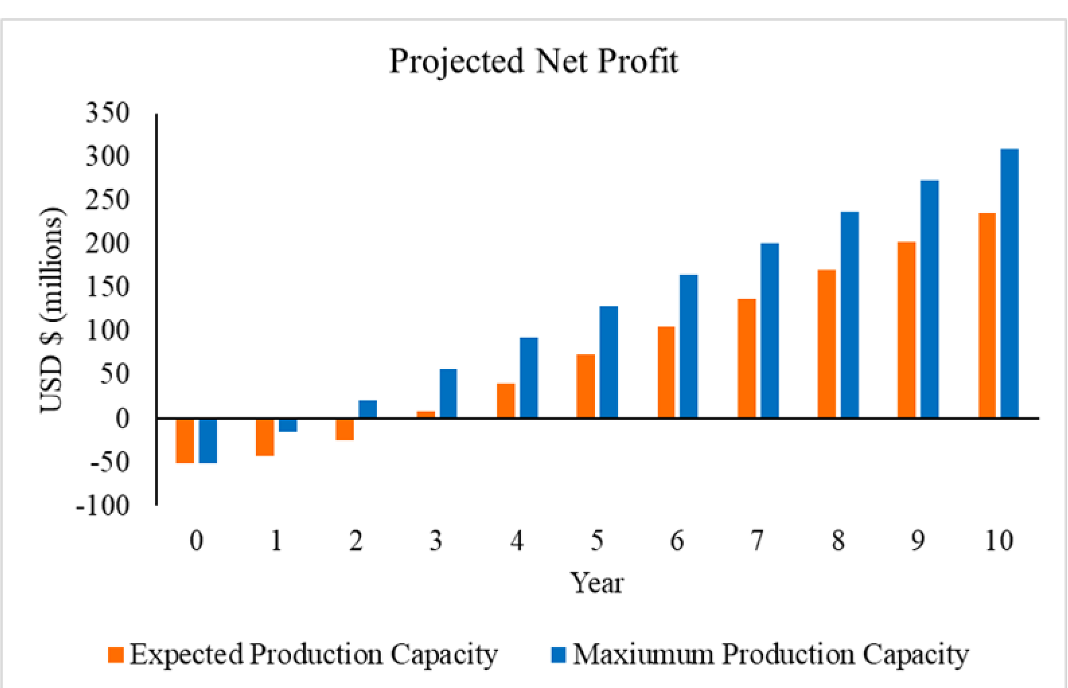
1. **Project effectively demonstrates the feasibility of upscaling thin-film Al_2O_3 produced via ALD as its both technically robust and economically sustainable.**

   Future Process Development
   - Use more robust systems to run more advanced simulations and heat exchanger network.
   - Integrate more advanced process control to increase operational productivity.

1. **Long term goals and projected profits are outlined and reflect the increasing market demand, ongoing advancements, and viability of the industry.**

   Future Business Direction
   - Pursue partnerships and licensing opportunities.
   - Build more ALD reactors and facilities.
   - Accommodate different precursors and implement more ALD reactor types

Economics



Annual Expenses	$424,036,975
Annual Net Earnings	$36,040,278
Total Capital Investment	$51,302,473
Return on Investment	70.25%
Payback Period	1.42 years
Adjusted Payback Period	2.75 years

Acknowledgments

We would like to extend our thanks to Dr. David M. Stewart, Dr. Nam Sun Wang, Ebenezer Kobina Sam, and the CHBE department for making this project possible.