# Integrated Hydrogen Electrolysis and Ammonia Production Process

## Dynamic Simulation Report

Modeled using Aspen Custom Modeler and Aspen HYSYS

Date: August 2025

This project presents the dynamic simulation of an integrated renewable energy-based ammonia production system, combining alkaline water electrolysis (modeled in Aspen Custom Modeler) with the Haber-Bosch process (modeled in Aspen HYSYS). The primary objective was to explore the dynamic behavior, control strategies, and energy integration of a "Power-to-Ammonia" system utilizing solar energy as the primary input.

The hydrogen production unit employed an alkaline water electrolyzer, dynamically modeled in ACM to reflect transient behavior under variable solar power input. The model captured the electrochemical kinetics, thermal balance, and mass transport phenomena of the electrolysis system. This hydrogen stream was integrated into a downstream Haber-Bosch loop simulated in Aspen HYSYS, where hydrogen reacts with nitrogen (from air separation) to produce ammonia at high temperature and pressure.

Dynamic simulations were carried out to analyze the open-loop responses of both subsystems to changes in solar power availability, feed composition, and flow disturbances. These simulations provided insight into system control and stability, identifying bottlenecks during ramp-up, cooldown, and fluctuating energy input conditions. The behavior of recycle compressors, reactors, and heat exchangers in the Haber-Bosch loop under dynamic conditions was specifically evaluated.

Process integration was a key focus, ensuring energy-efficient coupling between the electrolyzer and ammonia synthesis loop. A renewable energy model representing solar power variability was linked to the electrolyzer load, enabling power-to-gas analysis. Various case studies were conducted to simulate operational scenarios under different solar profiles, evaluating system flexibility, ramping capacity, and energy storage needs.

Finally, optimization studies were performed to improve overall process efficiency, reactor yield, and hydrogen utilization while maintaining system stability. Control strategies including cascade and feedforward loops were tested to mitigate power fluctuations and ensure steady ammonia output. This integrated simulation provides a foundation for designing flexible, renewable-powered ammonia production systems for future green energy infrastructure.