**PROJECT TITLE: Phase 2: Integrated Small-Scale Ammonia Synthesis**

**I. PROJECT STATEMENT** We want to continue making ammonia sustainably for the farm, using renewable energy and with no greenhouse gas emission − *but now in phase 2* focusing on a **single integrated reactor-separator module**, safer and more efficient than to date. This module is powered by electricity made from solar cells or wind turbines, and uses nitrogen extracted from air and hydrogen made from water. It has the potential to produce cheaper ammonia at small scale. In our recent work, the separator - an absorber - replaced the condenser used conventionally. The key in the currently proposed work is the integration of the reactor and separator. We have demonstrated proof of concept, but now need essential experimentation with this integrated reactor-separator, which greatly simplifies the equipment used in the industry standard, the century-old Haber-Bosch process. In addition to improved experiments, we will make additional calculations and process tests. The calculations center on areas where the integrated system can make ammonia more cheaply than Haber-Bosch. The experiments center on comparing the integrated system with two pilot plants at Morris - one based on a conventional Haber-Bosch, and the other more recent one with the condenser replaced by a separate absorber.

**II. PROJECT ACTIVITIES AND OUTCOMES**

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| **Activity 1 Title:** **Test absorbent materials, fabricate and test integrated reactor systems**  **Description:** *The idea on which this work is based is contrasted with conventional and recent technology in the figure below. In the conventional process on the left, hydrogen and nitrogen are reacted at 400oC. The resulting gas mixture is cooled in a condenser to -20oC to remove some of the ammonia, and the remaining ammonia and the unreacted gases are returned to the reactor. In the process developed in Phase 1 of the work with LCCMR (and with ARPA-E), shown in the center of the figure, the ammonia made is all removed by absorption at about 100oC (patent application filed).*  *In the work proposed now in Phase 2, shown at the right of the figure, the reactive gases are fed to the integrated unit containing* ***both*** *catalyst and absorber. This simpler process may make ammonia less expensively and at smaller scale. The research has four parts: better absorbents for integration, comparisons between processes, exploration of better catalysts, and test runs with comparative evaluations and technoeconomic analysis.*  *Absorbents: In the first phase of funding from LCCMR, we showed that materials like calcium chloride and magnesium bromide could absorb large amounts of ammonia, even at high temperatures. We improved the stability of these materials by coating them onto silica or another inert support, which is now covered in a patent application filed by the university. To combine reaction and separation in the integrated system, so far we have used an iron catalyst and salts like nickel and magnesium chlorides at 400oC. This system, also subject to a patent filing, is an integration that would not be possible at any pressure just with the condensation of ammonia, which would only be feasible well below the critical point of ammonia, 132oC. We also have developed an automated apparatus for screening large numbers of possible absorbents for ammonia.*  *Comparisons: In the original work, we used the WCROC Haber-Bosch process (built with money including from the State and from the Minnesota Corn Research and Promotion Council) as a standard for our development of ammonia-selective absorbents (developed using support from LCCMR and the US Department of Energy). We now have a second small pilot prototype being used to explore where the absorbent technology can compete with conventional. These two pilot operations give us a facility unique in the world for testing when the integrated technology can compete. Our new effort proposed here will focus on the integrated module - where the catalytic reactor and the absorber are combined into a single, integrated unit. We have completed work on a proof-of-concept; with this proposed work, we will expand our existing collaboration between the West Central Research and Outreach Center and the University of Minnesota to include more necessary work on the new integrated reactor-separator for optimal design, operation, and safety.*  **ENRTF BUDGET: $1,215,395** |  |

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| **Outcome** | **Completion Date** |
| *1. Year 1: Fabricate integrated reactor with proven materials, improve fabrication to ensure cycle reproducibility, develop and test improved absorbent materials* | *July 2021* |
| *2. Optimize operation with best materials to date; improve cycle durability and range of operation* | *July 2022* |
| *3. Extended runs for technoeconomic analysis (some at WCROC Morris); Technical partner development; Develop range of targeted fabrication/operation designs for different applications* | *July 2023* |

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| **Activity 2 Title: Modeling using physical experiment to develop a “virtual integrated reactor” for use in planning, design, and technoeconomic analysis**  **Description:** *As we gain experience in the physical fabrication and operation of integrated reactor systems, the project (and its prospects for realization in the market) will be assisted by the development of a mathematical model - a “virtual integrated reactor” - to predict and design sensors, control strategies, and actuators for optimal cyclic operation and assess safe operation procedures and parameters. This modeling effort will also allow technoeconomic analysis that will be essential for the development of commercial partners and to engage policy stakeholders.*  **ENRTF BUDGET: $292,520** |  |

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| **Outcome** | **Completion Date** |
| *1. Develop “virtual integrated reactor” model, parameterize* | *July 2021* |
| *2. Continue developing model; use to assess safe and optimal operation of physical system* | *July 2022* |
| *3. Use model for tailored design, optimal sensing and actuation, adapting to prospective partners* | *July 2023* |

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| **Activity 3 Title: Implement novel catalysts with different range of operation temperature**  ***Description:***  *In this research, we are largely accepting as ideal the catalysts used to make ammonia in the existing Haber-Bosch process. We understand that these catalysts are the product of over a century of focused development by the world’s best chemists. At the same time, we know on thermodynamic grounds that these catalysts are far less than optimal, that they require much higher temperatures and pressures than those theoretically required. Very recent developments suggest the possibility of lower-temperature catalysts, which might open useful new design options with lower temperature absorbents. In a high risk and high gain gamble, we want to seek these gains.*  **ENRTF BUDGET: $421,848** |  |

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| **Outcome** | **Completion Date** |
| *1. Ensure optimal treatment of current benchmark catalyst, comparison with alternatives* | *July 2021* |
| *2. Integration of new catalysts into the integrated reactor system* | *July 2022* |
| *3. Long-term stability runs with novel catalysts in integrated system* | *July 2023* |

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| **Activity 4 Title: Long-term stability runs of the integrated reactor system at WCROC**  **Description:**  *Though the systems we will devise are small scale, it is best to perform long runs in Morris for TEA analysis and for stability tests with the merit of WCROC safety and expertise at long-term hydrogen and ammonia handling.*  **ENRTF BUDGET: $178,756** |  |

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| **Outcome** | **Completion Date** |
| *1. Years 1 and 2: develop facility while working on leveraging projects* | *July 2022* |
| *2 Year 3: long-term testing of best systems fabricated by end of Year 2* | *July 2023* |

**III. PROJECT PARTNERS AND COLLABORATORS: Not at this time.**

**IV. LONG-TERM IMPLEMENTATION AND FUNDING:** We understand that the integrated reactor-separator must outperform the other processes for making ammonia, especially at small scale. We will investigate this at two levels. First, we will calculate how the capacities and rates of absorption which we measure affect the price at which ammonia is made; similarly, we must make the same calculation in reverse, to show what the measured parameters must be for the process to be profitable. Second, we must see how the entire integrated process must fit into the current economic environment, for example, how it is related to supply chains and energy on Minnesota farms. The first of these goals is important to exploring the feasibility of the integrated unit. The second, already begun with two papers, will connect these innovations with the overall distribution system of ammonia in the corn belt. The UMN Office of Technology Commercialization has been engaged in developing partner relations for the last year; for instance, our team was invited to the International Fertilizer Association meeting in New Orleans (April 2019), is arranging ongoing meetings with more than four potential corporate partners, and is regularly invited to other ammonia meeting venues. We will also apply for related federal support.

**V. SEE ADDITIONAL PROPOSAL COMPONENTS:**

**A. Proposal Budget Spreadsheet**

**B. Visual Component or Map**

**C. Parcel List Spreadsheet**

**D. Acquisition, Easements, and Restoration Requirements**

**E. Research Addendum (Not required at proposal submission stage. Required later in process, if proposal is recommended. Staff will provide further information at that time)**

**F. Project Manager Qualifications and Organization Description**

**G. Letter or Resolution**

**H. Financial Capacity**