

Supplementary Table S1 presents a structured and comprehensive quantitative dataset of all modelling studies included in this systematic review. To enhance clarity and readability, the dataset is organised into two complementary sections: **S1A**, which focuses on classification and modelling methodology, and **S1B**, which summarises catalyst systems, operating conditions, model parameters, and reported performance indicators. **Supplementary Table S1A** documents the ammonia decomposition pathway, modelling category (e.g., reactor-scale CFD, kinetic/microkinetic, multi-scale, thermodynamic/exergy-based), and key modelling assumptions adopted in each study. This section enables systematic comparison of modelling frameworks, computational scope, and assumptive conditions such as steady-state operation, equilibrium constraints, simplified heat-transfer treatment, or idealised transport behaviour.

Supplementary Table S1B compiles catalyst systems, operating temperature and pressure ranges, principal model parameters investigated (e.g., membrane permeance, plasma power, residence time, heat supply mechanism), and reported performance indicators such as ammonia conversion, hydrogen yield, space-time yield, or efficiency metrics. This section enables cross-study benchmarking of catalytic trends, operating envelopes, and performance reporting practices.

Supplementary Table S1A. Ammonia Decomposition Pathway, Modelling Category and Key Assumptions

	DOI	Modelling Category	Decomposition Category	Key Assumptions
1	10.1016/j.ces.2024.120439	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Integration of renewable electrical heating can replace fossil-based heat without compromising process integrity; assumes stable operation under electrified heating
2	10.1016/j.cattod.2024.114863	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Steady-state conditions in microchannel flow, Ideal gas behavior for NH ₃ and H ₂ , Uniform catalyst properties (thickness, porosity) across channels, Negligible radiation effects, Reaction kinetics governed

				by surface catalytic decomposition.
3	10.1021/acscatal.4c04415	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Adsorbed nitrogen migration into bulk dominates over recombinative desorption FeO-based bulk catalyst structure and active sites represented in MD simulations
4	10.1016/j.cej.2024.151875	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Renewable energy supply for operation, ideal PSA separation performance, integration of H2 off-gas to additional units, steady-state operation
5	10.1002/cite.202300166	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Surrogate model approximates detailed CFD results; integration assumes effective heat transfer from tail gas combustion; endothermic and exothermic reactions are coupled in reactor model
6	10.1016/j.fuel.2023.130243	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Idealized thermal behavior and catalyst distribution; reactor treated as optimized via heater positioning; comparative

				baseline cases assumed standard heat supply.
7	10.1016/j.memsci.2023.122345	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	No correlation fitting; all material properties obtained from experiments or tabulated data; emissivity included as an assumption
8	10.1016/j.jelechem.2023.118001	Generalized / Dimensionless / Conceptual Modelling	Electrocatalytic	The SOFC model assumes steady-state operation, ideal gas behavior for 9 reactants/products, and thermally coupled ammonia decomposition and electrochemical reactions. Validation shows less than 5% deviation from experimental data in the literature, suggesting simplified but accurate representation of physical processes.
9	10.1016/j.fuel.2023.129591	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	The model assumes steady-state operation under solar irradiation; uniform solar flux on reactor surface; consistent membrane permeation properties; constant inlet ammonia

				properties; and neglects re-radiation loss changes when channels increase.
10	10.1016/j.ces.2023.119449	Kinetic / Thermochemical Mechanism Modelling	Plasma-Catalytic	Assumes steady-state reaction kinetics; plasma activation treated as modifying reaction rates; catalyst surface reactions characterized using kinetic models; thermal and plasma modes compared under controlled laboratory conditions.
11	10.1016/j.cej.2023.147578	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	The model assumes a simplified equation set to compute effect of diffusional limitation by incorporating catalyst physical parameters (size, pellet geometry) rather than full detailed micro-scale modelling; the heterogeneous reaction kinetics + diffusion limitation are embedded in the CFD domain.
12	10.1016/j.apcatb.2023.123234	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Assumes steady-state reaction kinetics for evaluating catalyst

				performance; surface oxygen vacancies (OVs) influence N and H recombination/desorption; constant flow rate during experiments.
13	10.1002/cssc.202202370	Kinetic / Thermochemical Mechanism Modelling	Plasma-Catalytic	Steady-state plasma-catalytic operation; effect of catalyst support and plasma discharge incorporated into reaction kinetics; fixed space velocity and power input.
14	10.1016/j.fuel.2023.129320	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Steady-state reaction kinetics for experimental evaluation; DFT used to model adsorption/desorption and reaction energy barriers; nitrogen binding strength as descriptor for activity.
15	10.1016/j.cej.2023.145661	Generalized / Dimensionless / Conceptual Modelling	Thermocatalytic / Thermal Catalytic	Not specified; likely assumptions inherent to catalytic and reactor models (steady state, ideal flows).
16	10.1016/j.cej.2023.144623	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Enthalpy–entropy constraints were applied during model fitting. The

				model assumes elementary reaction steps and surface coverages can be described kinetically.
17	10.1021/acs.energyfuels.3c00760	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Not specified in abstract; likely assumptions relate to idealized mass transfer, membrane selectivity, and reactor kinetics.
18	10.1021/acs.energyfuels.3c01348	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Permeation of H ₂ and N ₂ follows Arrhenius behavior; reaction kinetics described using activation energy for NH ₃ decomposition; uniform catalyst distribution; ideal gas behavior
19	10.1016/j.fuel.2023.127879	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Validation against experimental data; use of Temkin–Phyzev kinetics; intermediate heating system considered; steady-state operation assumed
20	10.3390/catal13060920	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Steady-state operation; ideal H ₂ permeation through Pd-Ag membrane; mechanical stability and sealing considered in design; membrane

				selectivity and permeability assumed constant for H ₂ /N ₂ separation
21	10.1039/d3ra01596c	Generalized / Dimensionless / Conceptual Modelling	Thermocatalytic / Thermal Catalytic	Steady-state operation of membrane reactor; ideal selectivity for H ₂ permeation; negligible concentration polarization due to air bubbling ELP; uniform Pd layer thickness
22	10.1016/j.cej.2023.142474	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Vertically standing 2D support prevents nanoparticle sintering and aggregation; high flow rates do not significantly affect nanoparticle distribution; reaction occurs under steady-state conditions
23	10.1039/d3cy00055a	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Rate-determining steps derived from ab initio calculations; minimal parameter modification from theoretical values for fitting experimental data
24	10.1039/d2re00408a	Generalized / Dimensionless / Conceptual Modelling	Thermocatalytic / Thermal Catalytic	Agnostic (generalized) dimensionless model; kinetic and permeation

				parameters assumed representative for lab-made catalysts; reactor considered isothermal and non-isothermal scenarios
25	10.1016/j.cej.2022.141203	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Steady-state operation; reactor heated via electromagnetic induction using renewable electricity; cost assumptions for CAPEX/OPEX; ammonia feed and process scale impact LCOH
26	10.52292/j.laar.2023.1090	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	(1) Complete selectivity of the Pd–Ag membrane (100 % hydrogen selective). (2) Steady-state operation at moderate pressure (8 bar). (3) Total ammonia conversion achievable via equilibrium shift due to H ₂ removal. (4) Catalytic combustion of the retentate stream provides sufficient heat for the endothermic reaction (no external heating source).
27	10.3390/pr9122275	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Competitive adsorption of NH ₃ considered;

				adsorption-inhibition effects included; model focused on steady-state multiplicity; no Hopf bifurcation expected; simplified mixed model approach.
28	10.1016/j.apcatb.2021.119896	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Dehydrogenation of adsorbed ammonia is the rate-limiting step. Ammonia decomposition is inhibited by H ₂ . Surface reaction kinetics follow LHHW mechanism.
29	10.1016/j.cej.2021.128595	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Microreactor operates under kinetic-control conditions with negligible mass transfer resistance; CFD model assumes the kinetic rate expressions accurately represent the catalyst performance.
30	10.1016/j.fuel.2020.119111	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Assumes ideal thermochemical equilibrium; exhaust gas composition follows GDI engine conditions; Rh-Pt catalyst provides full

				conversion under these conditions.
31	10.1016/j.cherd.2020.11.004	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	heat transfer limitations are significant; NH ₃ supply rate can be controlled to achieve target conversion; packed-bed multi-tube configuration is feasible for industrial scale.
32	10.1016/j.memsci.2020.118483	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Membrane separation performance and H ₂ recovery modeled assuming efficient sweep gas operation; steady-state operation of membrane reactor; ideal mass transfer enhancement from steam sweep.
33	10.1021/acssuschemeng.8b06065	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	The model assumes first-order kinetics for ammonia decomposition due to efficient hydrogen removal through the Pd membrane. It also assumes idealized membrane permeation behavior and negligible transport resistances, as the catalyst and membrane were in intimate contact.

				Equilibrium constraints were bypassed through continuous H ₂ removal.
34	10.1016/j.cattod.2017.05.018	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Reactor channels assumed to allow effective heat transfer from exothermic to endothermic reactions. Flow uniformity and autothermal balance were assumed achievable under selected ammonia and combustible feed flow rates.
35	10.1007/s11814-018-0037-5	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Reactor models assume ideal behavior with H ₂ permeation described by membrane permeance; experimental kinetics accurately describe catalytic behavior; He sweep gas flow and temperature are controllable and uniform.
36	10.1007/s11051-018-4253-z	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	The 13-core/42-shell atom model (~1 nm) represents the nanoparticles; DFT calculations assume idealized nanoparticle geometries; surface

				reactions and N_2 desorption are modelled in vacuum or idealized conditions.
37	10.1016/j.jksues.2016.01.002	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Membrane plays a dominant role in shifting thermodynamic equilibrium; diffusion limitation confined to entrance region; inter-stage heating and fresh sweep gas used.
38	10.1252/jcej.14we431	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	The rate-limiting steps are catalyst-specific: recombinative $N_{2\text{}}$ desorption on Ru, $NH_{3\text{}}$ dehydrogenation on Ni. Elementary reaction steps are kinetically important and govern overall rates.
39	10.1039/c6cy01566b	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Rate-limiting steps influenced by catalyst composition; $H_{2\text{}}$ poisoning affects active sites; addition of Co, Ni, or

				Fe modifies recombinative N desorption and activity.
40	10.1021/jacs.5c15789	Multi-Scale / Cross-Scale Modelling	Plasma-Catalytic + Membrane-assisted integration	Membrane selectivity arises from adsorption-driven molecular sieving; MD captures preferential adsorption behavior governing NH ₃ /H ₂ and NH ₃ /N ₂ separation; plasma enhancement effectively lowers kinetic barriers compared to purely thermal catalysis
41	10.1002/aic.18781	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Catalyst particles are represented through effective porosity and pore-size parameters; reactor behaviour is assumed to be governed by coupled reaction kinetics and heat flux; segmentation allows decoupling of reaction rate and thermal gradients.
42	10.1002/aic.70187	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Reaction kinetics can be represented by rate expressions where N ₂ recombinative desorption is the rate-determining step; DFT accurately

				captures the effect of lattice strain on electronic structure and activation energies.
43	10.1016/j.applthermaleng.2025.128142	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	Realistic solar flux distributions were applied; steady-state operation implied; porous catalyst bed assumed with uniform properties; hydrogen selectively permeable membrane with defined permeability; no catalyst deactivation or heat losses beyond modeled radiation mentioned.
44	10.1016/j.seppur.2025.133723	Generalized / Dimensionless / Conceptual Modelling	Thermocatalytic / Thermal Catalytic	1. Idealized catalyst surface models (Ru and CeO ₂ interface). 2. Static adsorption and reaction pathways considered without dynamic reactor effects. 3. Electron transfer effects dominate catalytic performance. 4. No heat or mass transport limitations included.
45	10.1016/j.tsep.2025.104229	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Steady-state thermodynamic cycle

				analysis; ammonia decomposition driven by exhaust heat; hydrogen concentration in reformed gas up to 75%; comparison between CRCCGT and CCGT under similar operating conditions.
46	10.1021/acs.energyfuels.5c03995	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	1. Idealized catalyst surface used for DFT. 2. Static adsorption and reaction pathways considered. 3. Spin-state of Co influences adsorption and activation energy. 4. No heat/mass transport or reactor dynamics included.
47	10.1016/j.fuel.2025.135558	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	1. Steady-state reactor operation in the fixed-bed reactor. 2. Uniform heat and mass transfer in simulation. 3. Catalyst dispersion and pore structure assumed to influence activity in a predictable manner.
48	10.1021/acs.energyfuels.5c03034	Kinetic / Thermochemical Mechanism Modelling	Plasma-Catalytic	1. Reactor follows Temkin–Pyzhev kinetics. 2. Plasma and thermal effects can be

				superimposed in the model. 3. Energy flow analysis assumes steady-state operation. 4. Space velocity and plasma power are primary variables controlling performance.
49	10.1016/j.cej.2025.166903	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	1. CFD assumes steady-state flow and uniform catalyst coating. 2. Mass transfer limitations can be captured via concentration polarization coefficients (CPC). 3. Hydrogen extraction is driven by permeation through Pd membranes. 4. Porosity and baffles affect transport and reaction coupling.
50	10.1016/j.jcat.2025.116339	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	1. Free energy descriptors (NH_3 dissociation and N_2 adsorption energies) govern catalytic performance. 2. Correlation between electronic descriptors and turnover frequency is valid. 3. Catalyst surface structure

				remains stable under reaction conditions.
51	10.1007/s11814-025-00508-y	Thermodynamic, Energy & Exergy-Based Modelling	Thermocatalytic / Thermal Catalytic	1. Hydrogen conversion follows equilibrium thermodynamics. 2. Waste heat and cold energy recovery is feasible. 3. System is modelled under steady-state operation. 4. Energy distribution can be optimized via multi-objective criteria.
52	10.1016/j.fuel.2025.135311	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	DFT assumes idealized surfaces and active site models to calculate energy barriers; CoN and Co NP sites represent main catalytic sites.
53	10.3390/catal15090811	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Models assume idealized reactor conditions and typical kinetic parameters; catalyst activity is generalized based on literature.
54	10.1016/j.cherd.2025.07.044	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Nitrogen desorption is a rate-determining step; models assume idealized reactor and catalyst behavior; kinetic

				parameters are derived from experimental fitting
55	10.1016/j.ces.2025.121906	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Reactor operates under steady-state; diffusion and thermal transfer dominate reactor efficiency; washcoated SiSiC foam mitigates diffusion limitations.
56	10.1021/acs.energyfuels.5c01442	Reactor-Scale Numerical & CFD Modelling	Plasma-Catalytic	Assumes reaction mechanisms can be captured from molecular to reactor scales; models integrate kinetic and thermodynamic effects for decomposition efficiency and H ₂ separation.
57	10.1016/j.applthermaleng.2025.126172	Reactor-Scale Numerical & CFD Modelling	Photothermal	Non-uniform solar heat flux considered; fixed-bed reactor; reactor geometry and solar irradiation dominate temperature profile
58	10.1002/aic.18781	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Catalyst particle characteristics (porosity, pore diameter) affect reactor size and temperature profile; two-stage segmented reactor

				balances heat flux and reaction rate
59	10.1016/j.mcat.2025.115016	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Hydrogen inhibition affects N recombination and desorption; alkaline earth metal promoters enhance basicity and electron density around active sites
60	10.3390/catal15050488	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Kinetics of ammonia decomposition can be described by chosen models; space velocity and temperature are primary factors controlling conversion
61	10.1007/s10562-025-04992-z	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Rate-determining step occurs on Ru(0001) surface; activation barrier of first NH ₃ dehydrogenation governs kinetics.
62	10.1016/j.memsci.2025.124020	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Membrane selectivity and positioning significantly influence hydrogen flux; idealized H ₂ /N ₂ selectivity used as a model parameter
63	10.1039/d4cc06382a	Generalized / Dimensionless / Conceptual Modelling	Plasma-Catalytic	Machine learning models can simulate reaction mechanisms and predict high-performance

				catalysts; reduces trial-and-error experiments.
64	10.1016/j.combustflame.2025.113992	Reactor-Scale Numerical & CFD Modelling	Thermocatalytic / Thermal Catalytic	Local fuel composition variations and differential diffusion are captured; analytically reduced chemistry is valid for reactive LES; multi-fuel injection effects can be approximated by mixture fraction transport.
65	10.1016/j.fuel.2024.134043	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Bridge site adsorption is the most stable on Ru; rate-determining step is N ₂ formation; low Ru loading is sufficient; metal-support interactions dominate activity
66	10.1016/j.cej.2025.159443	Reactor-Scale Numerical & CFD Modelling	Plasma-Catalytic	Plasma and thermal decomposition pathways can be combined; quasi-1D reactor geometry; key reactions dominate H ₂ production and NH ₃ consumption.
67	10.1021/acssuschemeng.4c08899	Reactor-Scale Numerical & CFD Modelling	Plasma-Catalytic	Excess heat from the plasma reactor can support thermocatalytic ammonia cracking; lab-scale catalyst

				behavior representative for modeling
68	10.1021/acscatal.5c04795	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Dynamical lateral interactions on catalyst surface are fully accounted for; nitrogen recombination is the rate-determining step; FeCo alloying effects are represented at atomic scale.
69	10.1021/acscatal.5c01829	Kinetic / Thermochemical Mechanism Modelling	Thermocatalytic / Thermal Catalytic	Field-dipole interactions enhance reaction rates; NH dehydrogenation over Ru(1013) is rate-limiting step; turnover frequency as a key performance metric
70	10.1039/c5ra07818k	Multi-Scale / Cross-Scale Modelling	Thermocatalytic / Thermal Catalytic	Surface geometry and electronic structure determine active sites; defective surfaces influence adsorption energies and reaction barriers; NH ₃ adsorption follows energetically favorable paths

Supplementary Table S1B. Operating Conditions, Catalyst Systems, Model Parameters, and Performance Indicators

	DOI	Operating Conditions	Catalyst Systems	Main Parameters Tested	Key Findings
1	10.1016/j.ces.2024.120439	400-700°C		Reactor configuration type; heating mode (programmed/electrified vs. conventional); integration with renewable power input.	Electrified reactors can provide endothermic heat for ammonia decomposition using renewable energy, Demonstrated technical feasibility for hydrogen recovery while maintaining reactor/process integrity, Suggests potential for decarbonization of hydrogen supply chain through electrified thermal systems.
2	10.1016/j.cattod.2024.114863	701–722 K (≈428–449 °C)		Feeding velocity (0.2–2.5 m/s, Reaction temperature, Feeding temperature, Substrate material (thermal conductivity), Catalyst coating thickness and porosity	NH ₃ decomposition feasible in millisecond contact times in microchannel reactors. Increasing feeding velocity enhances H ₂ yield (0.549 → 2.213 mol H ₂ ·g ⁻¹ ·h ⁻¹) but reduces NH ₃ conversion (98.6% → 80.8%). High thermal conductivity materials improve

					performance but increase flow resistance. Optimized catalyst coating (thickness and porosity) minimizes transport limitations and maximizes catalyst utilization. Demonstrates effective reactor design guidelines for efficient CO_x-free hydrogen production.
3	10.1021/acscatal.4c04415	Not stated	Fe-based	Nitrogen migration and storage in bulk catalyst Stepwise formation and decomposition of Fe nitrides ($\text{Fe} \rightleftharpoons \text{Fe}_4\text{N} \rightleftharpoons \text{Fe}_2\text{N}$)	Fe₄N decomposition to Fe + N₂ is the rate-determining step (activation energy ~172–173 kJ/mol) MD simulations reveal that nitrogen migration into bulk affects N₂ release Provides insights into bulk Fe-based catalyst behavior under NH₃ decomposition conditions
4	10.1016/j.cej.2024.151875	400–600 °C	Pd	Process configuration (integration of PEMFC, SOFC, Pd membrane, burner), hydrogen production efficiency, thermal and exergy efficiency, levelized cost of hydrogen, CO₂ emissions	Pd membrane integration yields highest thermal and exergy efficiency; PEMFC integration provides lowest hydrogen LCOH; overall process allows carbon-free hydrogen production with

					improved thermodynamic and economic performance
5	10.1002/cite.202300166	400–700 °C		Reactor geometry, heat integration effectiveness, process efficiency metrics	The integrated reactor concept improves energy efficiency by using tail gas heat; the multi-scale modeling approach allows efficient evaluation and optimization compared to conventional reactor designs
6	10.1016/j.fuel.2023.130243	Not stated		Heater configuration (EH-AD, WAH-AD, NGH-AD), heater position, operating conditions (for optimization of conversion and thermal behavior)	EH-AD configuration significantly improves ammonia conversion and hydrogen yield compared to conventional heating; near 100% conversion achievable; up to 70.8% increase in H ₂ yield over NGH-AD.
7	10.1016/j.memsci.2023.122345	450–530 °C/ 0–0.4 MPa trans-membrane pressure		Geometry of membrane fittings, trans-membrane pressure, temperature, gas hourly space velocity (375–620 h ⁻¹), 16 design variables explored	Model predicts NH ₃ conversion (max 99.9%), H ₂ recovery (max 88%), and hydrogen purity (>99.8%) accurately; heat transfer and radial diffusion critical; including purity is rare and valuable for modeling
8	10.1016/j.jelechem.2023.118001	Simulations discuss temperature gradients within the		Operating voltage, inlet temperature, fuel flow rate, and ammonia pre-reforming degree were sys-	The model achieved <5% deviation from experimental results, confirming accuracy.

		SOFC, reporting temperature differences of 22 K to 167 K		tematically varied to study their effects on power density, temperature distribution, and heat balance.	A peak power density of 66.4 mW/cm ² was obtained at 0.45 V. Increasing inlet temperature and fuel flow rate enhanced efficiency but also increased temperature gradients. Adjusting ammonia pre-reforming degree significantly improved temperature uniformity — with a maximum temperature difference of only 22 K at 96% pre-reforming, compared to 167 K in direct ammonia feed. The study emphasizes optimizing pre-reforming to balance heat and electrochemical performance.
9	10.1016/j.fuel.2023.129591	multichannel reactors was about 47 °C, but the absolute temperature range is typically around 400–600 °C for Pd membrane ammonia decomposition		Number of membrane channels (1 to 6), catalyst volume (decreasing and increasing scenarios), and membrane permeation area.	Increasing the number of membrane channels enhances heat and mass transfer efficiency, leading to improved conversion. A six-channel reactor achieved 0.76 conversion, compared to 0.49 for a single-channel reactor under identical conditions. The temperature uniformity also improved (47 °C lower

					temperature difference), beneficial for Pd membrane stability.
10	10.1016/j.ces.2023.119449	~400–600 °C for thermal catalysis		Catalyst type (monometallic: Fe, Co, Ni, Mo; bimetallic: Fe-Co, Mo-Co, Fe-Ni, Mo-Ni), reaction mode (thermal vs plasma). Temperature-programmed surface reaction used to study kinetics.	Fe-Co catalyst is most active under thermal catalytic mode; Fe-Ni is best under plasma catalysis. Shows discrepancy between optimal catalysts for thermal and plasma NH ₃ decomposition. Kinetic factors and catalyst composition strongly affect hydrogen production performance.
11	10.1016/j.cej.2023.147578	inlet gas temperatures		Inlet gas temperature and catalyst pellet size were varied in the parametric study.	The proposed model is validated successfully for both steam-methane reforming and ammonia decomposition; the approach allows cost-effective 3-D CFD of large scale reactor systems with heterogeneous catalysts including internal diffusion effects; the parametric study gives insight into how catalyst size and feed temperature impact local transport phenomena and

					thermodynamic state in the SOFC hotbox system.
12	10.1016/j.apcatb.2023.123234	450 °C	Ru-based	Catalyst type (Ru/CeX/MgAl ₂ O ₄), Ce loading, calcination temperature, flow rate, reaction temperature, exposure time for stability.	Ru/Ce ₅ /MgAl(600) catalyst achieved high H ₂ formation rate (27.4 mmol H ₂ ·gcat ⁻¹ ·min ⁻¹) and stable performance after high-temperature exposure; CeO ₂ surface OVs enhance reaction kinetics and ammonia decomposition efficiency.
13	10.1002/cssc.202202370	Low-temperature decomposition, achieving near-complete NH ₃ conversion at 380 °C.	Ru/CeO ₂ , Ru/La ₂ O ₃ , Ru/SiO ₂ , Ru/Y ₂ O ₃	Catalyst type (Ru/Y ₂ O ₃ , Ru/La ₂ O ₃ , Ru/CeO ₂ , Ru/SiO ₂), NH ₃ conversion, H ₂ formation rate, plasma AC supply power, gas hourly space velocity (GHSV).	Ru/La ₂ O ₃ showed superior plasma-catalytic reactivity; combining plasma with Ru catalyst significantly enhanced conversion at low temperatures; H ₂ formation rate of 10.7 mol gRu ⁻¹ h ⁻¹ and high energy efficiency achieved.
14	10.1016/j.fuel.2023.129320	Moderate temperature, 550 °C, with continuous reaction stability tested for 18 h.	Co-doped	Catalyst type (Co-doped graphdiyne), reaction temperature, catalyst stability over time, DFT-derived reaction energy and adsorption properties.	Nearly complete NH ₃ decomposition at 550 °C; Co-doped graphdiyne exhibits high stability and activity; DFT shows nitrogen binding strength correlates with reaction kinetics and energy barrier.

15	10.1016/j.cej.2023.145661	Low temperature atmospheric pressure		Varied Reactor type, catalytic route, process conditions (temperature, pressure), hydrogen yield; simulations used to guide catalyst design.	
16	10.1016/j.cej.2023.144623	Not stated	Ba-promoted Co	Presence of Ba promoter, surface coverages, partial equilibrium indices, elementary reaction rates	Ba enhances ammonia decomposition by promoting N ₂ desorption and affecting NH ₂ dehydrogenation. Microkinetic analysis provides insight into the mechanistic role of Ba in improving the catalytic performance of Co–Ce catalysts.
17	10.1021/acs.energyfuels.3c00760	400–800 °C		Reactor configuration, membrane properties, operating conditions (temperature, pressure), catalysts, hydrogen purification steps.	Membrane reactors can enhance hydrogen purity and conversion compared to conventional reactors; selection of membrane type and catalyst are critical; operating conditions strongly affect performance.
18	10.1021/acs.energyfuels.3c01348	773.15 K (500 °C)	Ni–La / MXene-supported	H ₂ and N ₂ permeance, NH ₃ conversion, catalyst addition (Ni–La/γ-Al ₂ O ₃), membrane presence vs packed catalytic reactor	MXene membrane reactor improves NH ₃ conversion (99%) compared to packed catalyst alone; enhances H ₂ purity; activation energies

					determined for H ₂ N ₂ permeation and NH ₃ decomposition; modeling agrees with experimental data
19	10.1016/j.fuel.2023.127879	Not stated		Reactor temperature, pressure, fuel blending (NH ₃ /H ₂), equivalence ratio, flue gas recirculation, heat integration for energy saving	Optimized conditions achieved: thermal efficiency 59%, fuel saving 22%, NH ₃ conversion/product yield 77%; NO _x emissions are mitigated by flue gas recirculation and fuel blending; intermediate heating improves conversion efficiency; simulation results validated against experiments
20	10.3390/catal13060920	Above 475 °C for effective NH ₃ conversion	Pd–Ag membrane	Membrane type (metallic support vs ceramic support), surface modification (α-Al ₂ O ₃ /γ-Al ₂ O ₃), NH ₃ conversion, H ₂ recovery, temperature	>99% NH ₃ conversion at >475 °C; H ₂ recovery >60%; metallic-supported membranes show better mechanical stability and ease of integration than ceramic-supported membranes; demonstrates feasibility of simultaneous ammonia decomposition and H ₂ separation in one device

21	10.1039/d3ra01596c	723–748 K (450–475 °C)	Pd	Membrane fabrication method (air bubbling vs standard ELP), membrane dimensions, pressure difference, ammonia feed rate, permeation vacuum	Air bubbling ELP allows rapid, uniform Pd membrane formation; membranes achieved high H_2 purity (>99.999%), high permeation flux, reproducibility across multiple membranes; ammonia decomposition performance improved in membrane reactor vs packed bed without membrane
22	10.1016/j.cej.2023.142474	450 °C (723 K)	Ru	NH ₃ feeding rate (up to 32,000 mL g ^{−1} h ^{−1}), support structure (planar vs vertically standing 2D), catalyst loading, reaction temperature	Vertically standing 2D support prevents Ru nanoparticle sintering, retains catalyst activity, and enables high hydrogen production rates (95.17 mmol g ^{−1} min ^{−1}) even at high ammonia flow rates; catalyst shows stability at 450 °C Technoeconomic Analysis (TEA) Not available
23	10.1039/d3cy00055a	Not stated	Ru–K / Ru-based	Type of catalyst (Ru, Ru-K), rate-determining step assumptions in microkinetic models, ammonia	The microkinetic models accurately reproduce experimental ammonia conversions, allowing

				conversion validation against experiment	identification of the true rate-determining step; approach helps avoid over-reliance on empirical models and can be applied to other catalytic ammonia decomposition systems
24	10.1039/d2re00408a	likely 400–600 °C	Ru / Co / Pd–Au	Catalyst type (Ru vs Co), reactor operation (isothermal vs non-isothermal), membrane type (Pd–Au), coupling of operating conditions (temperature, pressure, flow), case studies for optimization	Holistic coupling of catalyst, membrane, and reactor parameters is essential for efficient hydrogen production; single-factor optimization (e.g., only catalyst) may be insufficient; optimized combinations can yield pressurized, high-purity hydrogen comparable or superior to Ru-based non-membrane systems
25	10.1016/j.cej.2022.141203	600 °C		Ammonia conversion, pressure (7 barg), hydrogen production capacity (150–500 Nm ³ /h), CAPEX, OPEX, LCOH	Achieved 90% ammonia conversion at 600 °C and 7 barg; exergy efficiency of 54.21%; LCOH of 6.98 USD/kgH ₂ at 150 Nm ³ /h, decreasing to 5.33 USD/kgH ₂ at 500 Nm ³ /h; confirms feasibility of on-site, carbon-free green hydrogen

					production using induction-heated reactors
26	10.52292/j.laar.2023.1090	300–650 °C	Pd	Operating temperature (300–650 °C), pressure (8 bar), hydrogen permeation efficiency ($\approx$ 86 %), and process scale (200 kg H ₂ /day) for a hydrogen refueling station.	The integrated shell-and-tube Pd–Ag membrane reactor achieved complete ammonia conversion and produced ultrapure hydrogen suitable for refueling applications. Hydrogen recovery reached 86 %, while the remaining fraction was combusted to supply process heat, making the system self-sustaining and energy-efficient. The study demonstrates feasibility and intensification potential for small-scale, carbon-free H ₂ production.
27	10.3390/pr9122275	Not stated	Ni–Ru / Ni / Ru	Feed ammonia concentration, reactor residence time, adsorption constant, membrane surface area, membrane permeability.	Steady-state multiplicity occurs due to competitive adsorption; exists over a wide range of feed concentration and residence times; membrane properties strongly influence multiplicity; no oscillatory (Hopf) behavior predicted.

28	10.1016/j.apcatb.2021.119896	400 °C	CoCeAlO-type	Metal loading (Ni: 2.4–5 wt%, Ru: 0.4–0.6 wt%), Ni/Ru ratio (~7), long-term stability, multicycle performance under pure ammonia.	Bimetallic Ni-Ru catalysts exhibit superior catalytic activity and stability compared to monometallic catalysts. Kinetic modelling indicates surface dehydrogenation of adsorbed NH ₃ is rate-limiting and inhibited by H ₂
29	10.1016/j.cej.2021.128595	Not stated	Pt / Rh–Pt	Reaction temperature, NH ₃ flow rate, microchannel flow properties.	CFD model accurately predicts microreactor performance; inkjet printing-assisted catalyst deposition is effective; design allows easy catalyst screening; kinetic models can reliably simulate reacting flow in microchannel.
30	10.1016/j.fuel.2020.119111	450 °C – 550 °C (typical gasoline direct injection engine exhaust gas temperatures)		Exhaust gas temperature, partial replacement of gasoline with H ₂ -N ₂ mixture, catalyst type (Rh-Pt).	Complete NH ₃ conversion achieved at GDI exhaust temperatures. On-board ammonia decomposition can increase energy output up to 15%, reduce CO ₂ emissions by up to 30%, and improve fuel efficiency. Life cycle CO ₂ benefits for NH ₃ use as an energy carrier are demonstrated.

31	10.1016/j.cherd.2020.11.004	~400–600 °C	Pd/Ta	NH ₃ flow rate, reactor tube length, reactor configuration (single-tube vs multi-tube).	Single-tube reactors at high flow rates cannot meet conversion due to heat transfer limitations; decreasing NH ₃ supply rate improves conversion; a packed-bed multi-tube reactor design is suitable for industrial-scale NH ₃ decomposition.
32	10.1016/j.memsci.2020.118483	<723 K (significantly reduced operating temperature compared to conventional catalytic decomposition)	Ru/YSZ	Reactor configuration, type of sweep gas (steam vs. noble gases), catalyst type and loading, membrane type (Pd/Ta composite), H ₂ recovery efficiency.	
33	10.1021/acssuschemeng.8b06065	500–600 °C		Key parameters include temperature (around 400 °C and above), Ru catalyst loading, Cs promoter addition, and reactor configuration (CMR vs. PBMR). The study also examined hydrogen recovery efficiency, conversion rates, and membrane performance (Pd layer thickness and hydrogen permeability).	he Ru/YSZ–Pd CMR system achieved >99.7% hydrogen purity and complete ammonia conversion at 400 °C without the need for a sweep gas. The Cs promoter enhanced catalytic performance, and the reactor model accurately predicted the observed behavior. Compared with the packed-bed membrane reactor (PBMR), the CMR reduced Ru

					loading by an order of magnitude and increased hydrogen recovery by 35%, demonstrating much higher volumetric productivity ($>30 \text{ mol m}^{-3} \text{ s}^{-1}$). The model validated that efficient hydrogen removal drives kinetic enhancement beyond equilibrium limits.
34	10.1016/j.cattod.2017.05.018	$>400 \text{ }^{\circ}\text{C}$		Ammonia flow rate, combustible feed flow rate, fuel equivalence ratio. Reactor performance metrics (NH_3 conversion, hydrogen production rate, reactor power density) were measured.	$>99\% \text{ NH}_3$ conversion achieved at optimal conditions (ammonia 0.4 NLPM , feed 0.8 NLPM , fuel equivalence ratio 1.2). Reactor could generate hydrogen for a 45 W_{e} fuel cell at $1.5 \text{ kW}_{\text{e}}/\text{L}$. Feasibility of distributed hydrogen production via autothermal microchannel reactors was demonstrated.
35	10.1007/s11814-018-0037-5	$400\text{--}600 \text{ }^{\circ}\text{C}$	Fe / Ni / Ru	H_2 permeance, He sweep gas flow, operating temperature. Comparison of membrane reactor (MR) vs conventional packed-bed reactor (PBR).	Membrane reactor achieved higher ammonia conversions and H_2 yields than PBR. He sweep gas flow improved NH_3 conversion up to a critical

					flow (5 kmol/h). Higher $H_{2\text{ permeance}}$ increased H_2 yield. Lower operating temperatures enhanced NH_3 conversion and H_2 yield in MR relative to PBR, providing natural gas cost savings.
36	10.1007/s11051-018-4253-z	Not stated		ore metal type (Fe, Ru, Ir) in M@Ni nanoparticles; electronic structure (partial density of states); adsorption energies of NH_3 and N_2.	Ru@Ni core-shell nanoparticles show catalytic activity comparable to pure Ru due to favorable adsorption energies and electronic structure; Fe@Ni and Ir@Ni are less active; d-band electrons of the core metal significantly influence catalytic performance.
37	10.1016/j.jksues.2016.01.002	Not stated	Ni / Ru	Reactor configuration (single FBR, FBMR, MSFBMR), number of beds, feed temperature, heat load, hydrogen permeation zone.	Multi-stage FBMR achieves 100% NH_3 conversion; FBMR outperforms FBR in conversion; linear correlation between feed temperature and number of beds; diffusion limitation is localized; MSFBMR has

					potential for on-site ultra-clean H ₂ production.
38	10.1252/jcej.14we431	Not stated	Co / Fe / Ni	Catalyst type (Ni, Ru), reaction conditions (unspecified, but varied across experiments).	The kinetic model successfully reproduces experimental data; rate-limiting steps differ by catalyst: Ru is limited by N ₂ desorption, Ni is limited by NH ₃ dehydrogenation.
39	10.1039/c6cy01566b	Not stated	Ru/SiO ₂	catalyst composition, nh ₃ and h ₂ partial pressure, particle size and surface area	Co, Ni, and Fe additives promote ammonia decomposition by facilitating recombinative N desorption; alleviate H ₂ poisoning; larger particle size and lower surface area do not negatively affect activity; Co, Ni, and Fe catalysts are more active than Mo ₂ N.
40	10.1021/jacs.5c15789	400 °C		Plasma integration, catalyst type (Ru/SiO ₂), membrane configuration and thickness, cascade staging, separation factors, effluent NH ₃ concentration, space-time yield, and removal efficiency.	Achieved high H ₂ space-time yield at reduced temperature, strong NH ₃ recovery via membrane cascades, MD-supported explanation of selectivity, substantial reduction of effluent NH ₃ ,

					and system intensification relative to conventional thermal processes.
41	10.1002/aic.18781	Low-temperature operation	Ru/Y ₂ O ₃	Catalyst porosity, pore diameter, reactor segmentation, precious metal loading, temperature profile, heat flux distribution, and reactor size.	Multiscale modelling reveals that catalyst structural properties strongly influence reactor sizing and thermal behaviour; a segmented, two-stage egg-shell catalyst design reduces precious metal usage by 61.6% and temperature drop by 42.9 K while maintaining efficient ammonia decomposition.
42	10.1002/aic.70187	Low-temperature regime		Catalyst strain level, Ru loading, reaction temperature, reaction rate, activation energy, and electronic structure descriptors (e.g. d-band centre).	Compressive strain (~4.9%) in Ru/Y ₂ O ₃ –MgO lowers the activation energy for N–N recombination, enhancing low-temperature ammonia decomposition; the catalyst achieves exceptionally high hydrogen production rates with ultralow Ru loading.
43	10.1016/j.applthermaleng.2025.128142	600–1000°C	Ru / CeO ₂	1. Number of channels (single vs. multi-channel) 2. Hydrogen partial-pressure control method (vacuum pumping vs. sweep gas) 3. Solar irradiation intensity (400–1100 W/m ²).	1. Multi-channel reactor increases H ₂ recovery by 13.2% and NH ₃ conversion by 5.9% compared to single-channel. 2. Vacuum pumping enhances NH ₃ conversion by

					32.5% and H ₂ recovery by 45% over sweep gas. 3. Increasing solar irradiance from 400 to 1100 W/m ² boosts NH ₃ conversion by 56.6% and H ₂ recovery by 25.8%. 4. Design optimization and operational control significantly improve hydrogen yield and conversion efficiency.
44	10.1016/j.seppur.2025.133723	Not stated		1. Catalyst supports (various metal oxides compared). 2. Electronic state of Ru influenced by support. 3. Energy barriers for NH ₃ activation and N–H dissociation.	1. Strong Ru–CeO ₂ interaction enhances electron density on Ru. 2. Electron back-donation lowers NH ₃ activation barrier and improves reaction rate. 3. The interfacial electronic environment is crucial for designing efficient NH ₃ decomposition catalysts.
45	10.1016/j.tsep.2025.104229	Turbine inlet temperature varied (exact values not given but typically 1000–1500 °C).	Ba / Co-based	Turbine inlet temperature, turbine pressure ratio, hydrogen fraction in reformed gas, thermal efficiency of cycle.	Exhaust-driven ammonia decomposition significantly increases turbine efficiency; CRCCGT reaches 47.6% peak efficiency; ammonia reforming yields hydrogen-rich gas (~75% H ₂) that increases flame speed and

					improves combustion behaviour.
46	10.1021/acs.energyfuels.5c03995	Not stated	Co-based (ZIF-67 derived)	1. La content to tune Co spin state. 2. Spin state of Co (high, medium, low). 3. Adsorption strength of NH ₃ , H ₂ dissociation, and N ₂ desorption energy barriers.	1. Intermediate (medium) spin state provides balanced NH ₃ adsorption and H ₂ /N ₂ reaction barriers. 2. Spin-state tuning significantly enhances catalytic NH ₃ decomposition performance. 3. Demonstrates a new strategy for catalyst optimization at the atomic level.
47	10.1016/j.fuel.2025.135558	550 °C		1. Catalyst type and composition (Co@CN-600 vs other variants). 2. Reaction tube diameter / reactor configuration (10 mm tube optimized). 3. Gas hourly space velocity (9,000 mL·g ⁻¹ ·h ⁻¹).	1. Nearly 100% NH ₃ decomposition and H ₂ production rate of 10 mmol·g ⁻¹ ·min ⁻¹ at 550 °C. 2. Lower activation energy (79.40 kJ·mol ⁻¹) and higher activity than typical Co-based catalysts. 3. Uniform Co dispersion and nitrogen-doped carbon support enhance electron transfer and ammonia activation. 4. Long-term stability of catalyst confirmed.
48	10.1021/acs.energyfuels.5c03034	Low to moderate temperature,		1. Operating temperature. 2. Plasma input power (40 W tested). 3. Space velocity. 4. Cata-	1. Ammonia conversion of 19% at 593 K with 40 W plasma input. 2. Plasma

		specifically 593 K (≈ 320 °C)		lyst and plasma coupling mode (closely coupled system).	enhances low-temperature activity but increases energy consumption. 3. Efficiency improves with higher space velocity, yet overall energy efficiency is limited by plasma input. 4. The optimized Temkin–Pyzhev model accurately predicts ammonia reforming performance, providing a foundation for engine-integrated simulations.
49	10.1016/j.cej.2025.166903	$\sim 400\text{--}600$ °C	Co / Ni / Rh / Ru–Ni	1. Gas Hourly Space Velocity (GHSV) (up to 1850 h^{-1}). 2. POCS porosity (0.6–0.8). 3. Baffle pres- ence/type. 4. Packing type and cell geometry (Kelvin 3-0.6).	1. Kelvin 3-0.6 POCS with baffles optimized hydrogen recovery at low GHSV. 2. At higher GHSV, baffles improve CPC but slightly reduce hydrogen recovery. 3. Optimal porosity (0.8) balances kinetics and hydrogen extraction. 4. Integration of POCS membranes can reduce membrane area required and protect membranes, offering potential economic benefits.
50	10.1016/j.jcat.2025.116339	Not stated		1. Catalyst type (Ru, Rh, Ir, Ni, Co, Ru-Ni alloys). 2. Monometallic vs.	1. Ru identified as the most effective monometallic

				bimetallic composition. 3. Electronic descriptors influencing NH_3 dissociation and N_2 adsorption.	catalyst. 2. Volcano-type relationship between NH_3 dissociation energy and N_2 adsorption energy determines activity. 3. Ru-Ni alloys offer balanced NH_3 activation and N_2 desorption. 4. Combining computational screening with experimental validation effectively guides catalyst design for scalable hydrogen production.
51	10.1007/s11814-025-00508-y	Not stated	CoCe / CoN	1. Net output power. 2. Thermal efficiency. 3. Specific energy consumption. 4. Exergy efficiency, heat exchange area per unit power, LCOH.	1. Highest net output power of 1391.83 kW at thermal efficiency of 42.37%. 2. Specific energy consumption is 6.33 kW/kg. 3. Optimized exergy efficiency = 63.297%, LCOH = 4.926 \$/kg-LH ₂ , and APR = 0.506 m ² /kW. 4. Waste heat recovery and system optimization enhance environmental performance and energy efficiency.
52	10.1016/j.fuel.2025.135311	600 °C	Co / Fe / Ni / Ru-based	1. Catalyst composition (CoN, Co NPs, N/Ce doping). 2. Active site type and configuration in DFT simulations.	1. CoCe-NC catalyst achieves complete NH_3 decomposition at 600 °C. 2. Hydrogen production rate: 1,840 mmol·g ⁻¹ ·h ⁻¹ . 3. Co NPs

					are optimal active sites; CoN synergistically enhances decomposition by lowering energy barriers. 4. N and Ce doping promotes formation of Co NPs and CoN structures.
53	10.3390/catal15090811	$\geq 500\text{ }^{\circ}\text{C}$		Catalyst type (Ru, Fe, Ni, Co), support materials, promoter type, reactor configuration, operating temperature.	1. Ru-based catalysts remain the benchmark. 2. Alternative transition metals require higher temperatures for comparable conversion. 3. Membrane reactors are promising for simultaneous reaction and product separation. 4. Trade-off between cost, performance, and scalability is critical for industrial application.
54	10.1016/j.cherd.2025.07.044	Wide range- not specified		Temperature, feed molar fractions of reactants and products, catalyst type/loading	Models considering nitrogen desorption as rate-determining best predict NH ₃ conversion; provides insights for reactor modelling, optimization, and catalyst performance improvement.
55	10.1016/j.ces.2025.121906	Up to 600 $^{\circ}\text{C}$		Reactor configuration (EWHR vs. IJHR), catalyst structure (particle	Internal Joule-Heated Reactor (IJHR) offers higher

				vs. washcoated foam), and temperature.	thermal efficiency, better catalytic performance, and lower energy consumption than conventional reactors; optimal efficiency at 600 °C.
56	10.1021/acs.energyfuels.5c01442	Not stated		Reaction pathways, catalyst properties, reactor design parameters, hydrogen separation strategies; multidimensional parameter analysis mentioned.	Provides critical insights into decomposition efficiency determinants, coupling of green ammonia production with H ₂ networks, and guidance for reactor modeling and sustainable hydrogen energy integration.
57	10.1016/j.applthermaleng.2025.126172	implied below 600 °C		Direct normal irradiation, ammonia inlet mass flow rate, reactor outer radius, cross-sectional temperature distribution	Ammonia conversion improves with higher irradiation and larger reactor radius, and lower inlet mass flow. Optimal conditions: 600 W/m ² irradiation, 12 kg/h ammonia flow, 35 mm outer radius. Solar-driven system achieves 87.12 % ammonia conversion and 28.83 % fuel savings.
58	10.1002/aic.18781	Not stated		Catalyst porosity, pore diameters, reactor segmentation strategy, precious metal loading.	Segmented reactor with two-stage egg-shell catalysts reduces precious metal usage by 61.6%, decreases temperature drop by 42.9 K,

					improves heat flux balance, and enables efficient low-temperature hydrogen production from ammonia.
59	10.1016/j.mcat.2025.115016	Low-temperature regime	Ni/CeO ₂	Catalyst composition (Ni/CeO ₂ with/without alkaline earth metals), hydrogen inhibition effect	Alkaline earth metals improve low-temperature activity, mitigate hydrogen inhibition, and the developed kinetic model accurately describes ammonia decomposition behavior.
60	10.3390/catal15050488	Ru-based catalyst: 250–450 °C; Ni-based catalyst: 400–600 °C	Ni/CeO ₂ / Ru/CeO ₂	Catalyst type, temperature, space velocity (2000–32,000 mL·g ⁻¹ ·h ⁻¹)	Ru/Ce–Zr–La–Nd–Pr–O catalyst showed superior NH ₃ conversion compared to Ni/Ce–Zr–O catalyst; NH ₃ conversion decreases with increasing space velocity; kinetic models reasonably predict experimental conversion; activation energies: 37.7 kJ/mol (Ru catalyst) and 66 kJ/mol (Ni catalyst)
61	10.1007/s10562-025-04992-z	350 °C	Ru/Pr ₆ O ₁₁	Ru precursor type, alkali metal type and concentration, catalyst composition and particle size.	Cs-modified Ru ₃ (CO) ₁₂ /Pr ₆ O ₁₁ catalyst shows highest activity; stronger alkali metals enhance H ₂ production via spillover and SMSI; first NH ₃

					dehydrogenation step is rate-limiting with 2.19 eV barrier.
62	10.1016/j.memsci.2025.124020	Not stated		Membrane position (offset), catalyst bed start position, reactor geometry (radii, lengths), temperature, pressure, feed flow rate, hydrogen selectivity	Optimizing membrane position can enhance hydrogen productivity; hydrogen flux responds differently to volumetric and flux-based optimization; membrane reactors do not always improve H ₂ productivity for all conditions
63	10.1039/d4cc06382a	Not stated		Catalyst/electrode type, reaction conditions (implied via AI/ML models), material properties.	Green ammonia decomposition technologies are progressing; AI/ML can accelerate catalyst design and mechanism understanding; technical challenges and recommendations are outlined.
64	10.1016/j.combustflame.2025.113992	Gas turbine operating conditions (exact range not specified).		Multi-fuel injection configuration, flame thickening, local equivalence ratio, ammonia–hydrogen fuel blends.	Extended MF-TFLES improves flame shape and structure prediction compared to conventional TFLES; allows simulation of partially-premixed multi-fuel flames and better understanding of pollutant formation from decarbonized fuels.

65	10.1016/j.fuel.2024.134043	500–525 °C	Ru/3Ce-type composite	Catalyst support composition (Ce-Al ratio), Ru loading, particle size, surface acidic sites.	Ru/3Ce-Al catalyst achieves 95% NH ₃ conversion at 525 °C with high durability; Ce-Al support enhances NH ₃ adsorption and lowers reaction energy barrier; DFT identifies stable adsorption sites and rate-determining step
66	10.1016/j.cej.2025.159443	Not stated		Reaction pathways, plasma vs thermal contribution, component sensitivity.	Both plasma and thermal decomposition contribute significantly; $\text{NH}_3 + \text{H} \rightarrow \text{NH}_2 + \text{H}_2$ is the fastest reaction, responsible for 51.9% of NH ₃ consumption and 82.1% of H ₂ production; thermal effects optimize pathways and energy efficiency.
67	10.1021/acssuschemeng.4c08899	Warm plasma conditions		Reactor design (reversed plasma vs. plasma-only vs. thermocatalysis), catalyst loading, ammonia conversion efficiency	Reversed plasma catalysis achieves ~98% ammonia conversion with up to 60% catalyst savings, reduces reactor size, maintains energy and exergy efficiency

					comparable to conventional plasma or thermocatalysis
68	10.1021/acscatal.5c04795	Not stated	Fe–Co nitrides	Catalyst composition (Fe vs FeCo alloys), surface dynamics, nitrogen migration and recombination behavior	Cobalt alloying lowers free energy barrier for nitrogen recombination, suppresses nitride formation, enhances ammonia conversion, and improves long-term stability of FeCo catalysts
69	10.1021/acscatal.5c01829	586 K to 823 K (temperature varies with applied electric field)		Applied electric field strength (e.g., $-1 \text{ V/\AA}$), temperature, turn-over frequency	Negative electric field significantly increases turnover frequency, lowers operating temperature for desired rates; NH ₃ dehydrogenation is identified as rate-limiting step; multiscale model provides mechanistic insights for field-enhanced catalysis
70	10.1039/c5ra07818k	Not stated	Co-based spinel	Surface orientation ((100), (110), (111)), presence of oxygen vacancies, adsorption energy, dissociation barrier	(111) surface is most favorable for NH ₃ adsorption and decomposition; oxygen vacancies can act as active sites; defective surfaces lower energy barriers for NH ₃

					dissociation; insights provide guidance for catalyst design
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