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Federal Department of the Environment,
Transport, Energy and Communications DETEC

Swiss Federal Office of Energy
Energy Research and Cleantech

Interim report from 21 November 2025

AMAZE

AmMoniA as a ZEro-carbon fuels and H2 carrier

Source: Created with AI Copilot 2025

Publisher:
Swiss Federal Office of Energy SFOE
Energy Research and Cleantech
CH-3003 Berne
www.energy-research.ch

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SFOE contract number: SI/502842-01

Summary

The AMAZE project brings together leading partners in the field chemical engineering, chemical production and catalysts for ammonia and hydrogen synthesis including CASALE SA, Clariant, HySytech, Kavala Novasolutions, CIECH, and several academic institutions (University of Messina, OST, SUPSI, University of Valladolid, UCLouvain, Power2X Analytics) to advance the pre-industrialization of green ammonia as a zero-carbon fuel and hydrogen carrier. The project addresses the urgent need to decarbonize ammonia production—traditionally a major source of CO_2 emissions—by developing new catalysts and integrated processes for producing ammonia using renewable hydrogen, and for efficiently converting ammonia back into hydrogen where needed.

Motivated by the global push for sustainable energy solutions, AMAZE targets two main technological breakthroughs: (1) distributed, small-scale green ammonia synthesis using non-critical raw material catalysts, and (2) innovative thermocatalytic and electrocatalytic technologies for ammonia cracking at lower temperatures and higher efficiencies. These advances are designed to make ammonia a practical, flexible energy vector for sectors such as shipping and long-term energy storage, leveraging existing infrastructure and logistics.

By the end of the project, AMAZE will have demonstrated a modular pilot plant capable of producing and cracking green ammonia at relevant scales, validated new catalyst formulations, and integrated digital twin and AI-based process optimization. Key achievements include the development of catalysts stable for hundreds of hours, energy-efficient ammonia cracking near ambient conditions, and successful operation of a pilot unit producing at least 4 tons of green ammonia per year. Life cycle and techno-economic assessments confirm that the AMAZE technologies can reduce greenhouse gas emissions by over 90% compared to conventional methods, while lowering production costs and enabling distributed renewable energy use.

The impact of AMAZE is significant: it paves the way for ammonia to become a cornerstone of the hydrogen economy, supporting the transition to renewable energy, reducing reliance on fossil fuels, and opening new business opportunities in energy, shipping, and sustainable agriculture. The project's results position its partners at the forefront of clean energy innovation, with validated solutions ready for industrial scale-up and broad market adoption.

Zusammenfassung

Das Projekt AMAZE vereint führende Partner aus den Bereichen Chemieingenieurwesen, chemische Produktion sowie Katalysatoren für die Ammoniak- und Wasserstoffsynthese – darunter CASALE SA, Clariant, Hy-Sytech, Kavala Novasolutions, CIECH sowie mehrere akademische Institutionen (Universität Messina, OST, SUPSI, Universität Valladolid, UCLouvain, Power2X Analytics) – mit dem Ziel, die Vor-Industrialisierung von grünem Ammoniak als CO_2-freiem Kraftstoff und Wasserstoffträger voranzutreiben. Das Projekt adressiert den dringenden Bedarf, die Ammoniakproduktion zu dekarbonisieren, die traditionell eine bedeutende Quelle von CO_2-Emissionen darstellt, indem neue Katalysatoren und integrierte Prozesse entwickelt werden: für die Herstellung von Ammoniak aus erneuerbarem Wasserstoff sowie für die effiziente Rückumwandlung von Ammoniak in Wasserstoff am Ort des Bedarfs.

Vor dem Hintergrund des globalen Vorstoßes hin zu nachhaltigen Energielösungen zielt AMAZE auf zwei wesentliche technologische Durchbrüche ab: (1) die dezentrale, kleinmaßstäbliche Synthese von grünem Ammoniak unter Einsatz von Katalysatoren auf Basis nicht-kritischer Rohstoffe und (2) innovative thermo-katalytische und elektro-katalytische Technologien für das Ammoniak-Cracking bei niedrigeren Temperaturen und höheren Wirkungsgraden. Diese Fortschritte sollen Ammoniak zu einem

praktikablen und flexiblen Energievektor für Sektoren wie die Schifffahrt und die langfristige Energiespeicherung machen, wobei vorhandene Infrastruktur und Logistikketten genutzt werden.Bis zum Ende des Projekts wird AMAZE eine modulare Pilotanlage demonstriert haben, die in der Lage ist, grünen Ammoniak in relevanten Maßstäben zu produzieren und zu spalten, neue Katalysatorformulierungen zu validieren und einen digitalen Zwilling sowie KI-basierte Prozessoptimierung zu integrieren. Zu den zentralen Ergebnissen zählen die Entwicklung von Katalysatoren mit Stabilität über Hunderte von Betriebsstunden, ein energieeffizientes Ammoniak-Cracking nahe Umgebungsbedingungen sowie der erfolgreiche Betrieb einer Piloteinheit mit einer Produktionskapazität von mindestens 4 Tonnen grünem Ammoniak pro Jahr. Lebenszyklus- und techno-ökonomische Bewertungen bestätigen, dass die AMAZE-Technologien die Treibhausgasemissionen im Vergleich zu konventionellen Verfahren um über 90 % reduzieren können – bei gleichzeitig sinkenden Produktionskosten und der Ermöglichung einer dezentralen Nutzung erneuerbarer Energien.

Die Wirkung von AMAZE ist erheblich: Das Projekt ebnet den Weg dafür, dass Ammoniak zu einem Eckpfeiler der Wasserstoffwirtschaft wird, unterstützt den Übergang zu erneuerbaren Energien, verringert die Abhängigkeit von fossilen Brennstoffen und eröffnet neue Geschäftsmöglichkeiten in den Bereichen Energie, Schifffahrt und nachhaltige Landwirtschaft. Die Projektergebnisse positionieren die Partner an der Spitze der Innovation im Bereich sauberer Energietechnologien – mit validierten Lösungen, die bereit für die industrielle Skalierung und eine breite Markteinführung sind.

Résumé

Le projet AMAZE réunit des partenaires de premier plan dans les domaines du génie chimique, de la production chimique et des catalyseurs pour la synthèse de l'ammoniac et de l'hydrogène, notamment CASALE SA, Clariant, Hy-Sytech, Kavala Novasolutions, CIECH, ainsi que plusieurs institutions académiques (Université de Messine, OST, SUPSI, Université de Valladolid, UCLouvain, Power2X Analytics), afin de faire progresser la pré-industrialisation de l'ammoniac vert en tant que carburant zéro carbone et vecteur de transport de l'hydrogène. Le projet répond au besoin urgent de décarboner la production d'ammoniac — traditionnellement une source majeure d'émissions de CO_2 — en développant de nouveaux catalyseurs et des procédés intégrés permettant de produire de l'ammoniac à partir d'hydrogène renouvelable, ainsi que de reconvertir efficacement l'ammoniac en hydrogène là où cela est nécessaire.

Porté par l'élan mondial en faveur de solutions énergétiques durables, AMAZE vise deux avancées technologiques majeures : (1) la synthèse distribuée de petite échelle d'ammoniac vert, reposant sur des catalyseurs à base de matières premières non critiques, et (2) des technologies innovantes de craquage de l'ammoniac, thermo-catalytiques et électro-catalytiques, opérant à plus basse température et avec des rendements plus élevés. Ces progrès ont pour objectif de faire de l'ammoniac un vecteur énergétique pratique et flexible pour des secteurs tels que le transport maritime et le stockage d'énergie de longue durée, en s'appuyant sur les infrastructures et la logistique existantes.

À la fin du projet, AMAZE aura démontré une unité pilote modulaire capable de produire et de craquer de l'ammoniac vert à des échelles pertinentes, aura validé de nouvelles formulations de catalyseurs et aura intégré un jumeau numérique ainsi qu'une optimisation des procédés basée sur l'IA. Parmi les principaux résultats attendus figurent le développement de catalyseurs stables sur plusieurs centaines d'heures, un craquage de l'ammoniac économe en énergie à des conditions proches de l'ambiante, ainsi que l'exploitation réussie d'une unité pilote produisant au moins 4 tonnes d'ammoniac vert par an. Des analyses de cycle de vie et des évaluations techno-économiques confirment que les technologies AMAZE peuvent réduire les émissions de gaz à effet de serre de plus de 90 % par rapport aux méthodes conventionnelles, tout en abaissant les coûts de production et en permettant une utilisation distribuée des énergies renouvelables.

L'impact d'AMAZE est considérable : il ouvre la voie à l'ammoniac comme pierre angulaire de l'économie de l'hydrogène, soutient la transition vers les énergies renouvelables, réduit la dépendance aux

combustibles fossiles et crée de nouvelles opportunités économiques dans les secteurs de l’énergie, du maritime et de l’agriculture durable. Les résultats du projet placent ses partenaires à l’avant-garde de l’innovation en matière d’énergie propre, avec des solutions validées, prêtes pour une montée en échelle industrielle et une adoption large par le marché.

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List of abbreviations

SFOE	Swiss Federal Office of Energy
AIMD	Ab Initio Molecular Dynamics
DFT	Density Functional Theory
LCOA	Levelized Cost of Ammonia
ML	Machine Learning
nCRM	Non Critical Raw Material
RHE	Reversible Hydrogen Electrode
TRL	Technology Readiness Level
WP	Work Package

1 Introduction

1.1 Context and motivation

Ammonia: From Fertilizer to Energy Vector. Ammonia (NH_3) is one of the most widely produced chemicals globally, with an annual output exceeding 150 million tons, primarily used as a fertilizer. The conventional Haber-Bosch process, developed over a century ago, synthesizes ammonia from nitrogen and hydrogen at high temperatures and pressures. While this process has been optimized for large-scale, centralized production, it remains heavily reliant on hydrogen derived from fossil fuels, particularly natural gas. As a result, ammonia production is responsible for approximately 1–2% of global CO_2 emissions, with a carbon footprint of 1.6–2.9 tons of CO_2 per ton of NH_3 produced (IEA, 2021; Appl. Energy, 2021, 282, 116009).

In recent years, ammonia has attracted renewed interest as a potential zero-carbon fuel and hydrogen carrier. Its high energy density, ease of liquefaction under mild conditions, and established global logistics infrastructure make it a promising candidate for large-scale energy storage and long-distance transport of renewable energy (IRENA, 2022; Chem. Eng. J., 2024, 486, 150132). Countries such as Japan and Australia are already investing in ammonia supply chains for power generation and shipping (IEA Ammonia Technology Roadmap, 2021).

Green Ammonia and Hydrogen Economy. The transition to a hydrogen economy is a cornerstone of global decarbonization strategies. However, hydrogen's low volumetric energy density and storage challenges hinder its widespread adoption. Ammonia offers a practical solution: it can be synthesized using green hydrogen (produced via water electrolysis powered by renewables), stored and transported efficiently, and then cracked back into hydrogen at the point of use (Energy Environ. Sci., 2021, 14, 3142–3176).

Recent advances in catalyst development and process engineering have enabled pilot-scale green ammonia plants, but significant barriers remain. The current state-of-the-art for green ammonia synthesis still relies on the Haber-Bosch process, which is not well-suited for distributed, small-scale, or flexible operation required by intermittent renewable energy sources (Chem. Sci., 2022, 13, 890). Furthermore, ammonia cracking technologies are at a lower technology readiness level (TRL), often requiring high temperatures (>550°C) and expensive noble metal catalysts, limiting their efficiency and scalability (Renew. Sustain. Energy Rev., 2022, 169, 112918).

Market Trends and Industrial Drivers. The global ammonia market was valued at over $200 billion in 2022 and is projected to grow at a compound annual growth rate (CAGR) of 5.4% through 2030, with even higher growth expected if ammonia is widely adopted as a hydrogen carrier and fuel (Market Analysis Report, 2023 IGVR-2-68038-207-5). The maritime sector, in particular, is exploring ammonia as a zero-carbon fuel to meet stringent emissions regulations (Sustainable Energy Fuels, 2021, 5, 2814).

Major industrial players, including CASALE SA and Clariant, are investing in the development of green ammonia technologies and catalysts, recognizing the strategic importance of decarbonizing ammonia production and leveraging ammonia's potential as an energy vector.

Key Challenges

1. **Decarbonizing Ammonia Production:** The main challenge is to replace fossil-derived hydrogen with green hydrogen in ammonia synthesis, while adapting the process for flexible, distributed production that can respond to variable renewable energy inputs.
2. **Efficient Ammonia Cracking:** To use ammonia as a hydrogen carrier, efficient, low-temperature, and scalable technologies for cracking ammonia back into hydrogen are needed. Current solutions are energy-intensive and rely on critical raw materials.
3. **Integration and Scalability:** Integrating green ammonia synthesis and cracking into a modular, scalable system suitable for diverse applications (from industrial to maritime) requires advances in catalyst design, process engineering, and digital optimization.

4. **Economic and Environmental Viability:** Achieving competitive costs and demonstrating significant reductions in greenhouse gas emissions are essential for market adoption. Life cycle assessment and techno-economic analysis are needed to validate the benefits.

The AMAZE project addresses these challenges through a coordinated, multidisciplinary effort (Figure 1):

- **Catalyst Innovation:** Developing advanced, non-critical raw material catalysts for both green ammonia synthesis and cracking, targeting high activity, stability, and lower operating temperatures.
- **Process Integration:** Designing and demonstrating a modular pilot plant that integrates green ammonia production with on-site catalytic and electrocatalytic cracking, supported by digital twin modelling for process optimization.
- **Distributed, Flexible Operation:** Focusing on small-scale, distributed production units that can utilize local renewable energy sources, enabling energy storage and hydrogen supply even in remote or off-grid locations.
- **Sustainability and Market Readiness:** Conducting comprehensive life cycle and techno-economic assessments to ensure environmental and economic viability, and engaging industrial partners to accelerate commercialization.

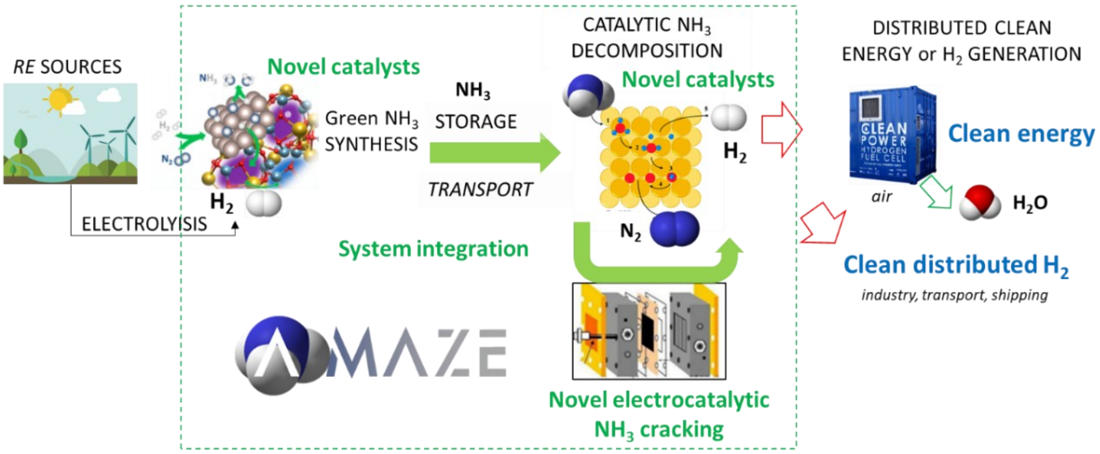

Figure 1: Amaze overall concept scheme

The AMAZE project is positioned at the forefront of the transition to a sustainable hydrogen economy. By addressing the technical, economic, and environmental challenges of green ammonia production and utilization, AMAZE aims to unlock ammonia's full potential as a zero-carbon fuel and hydrogen carrier. The project's outcomes will contribute to global decarbonization efforts, support the growth of renewable energy, and create new opportunities in energy, shipping, and chemical industries.

1.2 Project objectives

Purpose and Meaning of the Project. The AMAZE project is designed to address the urgent need for decarbonization in both the chemical and energy sectors by transforming ammonia from a traditional fertilizer feedstock into a cornerstone of the hydrogen economy. The project's central aim is to develop, demonstrate, and validate innovative, sustainable technologies for the distributed production of green ammonia and its efficient conversion back to hydrogen, thus enabling ammonia's dual role as a zero-carbon fuel and a hydrogen carrier.

How AMAZE Addresses Key Challenges

1. Decarbonizing Ammonia Production: AMAZE aims to enable distributed green ammonia production by developing new catalysts and process designs that can synthesize NH_3 using renewable-electricity-derived hydrogen while operating flexibly under variable energy (and hydrogen) availability, thereby overcoming the intrinsic limitations of conventional Haber-Bosch technology, which is highly heat-integrated and traditionally optimized for large, steady operation at high pressure and temperature. The project addresses critical "pre-stage" constraints that emerge in electrified, modular plants—most notably the need to ensure stable delivery and conditioning of make-up gases when H_2 production fluctuates, and the fact that (unlike conventional plants where nitrogen is introduced with process air) green configurations require dedicated nitrogen generation and tight control of the H_2:N_2 ratio under dynamic operation. At small and medium scales, these issues are amplified by the reduced economy of heat integration and by the energy penalties associated with pressurization and product separation, including the repeated cooling/re-heating/pressurization duties linked to ammonia removal, which become particularly burdensome when operation is frequently shifted away from design point. Within the synthesis loop itself, intermittent operation introduces mechanical and catalytic challenges, as each load change can induce thermal stresses in the ammonia converter and destabilize temperature management, making converter robustness and control strategies central to reliable flexible operation. Accordingly, AMAZE leverages low-temperature/pressure catalyst advances and a dedicated validation pathway—supported by a control-loop philosophy targeting 0–100% load flexibility and pilot-scale demonstration (minimum 4 t/y production)—to prove a modular process concept that can follow renewable profiles and reduce reliance on oversized upstream storage while maintaining safe, efficient NH_3 synthesis.

2. Efficient Ammonia Cracking: To unlock ammonia's potential as a hydrogen carrier, AMAZE will develop both thermocatalytic and electrocatalytic technologies for converting ammonia back into hydrogen at the point of use. The project aims to create catalysts that are free from critical raw materials, operate at lower temperatures, and deliver high efficiency and stability. This will make ammonia cracking more practical and scalable for applications such as shipping, remote energy supply, and industrial hydrogen use.

3. Integration and Digitalization: AMAZE will integrate these new synthesis and cracking technologies into a modular pilot plant, supported by advanced digital twin modeling and artificial intelligence. This will enable real-time process optimization, predictive maintenance, and flexible operation, further increasing the economic and technical viability of distributed green ammonia systems.

4. Sustainability and Market Readiness: The project will conduct comprehensive life cycle assessments (LCA) and techno-economic analyses to ensure that the developed technologies deliver significant reductions in greenhouse gas emissions and are cost-competitive with existing solutions. Industrial partners will play a key role in validating the technologies and preparing them for market adoption.

Issues to Be Investigated

- **Catalyst Development:** 1) Identification and optimization of non-critical raw material (nCRM) catalysts for both ammonia synthesis and cracking. 2) Investigation of catalyst stability, activity, and scalability under realistic operating conditions, including fluctuating renewable energy inputs.
- **Process Engineering:** 1) Design and demonstration of flexible, small-scale ammonia synthesis reactors.2) Development of efficient, compact ammonia cracking units suitable for distributed and mobile applications.
- **System Integration:** 1) Integration of synthesis and cracking technologies into a single, modular pilot plant. 2) Application of digital twin and AI tools for process monitoring, optimization, and predictive control.
- **Sustainability and Impact Assessment:** 1) Life cycle analysis to quantify environmental benefits, including CO_2 reduction and resource efficiency. 2) Techno-economic analysis to assess cost competitiveness and market potential.

Expected Results

- **Validated Pilot Plant:** Construction and operation of a modular pilot plant capable of producing at least 4 tons of green ammonia per year and demonstrating efficient on-site ammonia cracking.
- **Advanced Catalysts:** 1) Development of nCRM catalysts for ammonia synthesis with >90% efficiency and stability over 500 hours. 2) Thermocatalytic and electrocatalytic ammonia cracking technologies achieving high conversion rates at lower temperatures, with electrocatalytic cells targeting >70% energy efficiency at >100 mA/cm² near ambient temperature.
- **Digital Implementation:** Deployment of a digital twin for real-time process optimization and predictive maintenance.
- **Sustainability Validation:** Life cycle and techno-economic assessments confirming >90% reduction in greenhouse gas emissions compared to conventional ammonia production, and a targeted reduction in the levelized cost of ammonia (LCOA) by at least 15%.
- **Cross section and function collaboration:** A wide and practical scope of the project will involve the academic, the institutional and industrial players. It is targeted that they all will strengthen their relationship, provide opportunities to create and explore innovation and drive the project outcome into measurable and market driven outcome.

Qualitative Objectives:

- Enable flexible, distributed green ammonia production and utilization.
- Demonstrate the technical and economic feasibility of ammonia as a hydrogen carrier and zero-carbon fuel.
- Foster industrial adoption by involving key market players throughout the project.

Quantitative Objectives and KPIs:

OBJECTIVES (OB) and KEY PERFORMANCE INDEXES (KPI)	
OB1	**OB1:** Optimized nCRM (non-critical raw materials) catalysts for green NH_3 synthesis using H_2 from electrolysis **KPI1**: a nCRM catalyst, stable for 500h with catalyst efficiency (ratio of outlet ammonia concentration to the equilibrium ammonia concentration in a single pass) over 90%.
OB2	**OB2:** Development of nCRM thermocatalysts for NH_3 selective cracking **KPI2:** a nCRM catalyst, stable for >100h and activity which enables to reach the equilibrium in a single pass, at temperatures <50-100°C with respect to state of the art (a reference catalyst provided by industrial partners)
OB3	**OB3:** Development of nCRM electrocatalysts and zero-gap-type electrocatalytic cell for NH_3 cracking near ambient conditions **KPI3:** a nCRM electrocatalyst, gas-diffusion layer type electrode and zero-gap electrocatalytic cell giving energy efficiency > 70% at a current density > 100 mA/cm^2 at a temperature close to ambient
OB4	**OB4:** Demonstrate and validate the technology of green NH_3 distributed production **KPI4:** validate technology in a pilot-scale unit with minimum production of 4 tons/y of ammonia in green simulated conditions
OB5	**OB5:** Demonstrate and validate the technologies for cracking of NH_3 **KPI5:** validate the technology in a pilot-scale unit coupled to that developed in OB4

2 Approach, method, results and discussion

2.1 Approach

The AMAZE project adopts a **multidisciplinary, integrated approach** to develop and validate new technologies for green ammonia synthesis and cracking. The project is structured around the entire innovation chain—from fundamental catalyst research to pilot-scale demonstration and sustainability assessment—ensuring that scientific advances are rapidly translated into industrially relevant solutions.

Key features of the approach include:

- **Collaboration between industry and academia** to combine practical engineering, advanced modeling, and scientific discovery.
- **Parallel development** of both thermocatalytic and electrocatalytic ammonia cracking technologies.
- **Integration of digital tools** (digital twins, AI) for process optimization and predictive maintenance.
- **Continuous feedback loops** between laboratory research, modeling, pilot operation, and sustainability analysis.

2.2 Methods

2.2.1 Catalyst and Process Development

a) Catalyst Screening and Optimization

- **Non-critical raw material (nCRM) catalysts** for ammonia synthesis and cracking are developed using a combination of:
  - **High-throughput computational screening** (DFT, machine learning, molecular dynamics) to identify promising catalyst compositions and structures.
  - **Laboratory synthesis and testing** under realistic, fluctuating conditions (simulating renewable energy input).
  - **Scale-up and benchmarking** against industrial references, with stability tests exceeding 500 hours for synthesis and 100 hours for cracking.

b) Process Engineering

- **Design and construction of modular pilot units** for distributed green ammonia production and on-site cracking.
- **Process flow diagrams (PFD), energy and mass balances (E&M), and safety analyses (HAZOP)** are developed to ensure industrial relevance and safe operation.
- **Digital twin modeling** is implemented to simulate, monitor, and optimize pilot plant performance in real time.

2.2.2 Pilot Demonstration

- **Manufacturing and installation** of a containerized pilot plant at an industrial ammonia facility (Kavala NovaFert, Greece).
- **Integrated operation** of green ammonia synthesis and cracking units, with continuous data collection on performance, stability, and flexibility.
- **Testing under variable loads** to demonstrate compatibility with intermittent renewable energy sources.

2.2.3 Sustainability and Economic Assessment

- **Life Cycle Assessment (LCA):** Quantifies environmental impacts (GHG emissions, resource use) of the new technologies compared to conventional ammonia production.
- **Techno-Economic Analysis (TEA):** Evaluates the levelized cost of ammonia (LCOA), identifies cost drivers, and assesses market competitiveness.

- **Market and societal acceptability studies:** Engage stakeholders and assess readiness for adoption.

2.2.4 Digitalization and Data Management

- **Digital twin and AI tools** are developed for predictive maintenance, process optimization, and catalyst lifetime prediction.
- **Data management plans** ensure open access to research outputs and compliance with FAIR principles.

3 Results and Discussion

3.1 WP1: Optimisation of catalyst for Green NH_3 production

During the reporting period, WP1 of the AMAZE project achieved a significant milestone in catalyst development for green ammonia synthesis. CAS and UCL worked together to progress in a novel catalyst development. The consortium successfully designed and optimized a novel non-critical raw material catalyst, specifically tailored for low-temperature operation (target between 250 and 350°C compared to actual temperature that ranges from 350°C to 500°C). Conventional Haber–Bosch uses a bulk, promoted iron catalyst (iron-oxide–derived Fe with classical promoters such as K_2O/Al_2O_3) optimized for high-T/high-P steady operation, whereas the catalyst family we cite for green/flexible operation is a supported transition-metal system (e.g., Fe–Co on TiO_2/doped-TiO_2) combined with a Li-based hydride promoter (X–H_n, including Li), i.e., a different architecture and promoter concept than fused iron HB catalysts.This new catalyst exhibited a substantial improvement in ammonia productivity at low temperature where Haber Bosch catalyst usually does not work compared to the industrial reference catalyst under relevant conditions of temperature and pressure. The formulation was already patented and produced in different batches demonstrating both its technical viability. In addition, the principal mechanism of catalyst deactivation was identified, and targeted strategies for improved handling and protection are now being implemented. Overall, these results confirm the catalyst's strong potential for pilot-scale demonstration and future industrial application within the AMAZE project.

3.2 WP2: Understanding reaction mechanism on a molecular level

During the reporting period, WP2 of the AMAZE project made substantial progress in the computational modeling and mechanistic understanding of catalysts for both ammonia synthesis and ammonia cracking. The activities were structured around two main objectives: the modeling of NH_3 synthesis catalysts and the modeling of NH_3 cracking catalysts, with a strong emphasis on the integration of density functional theory (DFT), ab initio molecular dynamics (AIMD), and machine learning (ML) approaches. SUPSI and CAS worked mainly in the direction of ammonia synthesis, developing in silico models that are used for further development of the catalyst.

The molecular models are characterized by an integrated framework, utilizing DFT for quantum-mechanical accuracy, AIMD to capture the 500 K thermal fluctuations of the structured multi-component catalyst, and ML to accelerate and interpret atomistic simulations while decode key structural-dynamic features. The strategy involves a sequential pipeline where AIMD trajectories provide data on site persistence and intermediate formation (e.g., NH_2), which are then processed by ML to accelerate the screening and identification between active versus inactive sites. In this framework, Key Performance Indicators (KPIs) include activation energies of elementary steps and N_2 dissociation as well as ammonia desorption energies. These are optimized through the identification of specific active sites that favor the Langmuir–Hinshelwood mechanism, minimizing energy barriers for nitrogen activation while balancing the endothermic desorption of NH_3 to enhance overall turnover frequency.

For ammonia synthesis, the research team focused on single and bimetallic nanoparticles supported on TiO_2. Through extensive AIMD simulations at 500 K, the dynamic behavior of these nanoparticles was characterized, and the translation of these results for the understanding of the catalytic mechanisms. The studies led to the identification of specific active sites, which play a critical role in the adsorption and activation of nitrogen and hydrogen molecules. The research further elucidated the differences in reaction mechanisms among investigated metal nanoparticles, providing a nuanced understanding of their respective catalytic activities. So far, by means of DFT, 41 different configuration of possible active sites have been simulated (10 for Fe, 16 for Cobalt and 15 for Fe-Co alloy nanoparticles).

The mechanistic analysis revealed that the most probable pathway for ammonia formation on these catalysts is the Langmuir–Hinshelwood mechanism, particularly effective on the studied systems. The formation of NH_2 and NH_3 intermediates was mapped out, and the associated activation energies were calculated, offering quantitative insights into the energetics of each elementary step. Additionally, the desorption of NH_3 from the catalyst surface was found to be endothermic, with specific desorption energies determined for various active sites. These findings are significant as they provide a theoretical foundation for the rational design and optimization of next-generation catalysts. Specifically, these finding instruct catalyst synthesis by clarifying which active site should be targeted in order to ensure optimal NH_3 desorption rate.

In parallel, the team developed and trained machine learning models, including graph neural networks, to classify and predict the catalytic potential of adsorption sites based on structural and dynamic features extracted from AIMD trajectories. This approach enabled the identification of active versus inactive adsorption sites, the computation of their occurrence rates and persistence times, and the establishment of correlations with experimentally observed catalytic activity. So far, it has been identified that the N-N bond oscillation and elongation (upon interaction with a specific Fe, Co or Fe-Co adsorption site) is a key catalyst descriptor. If the N-N bond stretches below 1.3 Å, the site is considered at “low activity”. If the N-N bond elongation is between 1.3 Å and 1.4 Å, a “medium” activity pocket is present. Finally, if the stretch exceed 1.4 Å, a “high” activity site is identified. The integration of ML techniques not only accelerated the analysis of large-scale simulation data but also enhanced the predictive power of the modeling framework.

The computational and mechanistic insights derived from WP2 are directly applicable to the optimization of our multi-component catalyst by defining the electronic and structural descriptors required for high turnover frequencies. By leveraging the AIMD-dynamic profiles, the research will allow for the tuning and optimization of the Fe/Co ratio which impact the extent "back-donation" from the metals d-orbitals into the N_2 antibonding (π^*) orbitals. The ML-based identification of active sites will be used to predict how and in which extent the Li compounds (and their weight %) act as electronic promoters by lowering the rate-limiting N_2 dissociation barrier. Furthermore, the quantification of the NH_3 desorption energies will provide a target for optimization: the Li compounds as well as Fe/Co weight % and ratio will be balanced to ensure that while N_2 activation is accelerated, the site does not become "poisoned" by excessively strong ammonia binding.

For ammonia cracking, preliminary modeling activities were initiated, with a focus on screening potential catalyst compositions using AI-driven methods. This work was mainly done by SUPSI and CUT with the support of CAS. The team highlighted the need for further experimental input to guide the selection of suitable alloy elements, particularly for high-entropy alloy systems that may exhibit catalytic performance comparable to noble metals. The modeling of NH_3 cracking mechanisms and the identification of key factors influencing catalyst behavior are ongoing, with the expectation that these efforts will directly support the experimental work in subsequent project phases.

Overall, the results obtained in WP2 have provided a comprehensive mechanistic and computational foundation for the development of advanced catalysts within the AMAZE project. The combination of DFT, AIMD, and ML methodologies has enabled the detailed characterization of active sites, the elucidation of reaction pathways, and the establishment of structure–activity relationships for NH_3 synthesis.

These achievements not only inform the experimental activities in catalyst synthesis and testing but also position the project at the forefront of data-driven catalyst design for sustainable ammonia production and utilization.

3.3 WP3: Optimization of catalyst and technology for NH3 cracking

During the reporting period, WP3 of the AMAZE project achieved significant progress in the development and optimization of catalysts and technologies for ammonia cracking, addressing both thermocatalytic and electrocatalytic approaches. In this work package UNIME and CAS worked together to achieve the WP goals. UNIME was mainly dedicated to the electrochemical cell and catalyst development while CAS dedicated efforts to build and perform experiments on a wide range of conditions in the thermocatalytic ammonia cracking.

. The ammonia cracking catalysts developed within AMAZE differ from conventional industrial solutions primarily in terms of material composition, design objectives and targeted operating conditions. While state-of-the-art industrial crackers largely rely on Ru-based catalysts optimized for high-temperature, centralized hydrogen production, AMAZE investigates thermocatalytic systems based on Ni-, Co- and Fe-containing formulations, including hydrotalcite-derived mixed oxides, as well as multimetallic electrocatalysts supported on carbon. These catalysts emphasize the use of non-critical raw materials, tunable metal-support interactions and scalable synthesis routes. In addition, the inclusion of electrocatalytic ammonia cracking introduces a fundamentally different conversion pathway, potentially enabling operation at lower temperatures and closer to ambient pressure.

These materials were prepared via alkaline co-precipitation, followed by calcination at various temperatures to optimize their structural and catalytic properties. The catalysts underwent detailed physicochemical characterization, including advanced microscopy and diffraction techniques, to confirm their composition, morphology, and phase stability. The results demonstrated the successful formation of stable, single-phase structures, which are essential for robust catalytic performance under industrially relevant conditions. Catalyst are now ready to be tested in CAS Laboratories.

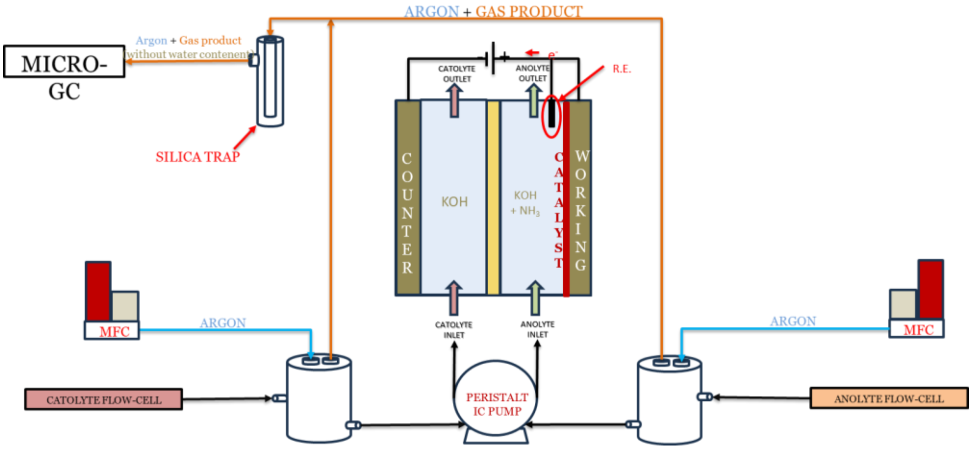

Figure 2: Setup for electrocracking

Parallel efforts were devoted to the development of electrocatalytic systems for ammonia cracking. The team designed and assembled an electrochemical cell equipped with both commercial and custom-prepared electrodes, including high-entropy alloy (HEA) catalysts supported on carbon substrates. The electrochemical setup was optimized for both liquid and gas-phase ammonia feeds, and the analytical system was upgraded to enable precise quantification of hydrogen production and faradaic efficiency. Testing of commercial Pt-Ru catalysts established baseline performance metrics, while subsequent experiments with HEA-based electrodes revealed promising activity for hydrogen evolution, with hydrogen productivity reaching up to 32.41 mmol H_2 per gram of catalyst per minute at 1.6 V versus RHE (Figure 2 and Figure 3).

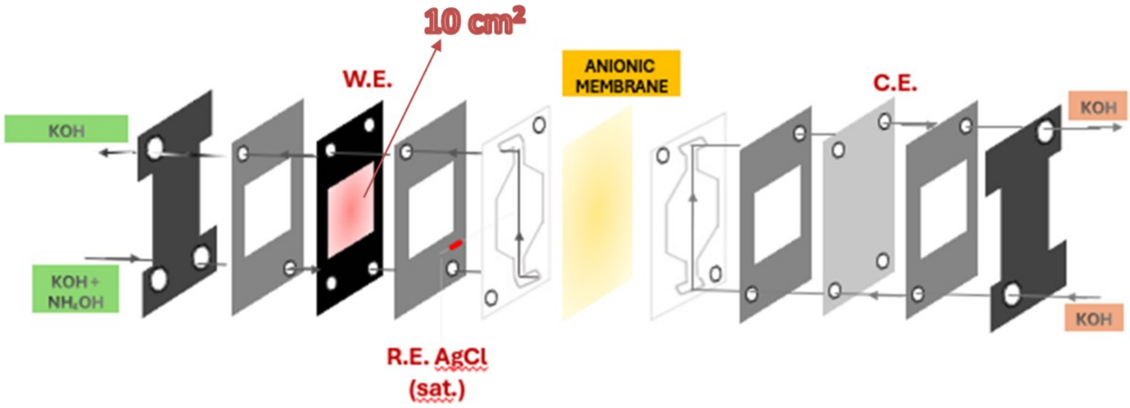

Figure 3:Cell for electrocracking Feeding NH3 (Liquid and gas-phases;4 mm gap)

Throughout the year, three distinct catalyst systems-Pt/C, HEA/C, and NiCo-hydrotalcite-were synthesized and subjected to comprehensive testing. The electrochemical cell and analytical instrumentation were successfully optimized, and the integration of an anionic membrane (Fumasep® FAA-3-50) was demonstrated. The results obtained thus far are directly relevant to the objectives of WP3, as they establish a robust foundation for the scale-up and further refinement of electrocatalytic ammonia cracking technologies. Notably, the project has reached key milestones, including the identification and initial scale-up of catalyst formulations suitable for possible electro ammonia cracking pilot-scale implementation. Notably, the project has reached key milestones, including the identification, synthesis, and initial scale-up of catalyst formulations relevant for electrochemical ammonia cracking. Multiple catalyst systems have been successfully prepared and characterized, including multi-metallic catalysts supported on carbon (5–20 wt%) for electrochemical testing, as well as Ni-based and Ru-based catalysts for ammonia decomposition benchmarks. The electrochemical catalysts have been tested under controlled half-cell conditions (alkaline electrolyte, varying ammonia concentrations, chronoamperometry, chronopotentiometry, and EIS), demonstrating stable operation and reproducible electrochemical behavior in line with literature. In parallel, gram-scale quantities (up to 2–3 g per batch) of selected catalyst formulations have been produced using scalable synthesis routes (e.g. solvothermal synthesis, co-precipitation, wet impregnation), representing an initial scale-up step beyond proof-of-principle. These results provide a robust experimental basis for further evaluation of catalyst performance in larger electrochemical configurations, supporting the feasibility of future pilot-scale electro-ammonia cracking concepts.

. Recent industrial announcements illustrate the rapid maturation of ammonia cracking technologies at large scale. In November 2025, Air Liquide commissioned the world's first industrial-scale ammonia cracking pilot at the Port of Antwerp-Bruges, with a capacity of about 30 t NH_3 per day, demonstrating centralized, high-throughput conversion of ammonia to hydrogen. In parallel, **KBR** reported the selection of its proprietary H2ACT® ammonia cracking technology by Hanwha Impact for a large hydrogen production project in Korea, further highlighting the readiness of conventional high-temperature cracking routes for large, continuous facilities. Topsoe and in several EU Clean Hydrogen / Hydrogen Joint Undertaking projects (e.g. COUPLE), which largely target centralized import terminals and industrial hubs. International assessments, including the IEA Ammonia Technology Roadmap and reviews by the Ammonia Energy Association, consistently note that while thermal cracking at scale is advancing toward deployment, flexible, lower-temperature and decentralized concepts-particularly electrochemical routes-remain at lower TRL and constitute a key research need. Within this context, AMAZE addresses complementary challenges by focusing on flexible thermocatalytic and electrocatalytic ammonia cracking concepts suitable for distributed and smaller-scale applications. Rather than targeting immediate deployment at the hundred-ton-per-day scale, the project emphasizes non-critical-raw-material catalysts, operation over a wide pressure range, exploration of water-assisted and lower-temperature regimes, and electrochemical cracking pathways that could enable ammonia-to-hydrogen conversion closer to ambient conditions. These developments aim to support decentralized hydrogen supply chains and pilot-scale implementations that complement emerging large, centralized ammonia cracking plants.

Thermocatalytic testing was conducted in a dedicated facility capable of operating across a wide range of pressures (1–50 bar) and temperatures (350–700°C), with and without water co-feed. CAS tested ten (10) commercial and pre-commercial catalysts. The results indicated that ammonia conversion increases with temperature, as expected from kinetic and equilibrium considerations, while higher pressures allow for greater volumetric throughput despite a slight reduction in per-pass conversion (Figure 4). Axial temperature profiling along the catalyst bed provided insights into reaction zone localization and heat distribution, highlighting the influence of catalyst composition on reactor performance.

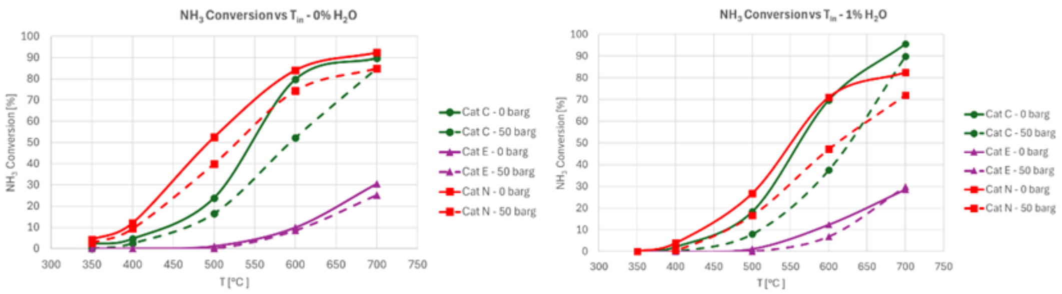

Figure 4: left, performances of three (3) catalysts for ammonia cracking tested at 0 and 50 barg in presence and absence of water at 10k GHSV (h^{-1}) in the temperature range 350-700°C.

In summary, the achievements of WP3 reflect a concerted effort to bridge fundamental catalyst development with applied reactor engineering, ensuring that the technologies under investigation are both scientifically sound and industrially viable. The ongoing work will focus on further optimization of catalyst composition, expansion of testing to additional operating regimes, and preparation for integration into the AMAZE pilot plant. These results position the project to make a substantive contribution to the advancement of sustainable hydrogen production via ammonia cracking.

3.4 WP4: Process Integration and Optimization

During the reporting period, WP4 focused on the systematic integration and optimization of the processes required for both ammonia synthesis and ammonia cracking within the AMAZE pilot system. The initial phase involved a collaborative effort among the project partners to define the technical and operational requirements for the pilot plant. The work was driven by CAS with KAV and HYS. This included specifying the target production and feed capacities (10 kg NH_3 per day for both synthesis and cracking), as well as establishing the maximum operating temperatures and pressures for each process unit (up to 520°C and 100 bar for synthesis, and up to 900°C and 50 bar for cracking).

Following the establishment of these requirements, the team developed comprehensive block-flow and process flow diagrams (BFD and PFD) for the integrated system. These diagrams provided a detailed representation of the process architecture, including all major equipment, streams, and control points. Preliminary heat and mass balances were calculated to support the engineering design phase, ensuring that all energy and material flows were accurately accounted for. Casale built a process model in Unisim steady state of the ammonia loop and cracking . The process flowsheet in Unisim also embedded Casale's proprietary models that enable to calculate the reactor process performance and informed on the reactor catalyst bed sizing. The key process information needed for the process design of the WP4 were generated by the Unisim flow sheet: e.g. energy balances, mass balances, equipment process parameters. These balances were done based on the PFD of the pilot unit –which included all process equipment (synthesis reactor, heat exchangers, coolers, separation columns etc.)– for an overall capacity of 10 kg NH_3 per day for both ammonia synthesis and cracking. All main streams were quantified in terms of mass flow, pressure, temperature and composition. This poses the basis for equipment sizing and selection. Likewise these data will be used for the reactor design. The perimeter of the calculations was agreed upon with KAV and included all required process steps, from the high-pressure gas supply and the main process steps for synthesis/cracking to the post-treatment of the gases needed to reach product quality required for further processing on the industrial site. For the synthesis case, it was agreed with KAV that the ammonia would be diluted with water for further use on-site. This means that the final process product is 40 kg/day ammonia solution (25 wt%). For the ammonia cracking, depending on process conditions, the 5 to 9 kg/day syngas produced (hydrogen and nitrogen mixture) would be vented.

The results of these activities were subsequently communicated to the engineering team responsible for pilot construction, serving as critical inputs for the next stage of the project. The process integration work also emphasized flexibility, with the design accommodating a wide range of catalyst types and operating scenarios. This approach ensures that the pilot plant will be capable of supporting both current and future experimental needs, thereby maximizing its value as a research and demonstration platform.

The process integration activities were executed in accordance with the project timeline and objectives. The collaborative approach facilitated effective alignment between research, engineering, and site operations. The emphasis on flexibility and adaptability in the design is a notable strength, as it allows for the evaluation of various catalyst technologies and process conditions. No significant deviations or issues were reported during this phase, indicating robust project management and technical execution.

Based on the development of detailed PFDs, mass and energy balances, and the steady-state process simulations implemented in Unisim, the evaluation of energy consumption and overall energy efficiency of the integrated ammonia synthesis and cracking pilot system is currently ongoing. The generated process data provide the necessary basis to assess energy demand at unit and system level, and to identify optimization opportunities as the design progresses and operating scenarios are further refined.

3.5 WP5: Construction of Pilot Unit and Safety Evaluation

WP5 advanced the project from conceptual design to initial engineering and preparation for pilot plant construction. The first step involved establishing the design basis in close coordination with the host site, Kavala Novafert. . More specifically, the Design basis agreed upon with Kavala Novafert defines:

- Flows and conditions of feed to be provided to the pilot from the site.
- Flows and conditions to be sent from the pilot back to the site.
    - Importantly the following aspects were already pre discussed with the site:
        - Ammonia produced will be diluted with water to reach a 25%_Wt solution with the advantage that the Site already has this product and a storage tank is located not far from the foreseen installation area. Therefore the ammonia water can simply be sent to this storage tank and mixed with the existing production.
        - Gases at the outlet of the plant will be in any case sent first to a water scrubber to remove most of the ammonia present. The remaining gases will have almost no ammonia and consdiering teh small quantities can be vented to atmosphere in a safe location.
- Norms applicable to the construction of the pilot, which include all European standard from PED, ATEX, Machine Directive etc.
- Weather conditions to be considered for the pilot design.

During a Site visit of CAS to Kavala, an installation area inside the premises of Kavalafert was already identified, which is near all required utilities but nevertheless is not currently a classified area, so the pilot will be only subjected to its own classification and will not impact other installations.

Considering that the temperature hardly ever goes below zero at Kavala, in agreement with the site the choice goes in the direction of an open skid (vs a containerized) because this allows much easier dispersion of potential leakages making it easier to comply with ATEX regulations.

The engineering team proceeded to develop the initial set of Piping & Instrumentation Diagrams (P&IDs), which translated the process flow diagrams into actionable engineering documents. These diagrams detailed all necessary instrumentation, control systems, and auxiliary equipment required for safe and efficient operation. The main auxiliary systems, such as thermal oil heating circuits and deep condensation chillers, were specified to support the isothermal operation of the reactors and ensure precise temperature control.

Conceptual and detailed drawings were produced for both the ammonia synthesis and cracking reactors. The synthesis reactor was designed with significant overcapacity and an isothermal configuration, allowing for the testing of a broad spectrum of catalysts, including those with narrow operating windows or high reactivity. The cracking reactor was designed as an electrically heated tube, capable of reaching the required high temperatures and pressures, and equipped with multipoint temperature control for enhanced safety and performance monitoring.

Throughout this phase, the team maintained a strong focus on safety and compliance with site-specific requirements. The design basis and auxiliary systems were developed to align with the operational protocols of the host site, ensuring seamless integration and minimizing potential risks.

The next step will be for HYS to organize an HAZOP with Kavala and Cas to finalize the P&ID before the procurement can start. The HAZOP will be executed at the site so that all relevant functions of the site can participate..

3.6 WP8: Sustainability Assessment

Task 8.1 Determination of process Sustainability Key Performance Indicators (S-KPIs)

Sustainability Assessment from the process point of view, determining S-KPIs (Sustainability Key Performance Indicators) according to a methodology previously designed. These metrics of sustainability will serve as a guidance for the project life cycle definition and analysis.

During the initial phase of the project, a comprehensive literature review on ammonia synthesis and cracking processes was carried out to select a set of indicators that best characterize both processes. The definition of these indicators followed the sustainability assessment methodology developed jointly by CASALE and UVa, based on the GREENSCOPE framework proposed by Ruiz-Mercado et al. (2012).

The selection of indicators and preparation of the assessment tools were performed following a literature-based methodology. From the literature review, an initial pre-selection of 120 potential indicators was compiled, covering three dimensions and six categories.

1. Environmental dimension: toxicity (toxic potential of chemicals involved and storage requirements) and atmospheric impacts (GWP, liquid and solid waste, and emissions associated with both processes).
2. Performance efficiency dimension: efficiency (reaction efficiency and catalyst performance improvements) and water consumption (fundamental process parameter).
3. Energy dimension: energy and exergy, key categories for monitoring and comparing energy consumption and energy quality, including renewable energy inputs.

The final selection was carried out with input from expert teams for each process. The resulting list includes 22 indicators for the synthesis process and 24 indicators for the ammonia cracking process. Figure 5 presents the selected indicators for both processes.

AMMONIA SYNTHESIS

	ENVIRONMENTAL
	Toxicity
#1_A	Specific toxic potential
#1_B	Specific toxic release/storage
	Atmospheric
#2	Global warming potential
#3	**Atmospheric acidification potential**
#4	Specific solid waste
#5	Specific liquid waste
#6	NOx emission index
	PERFORMANCE EFFICIENCY
	Efficiency
#7	Reaction yield
#8	Solvent and catalyst environmental impact parameter
#9	Recycled material fraction
#10	Product purity
	Water consumption
#11_A	Specific DMW consumption
#11_B	Specific CW consumption
	ENERGY
	Energy
#12	Energy efficiency
#13	Catalyst recovery energy
#14	Renewability energy index
#15	Energy for recycling
#16	Heat-recovery factor
	Exergy
#17_A	Exergy consumption
#17_B	Exergy intensity
#18	Resource exergy efficiency
#19	Renewability exergy index

AMMONIA CRACKING

	ENVIRONMENTAL
	Toxicity
#1_A	Specific toxic potential
#1_B	Specific toxic release/storage
	Atmospheric
#2	Global warming potential
#3	**Atmospheric acidification potential**
#4	Specific solid waste
#5	Specific liquid waste
#6	NOx emission index
#7_A	Ammonia slip – flue gas
#7_B	Ammonia slip – water
	PERFORMANCE EFFICIENCY
	Efficiency
#8	Reaction yield
#9	Solvent and catalyst environmental impact parameter
#10	Recycled material fraction
#11	Product purity
	Water consumption
#12_A	Specific DMW consumption
#12_B	Specific CW consumption
	ENERGY
	Energy
#13	Energy efficiency
#14	Catalyst recovery energy
#15	Renewability energy index
#16	Energy for recycling
#17	Heat-recovery factor
	Exergy
#18_A	Exergy consumption
#18_B	Exergy intensity
#19	Resource exergy efficiency
#20	Renewability exergy index

Figure 5. List of indicators selected for assessing the sustainability of ammonia synthesis and ammonia cracking.

To calculate and assess the sustainability indicators, an indicator-evaluation tool previously developed by CASALE and UVa was adapted to the selected dimensions, categories, and indicators. An inventory of process operation data is extracted from process simulation, currently under development. Includes mass and energy balance information obtained directly from process simulation (test case: Aspen Plus v.14). This sheet can be linked directly to the simulation to enable dynamic assessment. It compiles all inputs required for automatic indicator calculation. The assessment tool contains an executive report that summarizes the overall sustainability assessment results, as well as category- and dimension-level outcomes. It includes indicator values (using weighting and aggregation methods), along with radar plots to enhance visualization and facilitate comparison across dimensions, categories, baseline results and future targets. For each indicator, both the calculated and the normalized values, based on best- and worst-case sustainability limits, are presented.

Next steps

With the tools established, Aspen Plus v.14 simulations are being prepared for the different study cases to test and validate the assessment method. The simulations currently under preparation include:

- Conventional Haber–Bosch ammonia synthesis (baseline), with hydrogen and nitrogen from natural-gas steam reforming
- Conventional Haber–Bosch ammonia synthesis (baseline), with hydrogen from water electrolysis and nitrogen from cryogenic distillation
- Ammonia thermal cracking (baseline)
- Ammonia synthesis at lower temperature and pressure
- Ammonia electro-cracking

This task focuses on conducting a comprehensive Life Cycle Assessment (LCA) to evaluate the environmental impact of the AMAZE concept. The main objective is to identify and minimize contributions such as carbon footprint, resource scarcity and other environmental burdens associated with the ammonia synthesis and cracking processes throughout their life cycle.

During this initial project stage, a literature review was performed to define the objectives, boundaries and scope of the assessment, following the ISO 14040 framework for life cycle analysis. The review included the following key references:

Definition of study boundaries and objectives

The objective of the LCA is to conduct an integrated environmental assessment of the AMAZE proposal and compare it with conventional ammonia synthesis and cracking systems. AMAZE proposal includes green ammonia and hydrogen production using renewable energy sources, non-critical raw material catalysts, and improved operational conditions (lower temperature and pressure), all of which are expected to significantly reduce environmental impacts relative to conventional technologies.

Accordingly, the study adopts a cradle-to-gate scope. Based on the literature review, the functional units were defined as: (1) 1 kg of ammonia produced in the synthesis process, and (2) 1 kg of hydrogen produced in the cracking process.

The system boundaries are illustrated in the accompanying (6). They include construction materials and phases (catalysts included), land use and land occupation, and operation of the synthesis and cracking units. Scenarios for ammonia and hydrogen storage, as well as energy storage to account for renewable energy fluctuations, are also considered.

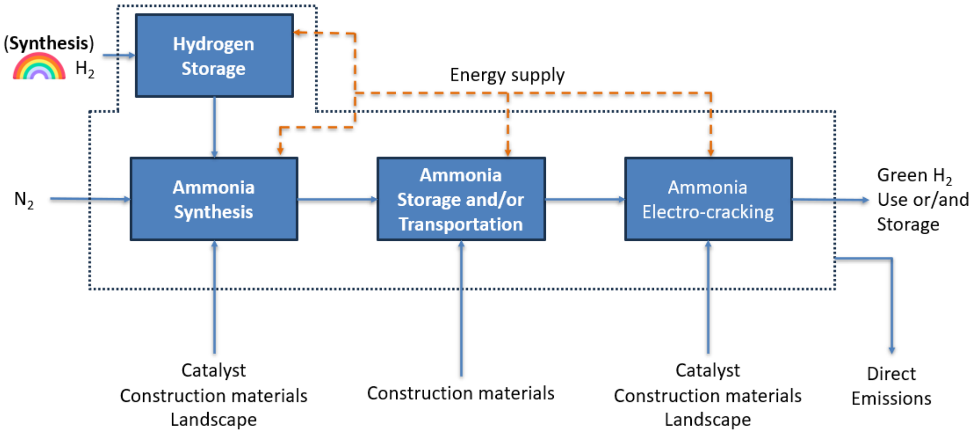

Figure 6: Sketch of boundaries of the study

Inventory

Life cycle inventory data will be obtained from process simulations (mass and energy balances). Inventory elements related to emissions, construction materials and land occupation will be derived from literature. All required background processes will be sourced from Ecoinvent v.2 or v.3, depending on the software version used.

Life Cycle Impact Assessment (LCIA) methodology

The assessment will be performed using SimaPro v7 and v9, with the corresponding Ecoinvent databases for background inventories. For classification and characterization, three widely used LCIA methods will be applied:

a) IMPACT 2002+. Includes, among others, categories such as ozone layer depletion, aquatic ecotoxicity, terrestrial ecotoxicity, land occupation, aquatic acidification, global warming potential and non-renewable energy use.

b) ReCiPe Midpoint (H), European normalization. Includes categories such as climate change, ozone depletion, human toxicity, freshwater acidification, water depletion, and urban/agricultural land occupation.
c) CML 2001 (baseline). Includes categories such as GWP100, acidification, freshwater aquatic ecotoxicity, ozone layer depletion, human toxicity and eutrophication.

Using the three methods allows assessing how methodological choices influence the final results and ensures robustness in the environmental evaluation.

Similarly to how a specific energy-related dimension was included in the process analysis using sustainability key performance indicators (SKPIs) in Task 8.1, special attention will also be given to results related to energy aspects during the life cycle analysis. In this regard, since the IMPACT 2002+ methodology includes a specific category related to energy renewability, this category will be calculated using the aforementioned methodology and included in the study and the final report. Two additional methodologies specifically related to energy aspects will be included: Cumulative Energy Demand (CED) and Cumulative Exergy Demand (CExD). Within the categorization of these methodologies are categories such as renewable and non-renewable energy in the areas of fossil, wind, and solar energy.

Sensitivity Case Studies

The following scenarios are considered for the sensitivity analysis:

a) Hydrogen source (SMR, PEM, other) and nitrogen source
b) Energy source and generation profile
c) Short- and mid-term climate characterization (GWP 10/20/100)
d) Hydrogen and/or ammonia losses (direct emissions)
e) Hydrogen and/or ammonia transport and storage (distance, direct emissions)
f) Water source, consumption and recycling
g) Catalyst material composition and performance (mass and energy balance), lifetime (disposal and/or recycling)
h) Process lifetime
i) LCIA method: ReCiPe Midpoint (H) / IMPACT 2002+ / CML baseline

Preliminary Results

A preliminary analysis was conducted by replicating the results of Vinardell et al. (2023) for ammonia production under different scenarios. This case study was adapted to the life cycle inventory using the Ecoinvent v2 database. The purpose of this preliminary assessment was to obtain an initial theoretical overview of the process and to anticipate the expected variability in the upcoming sensitivity analysis. This exercise also enabled the construction of a preliminary life cycle inventory, which will be further refined and updated once complete information from the AMAZE process design becomes available.

The case study by Vinardell et al. (2023) evaluates ammonia production via the conventional Haber–Bosch process with three different hydrogen sources:

a) Steam methane reforming using natural gas,

b) Water electrolysis powered by onshore wind electricity, and

c) Water electrolysis powered by solar photovoltaic (PV) electricity.

As shown in theFigure 7, the results indicate that the substitution of the electricity mix with renewable energy for hydrogen production can reduce the global warming potential (GWP) by more than 50%. In other words, switching the hydrogen source from grey to green leads to a reduction in the overall climate impact of up to 50%.

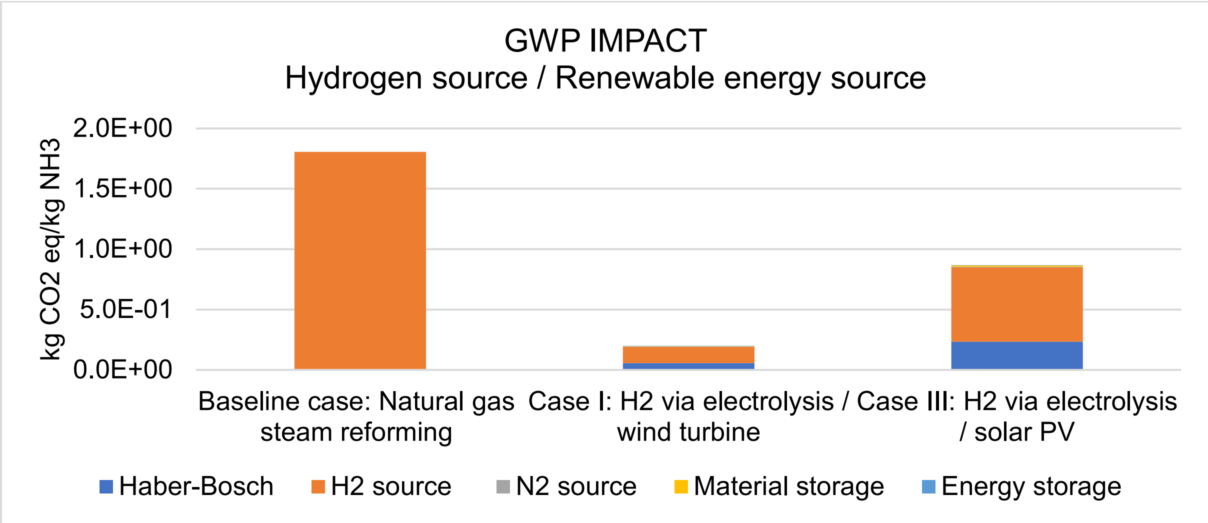

Figure 7: CO_2-equivalent emissions (kg CO_2eq per kg NH_3) for Haber–Bosch ammonia synthesis using three hydrogen sources: natural gas steam reforming, wind-powered electrolysis, and solar PV-powered electrolysis analyzed from Vinardell et al.

A more detailed analysis of the contribution of each process to the overall impact revealed that the largest share of the GWP in the baseline scenario is associated with the emissions generated during hydrogen production via natural-gas steam reforming, as well as the emissions arising in the ammonia synthesis unit as a consequence of the hydrogen source. Conversely, for the ammonia synthesis scenarios using renewable energy, the emissions, although substantially lower than those of the conventional process, are primarily linked to the energy generation stage (Figure 8).

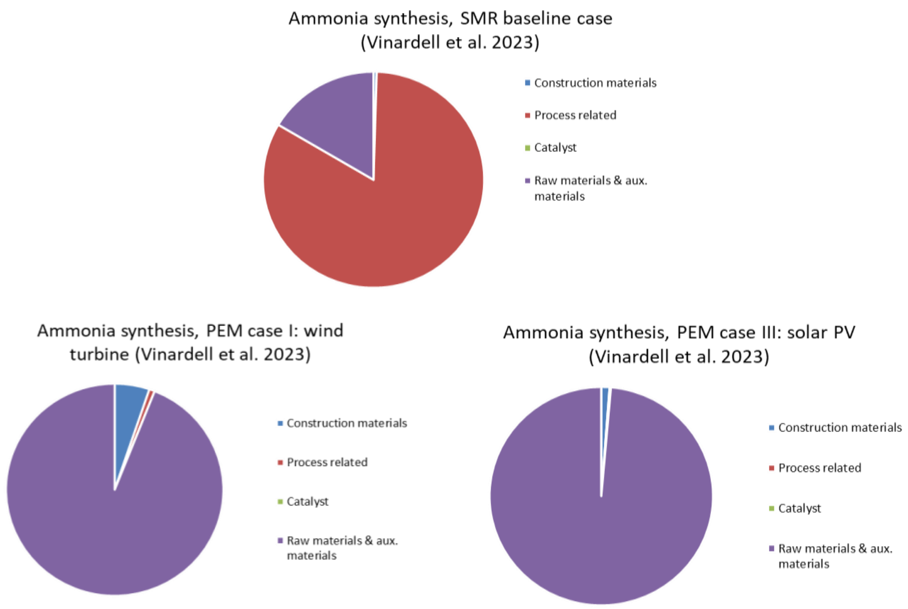

Figure 8: "Analysis of the contributions from construction materials, processes, catalysts, and raw materials to the global warming potential (GWP) for three scenarios for the NH_3 production: H_2 from steam methane reforming, H_2 from electrolysis powered by wind turbines, and H_2 from electrolysis powered by photovoltaics."

Next Steps

With the simulations generated for the calculation of sustainability indicators under Task 8.1, the next step will be to conduct the full LCA evaluation of the different study cases defined in Task 8.1, applying the three methodologies selected for the sensitivity analysis. Additionally, using the ReCiPe Midpoint (H) method, a preliminary assessment of the various sensitivity scenarios will be performed. These steps will provide an initial theoretical evaluation of the environmental impacts associated with the AMAZE proposal. These evaluations will consider and analyze all impact categories included in the selected methodologies, ensuring that impacts beyond global warming potential are also incorporated and assessed.

4 Conclusions and outlook

4.1 Conclusions

The AMAZE project has made substantial progress toward its goal of developing and demonstrating innovative, sustainable technologies for green ammonia synthesis and cracking. Over the first project period, the consortium has successfully:

- Developed and optimized a novel, non-critical raw material catalyst for low-temperature ammonia synthesis, achieving significant improvements in productivity and validating the formulation at both laboratory and pre-industrial scales.
- Advanced the mechanistic understanding of catalyst behavior through a combination of computational modeling (DFT, AIMD, ML) and experimental validation, providing a robust foundation for rational catalyst design.
- Designed, synthesized, and tested new catalyst systems for both thermocatalytic and electrocatalytic ammonia cracking, with promising results in terms of hydrogen productivity and operational stability.
- Completed the engineering design, site preparation, and permitting for the pilot plant, ensuring readiness for installation and operation in a relevant industrial environment.
- Established a comprehensive methodology for sustainability assessment, including the definition of process KPIs and the initiation of life cycle analysis, to quantify the environmental and economic benefits of the AMAZE technologies.
- Maintained effective international collaboration among industrial and academic partners, ensuring that all work packages are progressing according to schedule and within budget.

The project has met all major milestones and deliverables to date, with no significant deviations or budgetary concerns reported. The integrated approach combining fundamental research, process engineering, pilot demonstration, and sustainability assessment, positions AMAZE as a leading initiative in the transition to green ammonia and hydrogen technologies.

4.2 Outlook

Building on the achievements to date, the next steps for the AMAZE project will focus on:

1. **Pilot Plant Operation and Data Collection:**
    - Develop detailed engineering of the pilot, perform HAZOP with site, procure all equipment, build pilot, execute FAT.
    - Complete the installation and commissioning of the pilot plant at Kavala Solutions.

- Operate the pilot under real industrial conditions to validate the performance of the integrated synthesis and cracking technologies.
- Collect and analyze operational data, including catalyst stability, process efficiency, and hydrogen/ammonia yields.

2. **Advanced Testing and Optimization:**
   - Continue the optimization of catalyst formulations, particularly addressing issues of air/moisture sensitivity and mechanical stability.
   - Expand testing to additional catalyst compositions and operating regimes, including both thermocatalytic and electrocatalytic systems.
   - Refine the digital twin and AI-based tools for process monitoring, predictive maintenance, and lifetime prediction.
3. **Sustainability and Economic Assessment:**
   - Finalize the life cycle assessment (LCA) and techno-economic analysis (TEA) for the pilot-scale processes.
   - Benchmark the AMAZE technologies against conventional and emerging alternatives, quantifying reductions in greenhouse gas emissions and improvements in cost-effectiveness.
4. **Dissemination, Stakeholder Engagement, and Exploitation:**
   - Intensify dissemination activities, including scientific publications, conference presentations, and stakeholder workshops.
   - Engage with industry stakeholders and potential end-users to demonstrate the technology and gather feedback for future scale-up.
   - Prepare business models and exploitation plans to support the commercialization and broader deployment of AMAZE solutions.
5. **Reporting and Knowledge Sharing:**
   - Continue regular reporting to the CETPartnership Knowledge Community and other relevant bodies.
   - Share data, methodologies, and best practices with the broader research and industrial community to maximize impact.

5 National and international cooperation

The AMAZE project is founded on a strong framework of international cooperation, bringing together a consortium of leading industrial and academic organizations from across Europe. The partnership includes:

CASALE SA (Switzerland) – Project coordinator, responsible for process engineering, pilot plant design, and overall project management.

Clariant (CLA, Switzerland/Germany) – Industrial partner specializing in catalyst manufacturing, scale-up, and benchmarking.

HySytech (HYS, Italy) – Engineering company in charge of the design, construction, and commissioning of the pilot plant.

Kavala Solutions (KAV, Greece) – Industrial end-user and host site for the pilot demonstration, providing operational feedback and validation.

CIECH (Poland) – Chemical industry partner contributing industrial requirements and supporting technology validation.

Universitè Catholique de Louvain (UCL, Belgium) – Academic partner leading catalyst development and laboratory-scale testing.

Cracow University of Technology (CUT, Poland) – Academic partner specializing in computational modeling and mechanistic studies.

SUPSI (Switzerland) – University of Applied Sciences contributing molecular modeling and machine learning expertise.

Università di Messina (UNIME, Italy) – Academic partner focused on catalyst and electrochemical cell development for ammonia cracking.

Universidad de Valladolid (UVa, Spain) – Academic partner responsible for sustainability assessment and life cycle analysis.

P2X Analytics (US) – Specialist in techno-economic analysis and process optimization.

OST (Switzerland) – Partner providing digital twin modeling and process simulation support.

The collaboration among these partners is highly integrated and multidisciplinary. Academic institutions lead the fundamental research and modeling activities, designing and optimizing new catalyst formulations and reaction mechanisms. Industrial partners, such as Clariant and CASALE, are responsible for scaling up these innovations, conducting benchmarking under industrial conditions, and ensuring that the developed technologies are suitable for real-world application.

Engineering and technology providers, including HySytech, P2X Analytics and OST, work closely with both academic and industrial partners to translate laboratory-scale advances into pilot-scale demonstrations. This involves joint development of process flow diagrams, instrumentation, and digital tools, as well as shared responsibility for safety, commissioning, and operational validation.

End-users such as Kavala Solutions and CIECH play a crucial role by providing practical feedback, hosting the pilot plant, and ensuring that the solutions developed are aligned with market and regulatory requirements. Regular consortium meetings, technical workshops, and collaborative work packages facilitate open communication, knowledge exchange, and coordinated progress across all participating countries.

This international and cross-sectoral collaboration ensures that the AMAZE project benefits from a wide range of expertise, accelerates technology transfer, and maximizes the relevance and impact of its innovations for the European and global transition to sustainable ammonia and hydrogen technologies.

6 Publications and other communications

7 References

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