

Ammonia Combustion Technical Working Group meeting minutes
January 14, 2025

- Introductory remarks
- Michael Burke (Columbia) - Toward Predictive Kinetics for Ammonia Combustion and Emissions
 - Challenges in complex reactions worse for nitrogen than typical hydrocarbons
 - Deep dives on reactions relevant to N₂O emissions
 - Multiscale physics-based data driven models
- Columbia Q&A
 - Clint Bedick, NETL: Have you looked at trying to update existing mechanisms?
 - Updated third-body reaction efficiencies probably will matter for other mechanisms - it did for Glarborg
 - Stephen Klippenstein - Pure ammonia pyrolysis reaction?
 - They are looking at, but haven't done a deep dive yet
 - John O'Halloran - What was the diluent used in optical experiments
 - Helium, could also use argon or nitrogen
 - Clayton Mulvihill - What are your thoughts on synthesizing old data from previous papers?
 - They have tried to reverse engineer data, but have not had success in extracting raw data in an unambiguous way
- Stephen Klippenstein (ANL) - Theory Informed Kinetics for NH₃ Oxidation and Pyrolysis
- ANL Q&A
 - Rob Barlow - What do we have to learn about NH₃/H₂ blends? What about a GRI type mech?
 - NH₃/H₂ pyrolysis reactions should be important. Maybe some interesting considerations with non-thermal interactions. Non-thermal reactions particularly important with co-fuels, like H₂.
 - Clint Bedick - CFD
 - Haven't properly learned co-fuel cross reactions. Huge holes in current NH₃-hydrocarbon reactions. Even a model that reproduces IDT or flame speed will probably will not cover all of the conditions of a real ammonia combustion device.
 - M. Gilles Bourque - Could we build a roadmap of what data is needed for mechanism development?
 - That's not a thing that is normally published but it should be published. Maybe we should also think about developing mechanisms for a specific application and thinking about what reactions are needed, rather than developing them around the data available.
- AEA Turbines Panel Summary
 - Need data in the 15-25 atm range to be gas turbine relevant
 - Need much more ammonia production to meet potential demand for gas turbine usage
- Open discussion
 - Are people concerned about N₂O? Yes, very concerned about N₂O (Rob Steele)

Closing remarks