Modelling of Nitridation Kinetics for Chemical Looping Ammonia Synthesis

Adaeze Maduako, Laron Burrows and George Bollas

Department of Chemical and Biomolecular Engineering, University of Connecticut, Storrs, CT

adaeze.maduako@uconn.edu

Ammonia

2nd Most produced chemical worldwide

70% of the World population relies on ammonia-based fertilizers

20% [1] of global energy consumption for ammonia production

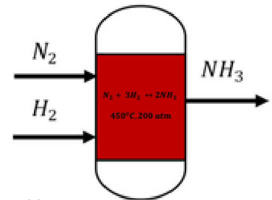
200 Million tons of annual ammonia production

3 KWh/l Energy density of liquid ammonia; highest zero-carbon fuel

500 Billion USD market value for green ammonia in maritime transport

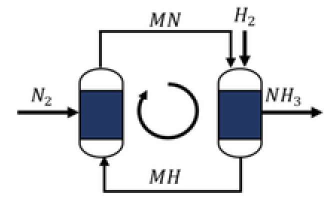
How is it produced?

Haber-Bosch Process



- Nitrogen activation
- High Energy Consumption
- High Associated emmissions
- High Operational Costs.

Chemical Looping Ammonia Synthesis

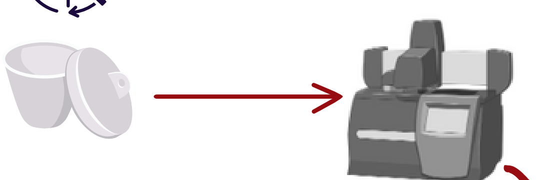


- Decouples the ammonia synthesis reaction
- Mild reaction conditions
- Integration with renewable energy.

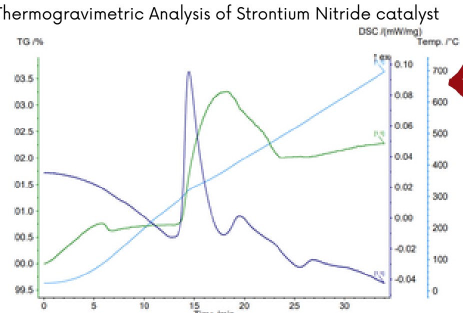
Objective

- Calculate the thermodynamic properties for the nitridation reaction
- Develop a comprehensive kinetic model for Sr3N2 nitridation reaction
- Validate model against experimental data
- Compare Isothermal and Non-isothermal methods

Methodology



Thermogravimetric Analysis of Strontium Nitride catalyst



Thermogravimetric analysis (TGA) was used to measure the weight gain of the catalyst in a Nitrogen environment, under Isothermal and Non-Isothermal conditions

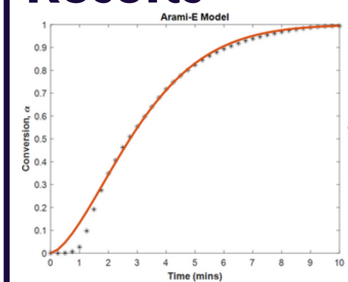
Isothermal:

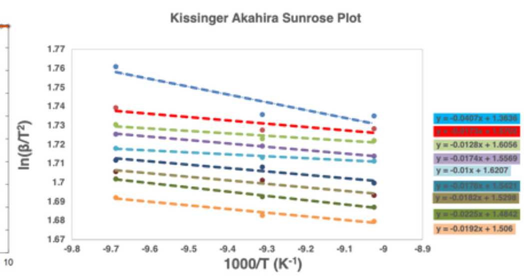
- Temperature range: 200-700°C.

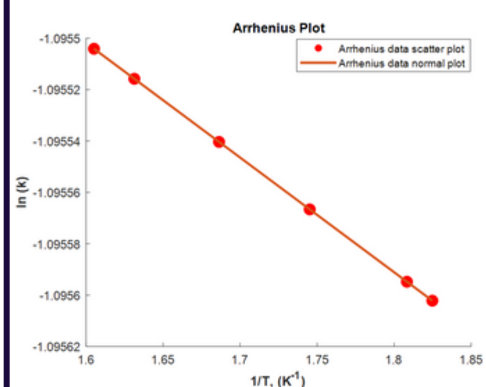
Non-Isothermal

- Heating Rates: 20°C/min, 30°C/min , and 40°C/min.

Results







$$\frac{d\alpha}{dt}\ 0.458e^{\frac{-3153.03}{RT}} f(\alpha)$$

$$f(\alpha) = 1.6616(1-\alpha)[-\ln(1-\alpha)]^{0.3932}$$

Kinetic Parameter	Value
Rate constant, k (M/s)	-0.24206
Activation Energy, Ea (J/mol)	-3153.03
Temperature (°C)	321
Pre-exponential factor, A	-0.458
Heating Rate, β (°C/min)	20
ΔS (J/mol)	-294.11
ΔH (J/mol)	-1785.48
ΔG (J/mol)	-172913.24

Conclusion

- Our results shows that the Avrami Nucleation model accurately describes the reaction kinetics
- A comprehensive kinetic model for Sr3N2 nitridation was obtained and validated against experimental data
- Thermodynamic analysis reveals that the activation energy for the process is 3153 J/mol
- The Isothermal method yields a more realistic estimation of reaction thermodynamic properties.

References

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- Peterson, B. A., Pfromm, P. H., & Peterson, A. A. (2015). Chemical looping of metal nitride catalysts: low-pressure ammonia synthesis for energy storage. Chem. Sci, 6(7)
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