Supplementary material for: Generative AI in Process Design Instruction: A Survey of Students and Faculty

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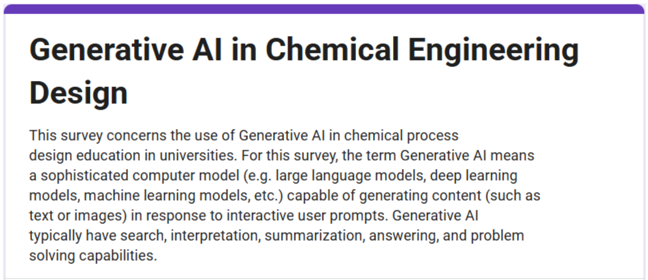
1 SURVEY QUESTIONS

All participants received the following text and prompts through Google Forms. Back and Next buttons were provided for easy of navigation, and participants were allowed to change answers before final submission of the survey. The desktop version is shown below.



Generative AI in Chemical Engineering Design

This survey concerns the use of Generative AI in chemical process design education in universities. For this survey, the term Generative AI means a sophisticated computer model (e.g. large language models, deep learning models, machine learning models, etc.) capable of generating content (such as text or images) in response to interactive user prompts. Generative AI typically have search, interpretation, summarization, answering, and problem solving capabilities.

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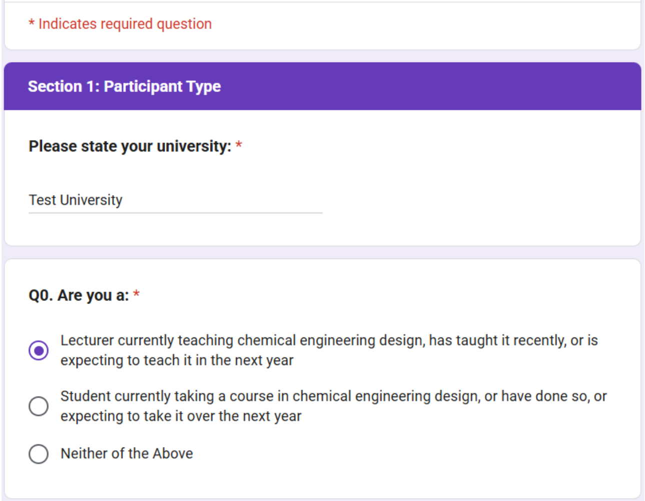


* Indicates required question

Section 1: Participant Type

Please state your university: *

Test University

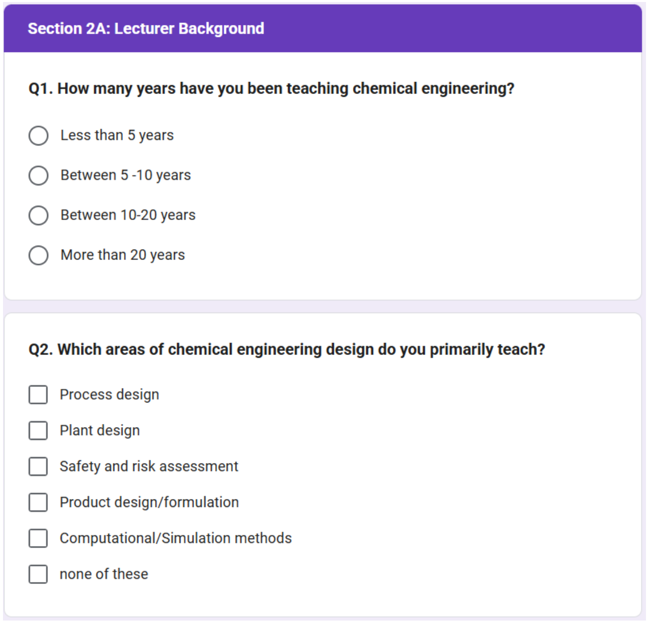
Q0. Are you a: *

● Lecturer currently teaching chemical engineering design, has taught it recently, or is expecting to teach it in the next year
○ Student currently taking a course in chemical engineering design, or have done so, or expecting to take it over the next year
○ Neither of the Above

[Back / Next buttons]

Participants who answered "Lecturer" were taken to the Lecturer set of questions. Participants who answered "Student" were taken to the student set of questions. Participants who answered "Neither" were presented with no further questions (the survey ended).

1.1 Questions for Lecturers



Section 2A: Lecturer Background

Q1. How many years have you been teaching chemical engineering?

○ Less than 5 years
○ Between 5 -10 years
○ Between 10-20 years
○ More than 20 years

Q2. Which areas of chemical engineering design do you primarily teach?

☐ Process design
☐ Plant design
☐ Safety and risk assessment
☐ Product design/formulation
☐ Computational/Simulation methods
☐ none of these

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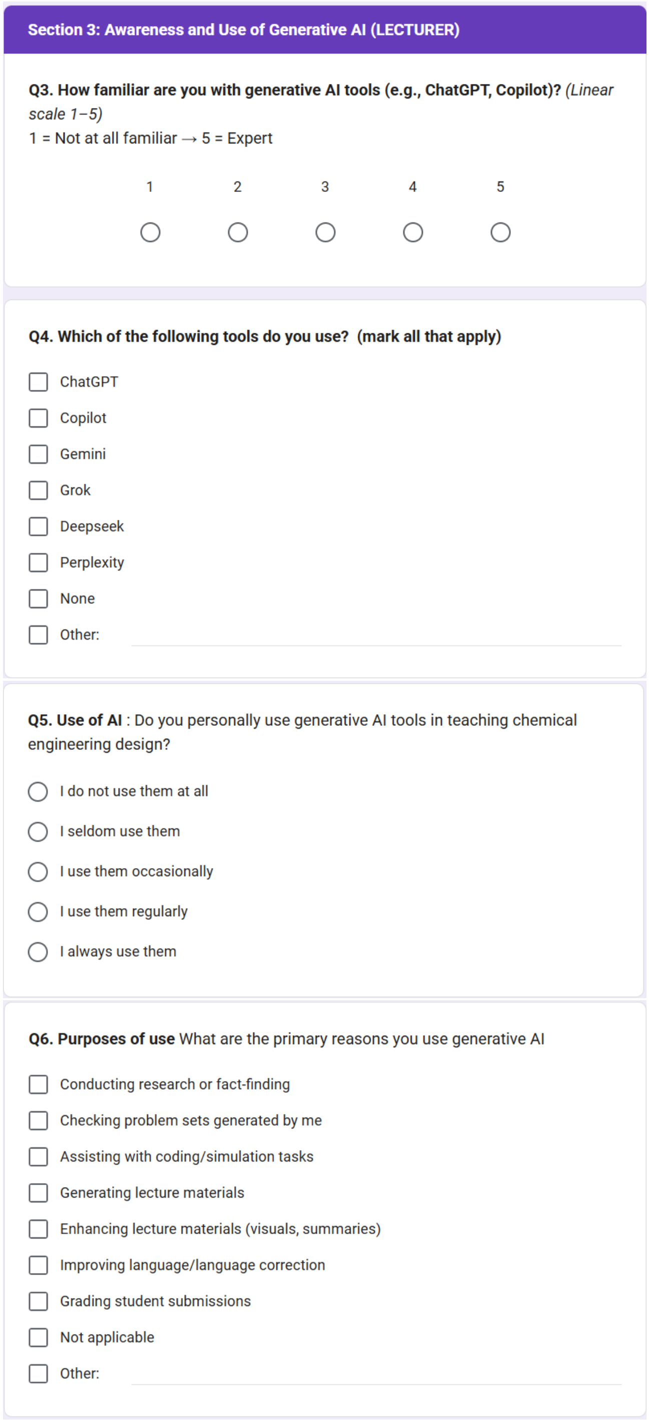

Section 3: Awareness and Use of Generative AI (LECTURER)

Q3. How familiar are you with generative AI tools (e.g., ChatGPT, Copilot)? *(Linear scale 1–5)*
1 = Not at all familiar → 5 = Expert

1	2	3	4	5
○	○	○	○	○

Q4. Which of the following tools do you use? (mark all that apply)

☐ ChatGPT
☐ Copilot
☐ Gemini
☐ Grok
☐ Deepseek
☐ Perplexity
☐ None
☐ Other: ________

Q5. Use of AI : Do you personally use generative AI tools in teaching chemical engineering design?

○ I do not use them at all
○ I seldom use them
○ I use them occasionally
○ I use them regularly
○ I always use them

Q6. Purposes of use What are the primary reasons you use generative AI

☐ Conducting research or fact-finding
☐ Checking problem sets generated by me
☐ Assisting with coding/simulation tasks
☐ Generating lecture materials
☐ Enhancing lecture materials (visuals, summaries)
☐ Improving language/language correction
☐ Grading student submissions
☐ Not applicable
☐ Other: ________

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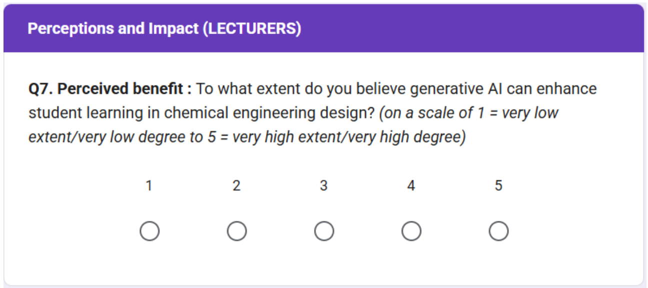
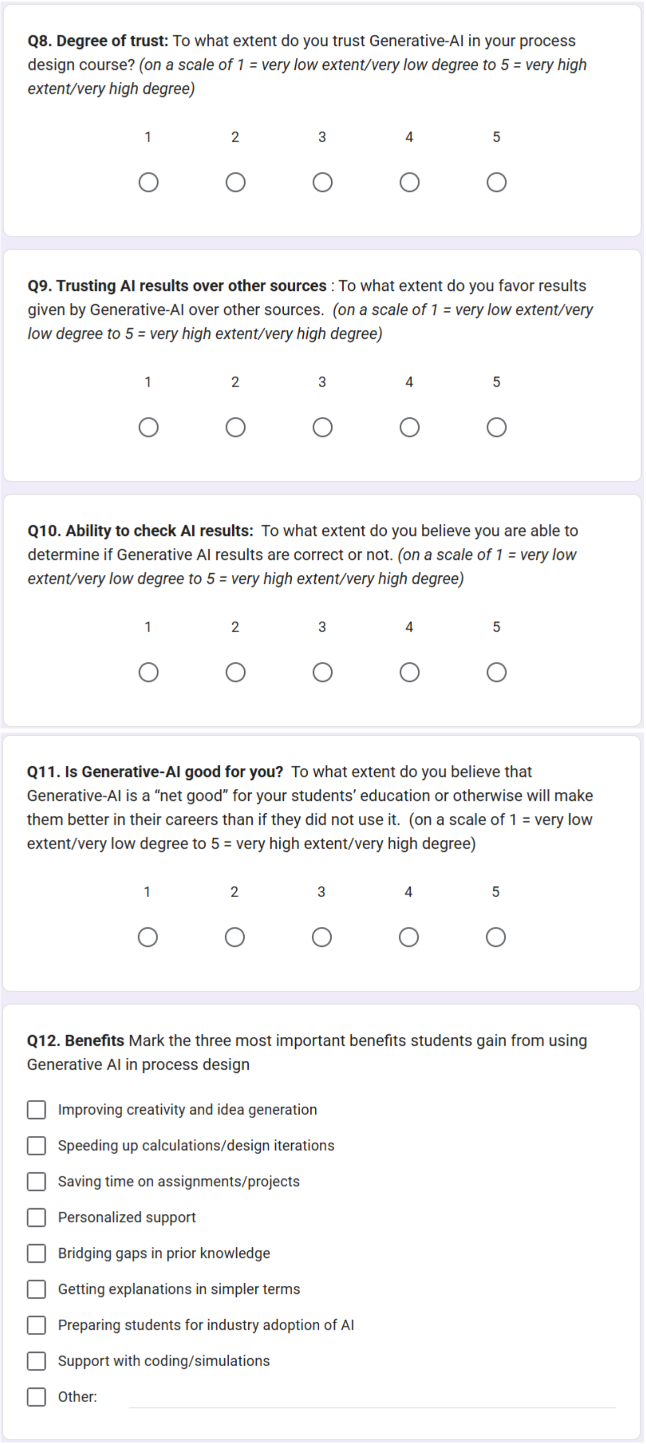


Perceptions and Impact (LECTURERS)

Q7. Perceived benefit : To what extent do you believe generative AI can enhance student learning in chemical engineering design? *(on a scale of 1 = very low extent/very low degree to 5 = very high extent/very high degree)*

1	2	3	4	5
○	○	○	○	○



Q8. Degree of trust: To what extent do you trust Generative-AI in your process design course? *(on a scale of 1 = very low extent/very low degree to 5 = very high extent/very high degree)*

1	2	3	4	5
○	○	○	○	○

Q9. Trusting AI results over other sources : To what extent do you favor results given by Generative-AI over other sources. *(on a scale of 1 = very low extent/very low degree to 5 = very high extent/very high degree)*

1	2	3	4	5
○	○	○	○	○

Q10. Ability to check AI results: To what extent do you believe you are able to determine if Generative AI results are correct or not. *(on a scale of 1 = very low extent/very low degree to 5 = very high extent/very high degree)*

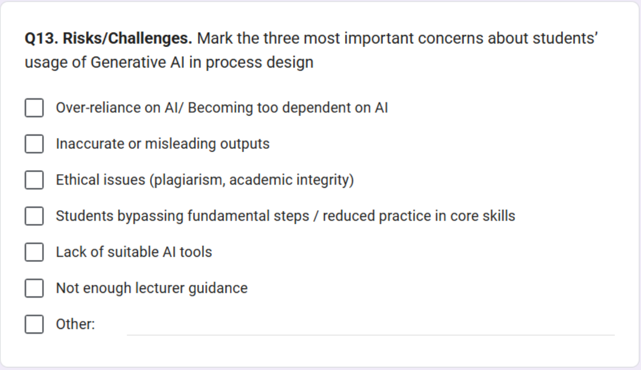
1	2	3	4	5
○	○	○	○	○

Q11. Is Generative-AI good for you? To what extent do you believe that Generative-AI is a “net good” for your students’ education or otherwise will make them better in their careers than if they did not use it. (on a scale of 1 = very low extent/very low degree to 5 = very high extent/very high degree)

1	2	3	4	5
○	○	○	○	○

Q12. Benefits Mark the three most important benefits students gain from using Generative AI in process design

☐ Improving creativity and idea generation
☐ Speeding up calculations/design iterations
☐ Saving time on assignments/projects
☐ Personalized support
☐ Bridging gaps in prior knowledge
☐ Getting explanations in simpler terms
☐ Preparing students for industry adoption of AI
☐ Support with coding/simulations
☐ Other: ________



Q13. Risks/Challenges. Mark the three most important concerns about students' usage of Generative AI in process design

☐ Over-reliance on AI/ Becoming too dependent on AI
☐ Inaccurate or misleading outputs
☐ Ethical issues (plagiarism, academic integrity)
☐ Students bypassing fundamental steps / reduced practice in core skills
☐ Lack of suitable AI tools
☐ Not enough lecturer guidance
☐ Other: ____

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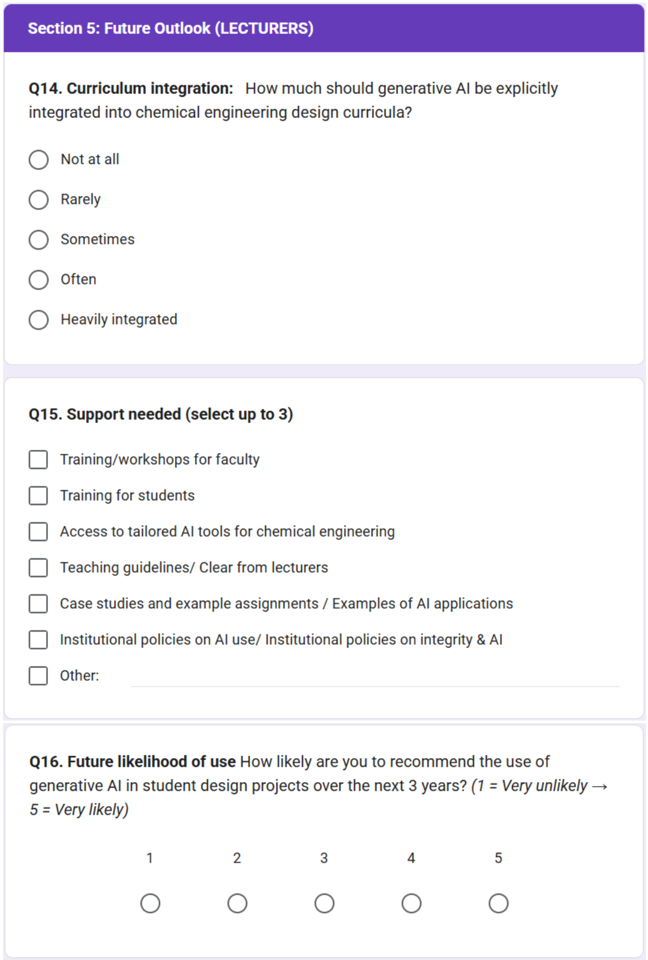

Section 5: Future Outlook (LECTURERS)

Q14. Curriculum integration: How much should generative AI be explicitly integrated into chemical engineering design curricula?

○ Not at all
○ Rarely
○ Sometimes
○ Often
○ Heavily integrated

Q15. Support needed (select up to 3)

☐ Training/workshops for faculty
☐ Training for students
☐ Access to tailored AI tools for chemical engineering
☐ Teaching guidelines/ Clear from lecturers
☐ Case studies and example assignments / Examples of AI applications
☐ Institutional policies on AI use/ Institutional policies on integrity & AI
☐ Other: ____

Q16. Future likelihood of use How likely are you to recommend the use of generative AI in student design projects over the next 3 years? *(1 = Very unlikely → 5 = Very likely)*

1	2	3	4	5
○	○	○	○	○

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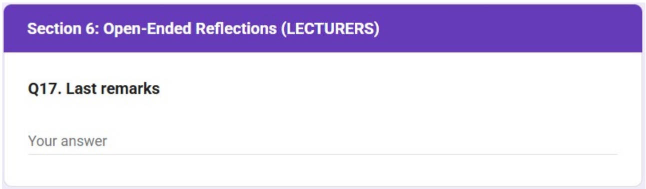

Section 6: Open-Ended Reflections (LECTURERS)

Q17. Last remarks

Your answer ____

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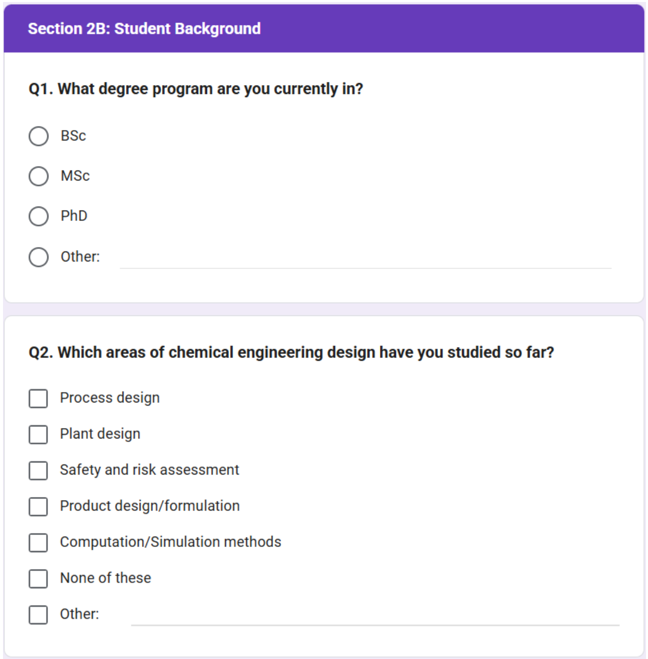
1.2 Questions for Students



Section 2B: Student Background

Q1. What degree program are you currently in?

○ BSc
○ MSc
○ PhD
○ Other: ____

Q2. Which areas of chemical engineering design have you studied so far?

☐ Process design
☐ Plant design
☐ Safety and risk assessment
☐ Product design/formulation
☐ Computation/Simulation methods
☐ None of these
☐ Other: ____

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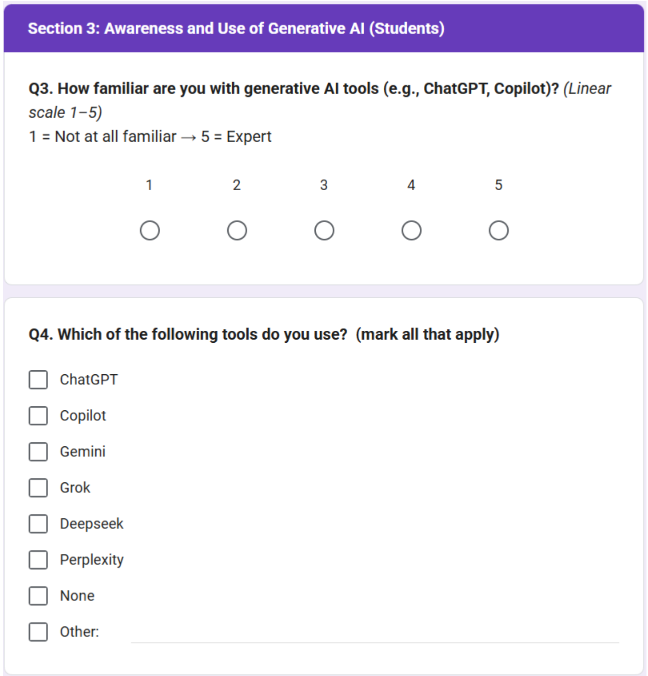

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☐ Grok
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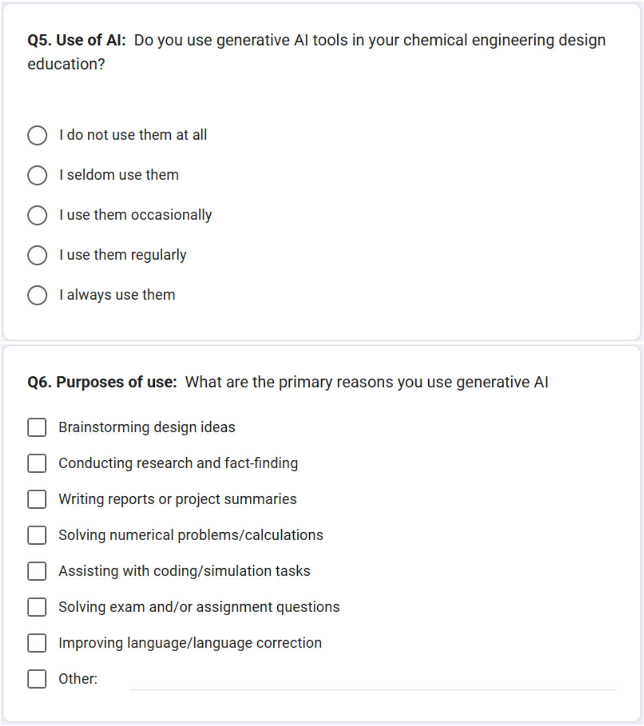
☐ None
☐ Other: ____



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○ I do not use them at all
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Q6. Purposes of use: What are the primary reasons you use generative AI

☐ Brainstorming design ideas
☐ Conducting research and fact-finding
☐ Writing reports or project summaries
☐ Solving numerical problems/calculations
☐ Assisting with coding/simulation tasks
☐ Solving exam and/or assignment questions
☐ Improving language/language correction
☐ Other: ________

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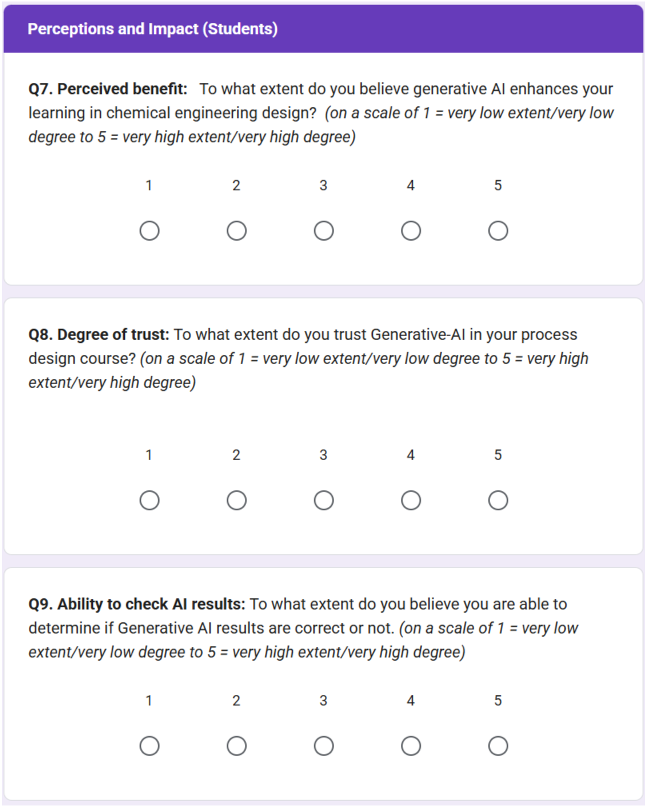
Note, in the next section, a technical error caused an intended question 9 about trusting AI results over other sources to be skipped and for no Q13 to exist. Therefore Q9-12 correspond to Q10-13 in the lecturer portion.



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○	○	○	○	○

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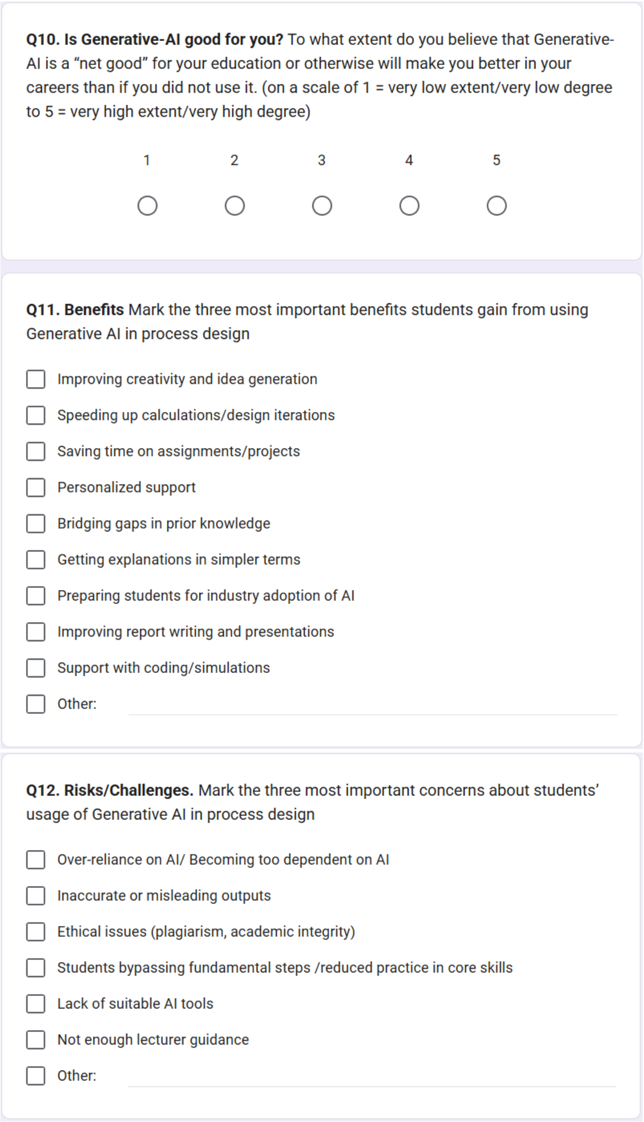
○	○	○	○	○



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○	○	○	○	○

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☐ Getting explanations in simpler terms
☐ Preparing students for industry adoption of AI
☐ Improving report writing and presentations
☐ Support with coding/simulations
☐ Other: ________

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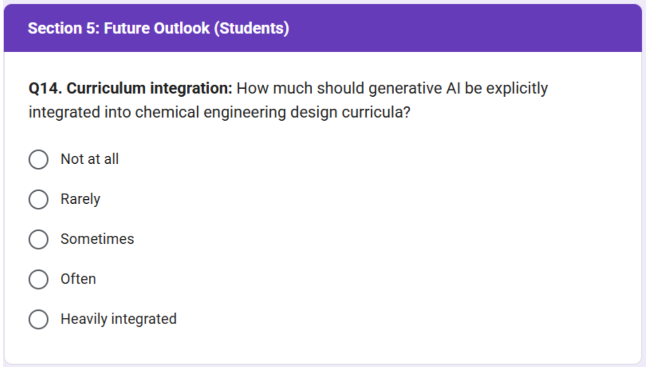

Section 5: Future Outlook (Students)

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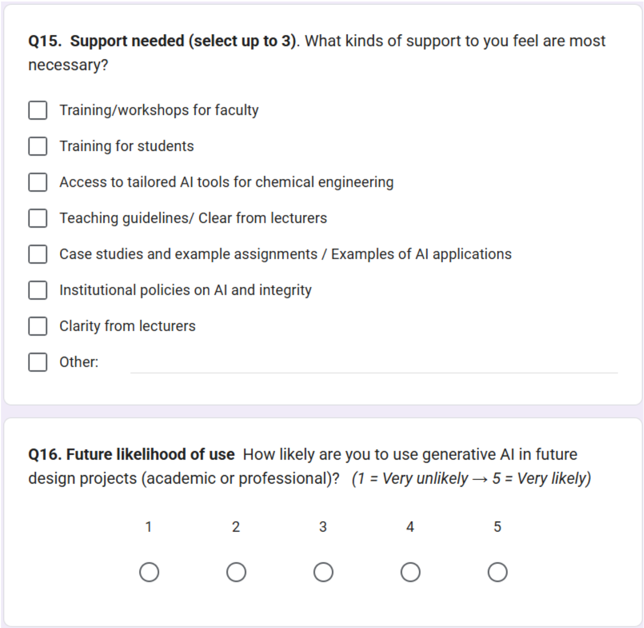


Q15. Support needed (select up to 3). What kinds of support to you feel are most necessary?

☐ Training/workshops for faculty
☐ Training for students
☐ Access to tailored AI tools for chemical engineering
☐ Teaching guidelines/ Clear from lecturers
☐ Case studies and example assignments / Examples of AI applications
☐ Institutional policies on AI and integrity
☐ Clarity from lecturers
☐ Other: ______

Q16. Future likelihood of use How likely are you to use generative AI in future design projects (academic or professional)? *(1 = Very unlikely → 5 = Very likely)*

1	2	3	4	5
○	○	○	○	○

2 SURVEY RESULTS

Raw survey data are provided in the accompanying Microsoft Excel file. For privacy reasons and to prevent participant identification, answers for a participants' university were redacted, date-stamps of the survey were removed, and the responses are presented in randomized order. Free-form comments were redacted when necessary for privacy reasons.

3 CHATGPT TRANSCRIPT

As described in the paper, the next page contains the transcript with ChatGPT concerning the synthesis of an ammonia production plant. Input text is in red. Some items formatted for clarity.

ChatGPT Transcript

Generate a preliminary flowsheet for the production of ammonia from air and water

Thought for 27s

Nice — here's a clear, engineering-style **preliminary flowsheet** (text + stream table + notes) for producing **ammonia from air and water**. I'll present a block/process diagram, key unit operations, a material-basis example (1000 kg NH_3 / hr), typical operating conditions, and important design/safety notes you'll want to consider next. This is a practical starting point you can refine into P&ID and detailed mass/energy balances.

Process summary (block flow)

Air ---> (1) Air Compressor ---> (2) Air Separation Unit (ASU: cryogenic or PSA) ---> N2

|

v

Water ---> (3) Electrolyzer ($H_2O \rightarrow H_2 + \frac{1}{2} O_2$) ---> H2

|

H2 Compressor <--- (optional) ---|

v

(4) Feed Compression & Purification (remove O_2, dry, adjust H_2:N_2 ratio)

|

(5) Preheat / Reactor Feed Conditioning (remove steam, EQT)

v

(6) Haber–Bosch Reactor (Fe or promoted catalyst; 150–250 bar, 400–500 °C)

|

(7) Cooler / Condenser (liquid NH_3 out)

|

(8) NH_3 Separator (liquid product)

|

(9) Recycle Compressor -> Recycle to (6) (unconverted H_2/N_2)

|

(10) Purge & Tail Gas Treatment (to avoid inert buildup, e.g. Ar)

Key unit operations (short descriptions)

1. **Air compressor** — compress ambient air to ASU feed pressure.

2. **ASU (Air Separation Unit)** — produce high-purity N_2. For large plants: cryogenic distillation; for modular/smaller plants: PSA or membrane separation (lower purity/cost tradeoffs).
3. **Electrolyzer** — produce H_2 by splitting water (PEM, alkaline or AEM). Oxygen is produced as a coproduct. Electrolyzer product typically contains water vapor; drying/purification needed.
4. **Gas cleanup & compression** — remove oxygen traces (oxygen poisons HB catalyst), dry gases, control H_2:N_2 ratio (stoichiometric or slight H_2 excess), and compress to synthesis pressure.
5. **Haber–Bosch synthesis loop** — high-pressure reactor over iron or promoted catalyst; partial conversion per pass; downstream condenser to separate NH_3; recycle unconverted gases.
6. **NH_3 liquefaction & storage** — condense ammonia (liquid under pressure/cooling), store in refrigerated tanks or pressurized spheres as required.
7. **Utilities & heat integration** — recuperate heat from reactor effluent to preheat feeds, provide steam/electricity for electrolyzers, refrigeration for NH_3 condensation.

Basis & stoichiometry (design basis)

Basis: 1,000 kg NH_3 per hour (≈ large pilot/moderate plant size).
Reaction: $N_2 + 3\,H_2 \rightarrow 2\,NH_3$
Molar mass: NH_3 = 17.031 g·mol^{-1}

From stoichiometry (per 1000 kg/hr NH_3):

- NH_3 production: **1,000 kg/hr** → **58,716 mol/hr** NH_3
- Required N_2 (stoich): **0.5 mol N_2 per mol NH_3** → **29,358 mol/hr N_2** → **≈ 822.4 kg/hr N_2**
- Required H_2 (stoich): **1.5 mol H_2 per mol NH_3** → **88,075 mol/hr H_2** → **≈ 177.5 kg/hr H_2**

To supply N_2 from air (air ≈ 78.08% N_2 by volume):

- Air needed ≈ **37,600 mol/hr** → **≈ 1,089 kg/hr** air

To supply H_2 from water electrolysis:

- H_2 produced mol ≈ 88,075 mol/hr → water consumption ≈ 88,075 mol/hr H_2O → **≈ 1,586.7 kg/hr** water
- O_2 co-product from electrolysis ≈ 44,037 mol/hr → **≈ 1,409 kg/hr** O_2 (use/store/sell if feasible)

Note: numbers above assume **100% Faradaic efficiency** and no losses — account for electrolyzer inefficiencies, purge, and leakages in detailed design.

Typical operating conditions (preliminary)

- **ASU:** depends on technology — cryogenic yields very high purity N_2 (>99.9%) at low temperatures; PSA yields up to ~99% N_2 at lower CAPEX but with more purge.
- **H_2 electrolyzer:** PEM/alkaline — produces H_2 at low to moderate pressure (1–30 bar depending on system).
- **Synthesis (Haber–Bosch) reactor:** Pressure typically **150–250 bar**; temperature **400–500 °C** (tradeoff: higher T increases rate but lowers equilibrium conversion). Typical per-pass conversion ~10–20%; recycle unconverted gas.

- **NH_3 condensation:** at synthesis pressure the product is cooled to condense NH_3 (liquid) — cooling duty depends on pressure and condenser design.

Preliminary stream table (summary — molar & mass flows)

(rounded values; only main species shown; inert species like Ar, CO_2, moisture not shown)

Stream	Mol/hr (approx)	Mass kg/hr (approx)	Composition
Air feed	37,600 mol/hr	1,089 kg/hr	air (N_2 ~78 vol%)
N_2 (to synthesis)	29,358 mol/hr	822.4 kg/hr	N_2 (after ASU)
Water feed (electrolysis)	88,075 mol/hr	1,586.7 kg/hr	H_2O
H_2 (to synthesis)	88,075 mol/hr	177.5 kg/hr	H_2 (after electrolyzer & cleanup)
O_2 (electrolyzer off-gas)	44,037 mol/hr	1,409 kg/hr	O_2 (can be vented or used)
NH_3 product	58,716 mol/hr	1,000 kg/hr	NH_3 (liquid after condenser)
Recycle gas (approx)	depends on per-pass conv. (assume 15% per pass)	large recycle compressor duty	unconverted H_2/N_2

Mass & energy considerations (high-level)

- **Energy for H_2 production** will dominate if electrolytic H_2 is used. Typical cell energy intensity: roughly **40–55 kWh per kg H_2** (order-of-magnitude; depends on electrolyzer type & efficiency). For ~177.5 kg $H_2 \cdot hr^{-1}$ this implies several MW of continuous electrical load (tens of MW); do detailed power balance for your specific electrolyzer.
- **Compression duties** (compressing H_2/N_2 to 150–250 bar) are significant — compressors and heat-rejection equipment must be sized appropriately.
- **Heat integration**: recover reactor waste heat to preheat feed gases and generate steam for other uses — critical to improve overall plant efficiency.

Process control & safety highlights

- **Oxygen traces are catalyst poisons** — oxygen must be removed to < ppm levels before the HB reactor.
- **Inert build-up** (Ar, CH_4, N_2O in feed) — purge stream required to avoid inert accumulation; purge requires handling and possible treatment.
- **Hydrogen safety** — H_2 leak detection, explosion-proof areas, appropriate ventilation, and flame arrestors.
- **Ammonia hazards** — toxicity and corrosiveness. Provide refrigeration, spill containment, scrubbers for vent streams.
- **Pressure safety** — high-pressure equipment (150–250 bar) requires rigorous mechanical design and relief systems.

Alternatives & variants (pick depending on scale/cost)

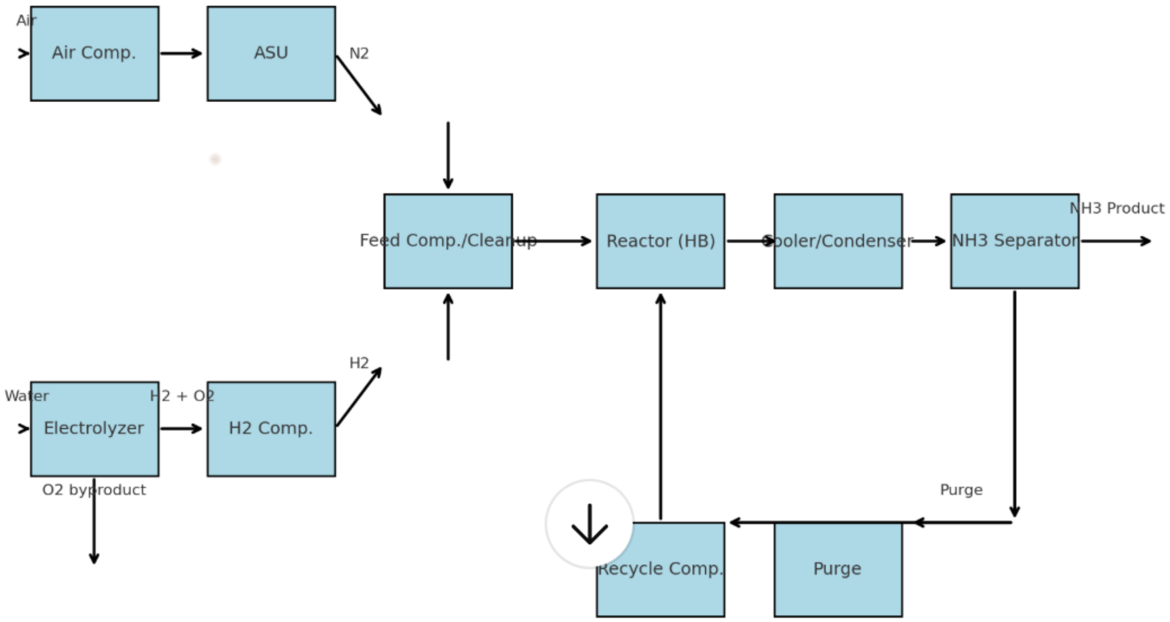
- **H_2 source alternatives:** steam-methane reforming (SMR) + CCS (cheaper but fossil feed) vs. water electrolysis (low-carbon if using renewable electricity). You specified *air and water* — so electrolysis is the natural fit.
- **N_2 source alternatives:** PSA / membrane separation (lower CAPEX for modular plants) vs. cryogenic ASU (higher purity, efficient for large scale).
- **Catalysts/conditions:** newer catalysts and lower-pressure routes (electrochemical ammonia synthesis) are still emerging; for near-term engineering the Haber–Bosch route is proven.

Next steps (recommended)

1. Choose **plant scale** (this example used 1,000 kg/hr NH_3). Confirm target and perform full mass & energy balances including electrolyzer efficiency, ASU efficiency, compressors, boil-off and purge.
2. Select technology options (PEM vs alkaline electrolyzer; PSA vs cryogenic ASU). Each choice changes utilities & economics.
3. Carry out **process simulations** (Aspen Plus / HYSYS / gPROMS) to size compressors, heat exchangers, and calculate recycle fractions and per-pass conversion.
4. Generate P&IDs and a preliminary equipment list (electrolyzer stacks, compressors, reactor, heat exchangers, condenser, storage).
5. Do safety & environmental risk assessment (HAZOP, LOPA, dispersion modeling for ammonia).
6. If you want, I can: (a) convert this into a PFD with labeled streams, (b) run a numerical mass/energy balance for the 1,000 kg/hr basis including electrolyzer power (you tell me assumed electrolyzer efficiency in kWh/kg H_2), or (c) produce a simplified Aspen/HYSYS input spec.

Would you like me to **(A)** draw a PFD (graphic) of the flowsheet, **(B)** run a numerical energy estimate using an assumed electrolyzer efficiency and compressor polytropic efficiencies, or **(C)** prepare a P&ID checklist and equipment list next? You're doing great — pick one and I'll jump straight in.

Please draw a PFD



Here's the **Preliminary Process Flow Diagram (PFD)** for **ammonia synthesis from air and water**.

It shows:

- **Air → ASU → N_2 stream**
- **Water → Electrolyzer → H_2 + O_2 coproduct**
- **Compression/purification** → **Haber–Bosch loop** (reactor, condenser, separator)
- **Recycle & purge streams**

Would you like me to also prepare a **stream table (with molar/mass flows and conditions)** alongside this PFD so it can serve as a complete handout for teaching or reporting?

What opportunities are there for heat integration?

Thought for 8s

Great question — there's a lot of low-hanging and high-value heat integration in an electrolytic Haber–Bosch ammonia plant. Below I list the main heat sources and sinks, practical integration patterns (how to match them), useful technologies to upgrade or store heat, and next steps (including pinch analysis). I'll keep it concrete and actionable so you can start sketching a heat-exchanger network (HEN).

Main heat sources (where heat is available)

- **Haber–Bosch reactor effluent (reaction exotherm + gas temperature):** very hot gas (reaction conditions/exit depend on catalyst & recycle, but reactor and interstage temperatures are high). This is the largest high-grade thermal source in the synthesis loop.
- **Interstage / reactor outlet cooling:** heat removed to condense NH_3 and cool synthesis gas — a medium-to-high temperature source when cooled from reactor outlet to condenser temperature.

- **Compressor intercooling / aftercoolers (air, N_2, H_2, recycle):** moderately hot streams (single- or multi-stage compressors produce significant heat at ~40–120 °C depending on compression ratios and cooling utilities).
- **Electrolyzer waste heat:** electrolyzers (PEM, alkaline, AEM) reject low-to-moderate grade heat (often <80–90 °C for stacks; some designs allow hot water at ~60–90 °C). Modern high-current stacks can have considerable heat to recover.
- **Condensers & refrigeration rejects (NH_3 condensation):** cold and warm sinks — the condenser releases heat at the condensation temperature (depending on pressure) to the cooling system; refrigeration rejects to ambient (low-grade).
- **Utility steam cycle rejects and power generation (if present):** any onsite turbines or ORC will generate lower-grade heat in condensers.
- **Purge/gas compression heat:** purge compressors and tail-gas units also reject useful heat.

Main heat sinks (where heat is needed)

- **Feed preheating to reactor (synthesis feed):** N_2/H_2 feed must be preheated to reactor inlet temperature (high value sink).
- **Steam generation for plant (process steam):** for cleaning, turbine sealing, heating electrolyzer balance-of-plant, or other internal uses.
- **Electrolyzer water pre-warming:** warming feed water to electrolyzer reduces electrical energy per kg H_2 (preheat to stack inlet temperature improves efficiency).
- **Evaporation / drying duties:** drying of gases, removing moisture from N_2 or feeds before reactor (requires moderate heat).
- **District heating or on-site heating load:** if available, low-grade heat can be exported to buildings or other processes for value.
- **Desalination / water pre-treatment:** preheating make-up water or low-grade desalination heat (if water source desalination is needed).
- **Regeneration/desorption (adsorbent beds):** heat for PSA bed regeneration (if PSA used) or membranes can require moderate heat.

Practical integration patterns (how to match sources → sinks)

1. **Use reactor effluent to preheat feed gases (direct heat cascade).**
   - Hot reactor effluent (high T) → train of heat exchangers that first preheat feed N_2/H_2 to reactor inlet, then produce/raise steam or heat water. This recovers the highest-quality heat where it's most valuable (feed preheat).
2. **Generate process steam from reactor and intercooler heat.**
   - High/medium grade heat can drive a steam drum → steam used for heaters, cleaning, or to drive a small steam turbine/expander to produce electricity for compressors.
3. **Recover compressor intercooling heat to preheat electrolyzer water and feed gases.**
   - Intercooler water (moderate T) is an excellent match for raising water to electrolyzer inlet temperature or for preheating N_2 feed before final heater.

4. **Electrolyzer heat → use for balance-of-plant and local heating.**
    - Low-grade electrolyzer heat can supply domestic/process hot water, regenerate adsorption beds, or preheat feed water using plate-heat exchangers.
5. **Cascade cold and hot utilities:** use cascade approach — highest temperature source to highest temperature sink, then next highest to next, etc., to maximize ΔT driving force and minimize external utilities.
6. **Cold integration and refrigeration reuse:** consider using cold from NH_3 refrigeration to cool other streams that require low temperature (e.g., product conditioning, liquid storage coolers), and use cascade refrigeration stages to minimize overall work.
7. **Heat pumps / electrically driven heat upgradeers:** if you have a lot of low-grade heat (electrolyzer, condenser rejects) but need medium/high T for feed preheat, use a heat pump to upgrade heat efficiently compared with firing extra electrical heaters.
8. **Power cogeneration (steam turbine or ORC):** convert part of high-grade heat to electricity for compressors or electrolyzers; ORC is useful if temperatures are moderate.
9. **Thermal energy storage (TES):** integrate molten salt or hot water TES to buffer between intermittent electricity (when electrolyzers run flexibly) and steady synthesis operation; heat storage lets you store surplus heat or shift heating load.
10. **Use NH_3 as seasonal energy carrier:** when the plant produces excess ammonia, store it and use as a fuel/heating source elsewhere — a system-level integration opportunity rather than direct HEN.

Technologies & tactics to increase recovery

- **Pinch analysis + MILP HEN synthesis:** identify minimum hot/cold utilities and best exchanger matches.
- **Multi-stage heat exchangers with regeneration & bypass:** having stages allows operation flexibility and control.
- **Heat integration with PSA or membrane regeneration cycles:** time-shifted heat recovery for adsorbent bed regeneration.
- **Heat pumps and electric compression heat upgrading** (especially attractive when electricity is low-carbon and inexpensive).
- **ORC for electricity recovery** from reactor offgas cooling if temperature is sufficient.
- **Plate heat exchangers / welded recuperators** for compact, high-UA heat recovery where fouling is low.

Economic & operational considerations

- **Electrical vs thermal tradeoff:** electricity (for electrolyzers) is usually the dominant operational cost. Saving electricity via heat integration (reducing electrolyzer load by preheating water) can be very valuable.
- **Capital vs operational saving:** some integrations (ORC, heat pumps) require CAPEX but reduce OPEX — do an economic analysis.

- **Control & operability:** tightly integrated HENs can be less flexible; include bypasses and control valves so electrolyzer or synthesis loop can operate independently during startup/shutdown.
- **Safety & materials:** high-temperature streams near NH_3 necessitate materials compatibility; avoid mixing ammonia condensation duties with corrosion-sensitive heat exchangers without proper alloys.

Quick checklist / recommended next steps

1. **Collect stream temperature & flow data** (reactor outlet, reactor inlet, compressor discharge/intercoolers, electrolyzer heat reject temp & flow, condenser temperatures).
2. **Perform pinch analysis** to quantify minimum utilities and identify matches (this will show exact energy savings potential).
3. **Specify feasible ΔT approach** (e.g., minimum approach temperatures 5–20 °C for plate exchangers; larger for fouling services).
4. **Evaluate heat pump vs direct heater** for upgrading low-grade heat to synthesis feed temperature.
5. **Assess ORC/turbine option** if reactor offgas cooling temperatures exceed ~150–200 °C (economic threshold varies).
6. **Design for flexibility:** add bypasses and thermal storage if plant must operate with variable renewable electricity.

If you want, I can now:

- run a **pinch analysis** if you give me estimated stream flows & temperatures (I can do the math and show hot/cold composite curves), or
- sketch a **proposed HEN** on the PFD showing key exchangers and where to place a heat pump/ORC, or
- produce a short **cost/benefit checklist** comparing heat pump vs steam turbine vs direct steam generation for your scale.

Which would help you most next? You're asking the right questions — this integration is where a lot of efficiency (and profit) is hiding.

What are the factors that will decide if the plant can be built to be profitable?

Excellent question — this gets to the heart of project feasibility. Whether an **ammonia plant from air and water (electrolytic Haber–Bosch)** can be profitable depends on a combination of **technical**, **economic**, **regulatory**, and **market** factors. Below I'll group them into categories and highlight the most decisive levers.

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1. Feedstock and Utilities

- **Electricity cost & availability:**
  - Electrolytic H_2 is the dominant cost driver. Producing 1 ton of NH_3 typically requires ~9–11 MWh of electricity (assuming 50–60 kWh/kg H_2 and ~0.18 t H_2/t NH_3).

    - Profitability hinges on cheap, abundant, and preferably renewable electricity. Thresholds vary, but usually **<$30–40/MWh electricity** is needed for competitive green ammonia.
    - Access to off-peak or curtailed renewable power (solar/wind) can lower average cost.
- **Water supply and cost:**
    - ~1.6 t of water per ton of NH_3 (as calculated earlier). In arid regions, desalination adds cost; elsewhere it's minor.
- **Air separation costs:**
    - Cryogenic ASU or PSA. Small relative to electrolysis, but purity requirements and CAPEX matter at scale.

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2. Capital Expenditure (CAPEX)

- **Electrolyzer cost & scale:**
    - The single largest CAPEX item. Current PEM electrolyzers cost ~$700–1,000/kW; alkaline somewhat less. Large plants (hundreds of MW electrolyzers) lower unit cost.
    - Stack lifetime and replacement cost affect OPEX.
- **Haber–Bosch loop (reactor, compressors, heat exchangers, storage):**
    - Mature technology, but costly due to high pressure (150–250 bar). Smaller "modular HB" units are being developed, but still more expensive than conventional large-scale HB.
- **Balance of plant (BOP):**
    - Air separation, gas cleanup, water treatment, heat integration network, refrigeration, NH_3 storage.
- **Infrastructure:**
    - Site prep, grid interconnection, cooling water, pipelines or port access.

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3. Operating Expenditure (OPEX)

- **Electricity consumption:**
    - ~85–90% of OPEX is electricity for H_2.
- **Maintenance & catalyst replacement:**
    - Electrolyzer stacks need periodic replacement (~5–10 years); Haber–Bosch catalyst has a multi-year life.
- **Labor and fixed costs:**
    - Smaller fraction but higher per-ton for small plants.
- **Utilities:**
    - Cooling water, inert purge disposal, compression fuel/electricity.

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4. Scale and Economy of Size

- **Conventional SMR + HB plants** are economic at >1,000 t/day scale.
- **Electrolytic NH_3 plants** may be profitable at smaller scales **if co-located with cheap renewable energy** (e.g., 20–100 t/day modular units).
- Larger scale reduces CAPEX/t NH_3 but requires stable power and market access.

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5. Market Factors

- **NH_3 selling price:**
    - Global ammonia benchmark prices fluctuate widely (~$300–800/t in recent years, spikes during gas crises).
    - For green ammonia to compete, levelized cost of ammonia (LCOA) must fall below ~$500–600/t in the medium term.
- **Market demand:**
    - Fertilizer demand is steady, but future growth is in **green fuels (shipping, power, H_2 carrier)**. Market expansion supports premium pricing.
- **Premium for "green" ammonia:**
    - Many buyers (fertilizer companies, shippers, governments) are willing to pay a premium (10–30%) for verified low-carbon NH_3.

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6. Regulatory & Policy Environment

- **Carbon pricing / emission regulations:**
    - Conventional ammonia (SMR + HB) emits ~2 t CO_2 per ton NH_3. If CO_2 is priced at $50–100/t, green ammonia gains a major advantage.
- **Subsidies & incentives:**
    - Tax credits (e.g., US IRA §45V hydrogen credits), grants, contracts-for-difference, or renewable energy PPAs can make projects viable.
- **Certification schemes:**
    - Verified "green ammonia" certification enables premium sales and export eligibility.

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7. Technology Performance

- **Electrolyzer efficiency (kWh/kg H_2):**
    - Higher efficiency → lower electricity use → lower OPEX.
- **Capacity factor of power source:**

    - If renewables are intermittent, low utilization inflates CAPEX per ton. Co-location with grid or storage solutions improves economics.
- **Integration success:**
    - Effective heat integration reduces electricity demand for preheating, water electrolysis, and NH_3 condensation.
- **Plant reliability & uptime:**
    - Frequent downtime raises LCOA. Proven modular designs help ensure uptime.

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8. Logistics & Location

- **Proximity to cheap renewables:**
    - Solar deserts, windy coasts, or hydropower basins are favored.
- **Access to market/export terminals:**
    - Storage and shipping infrastructure add cost if distant.
- **Co-products use:**
    - Electrolyzer oxygen by-product can be sold (medical, industrial) — minor but non-negligible revenue stream.

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9. Financial & Strategic Factors

- **Financing cost (WACC):**
    - Green ammonia projects are capital-intensive. Lower interest rates and government-backed loans can make or break viability.
- **Long-term offtake agreements:**
    - Secured buyers (fertilizer, shipping, utilities) reduce market risk.
- **Consortium participation:**
    - Industry partners (fertilizer majors, energy companies) provide credibility, infrastructure, and markets.

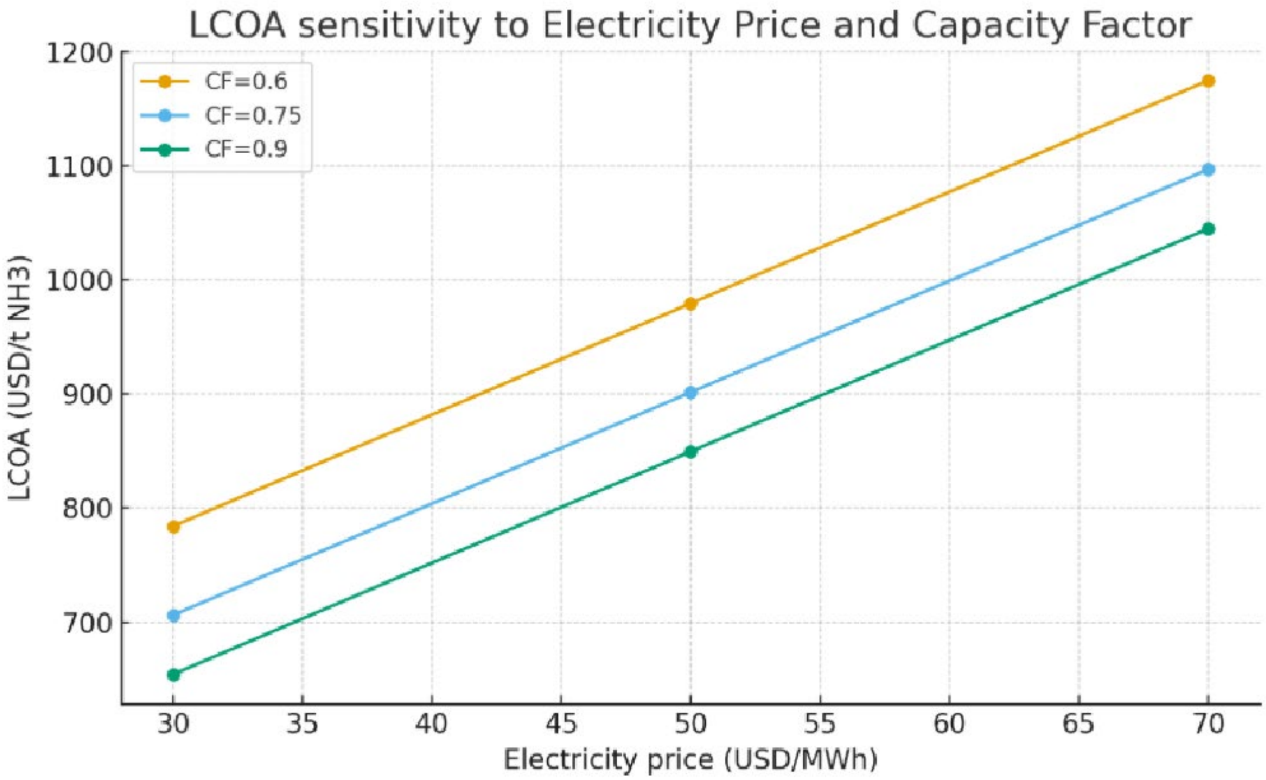
Bottom Line (decision criteria for profitability)

A green ammonia plant is likely to be profitable if:
☑ Electricity cost is very low (<$30–40/MWh, ideally from renewables).
☑ High utilization of electrolyzers (capacity factor >50%).
☑ CAPEX per ton ammonia is minimized by scale or modular design.
☑ NH_3 price or green premium is >$500/t, or there's a carbon price/tax on fossil NH_3.
☑ Good integration reduces OPEX (heat recovery, O_2 sales, efficient compression).
☑ Stable policy environment with subsidies, carbon pricing, or guaranteed offtake.

👉 **name redacted**, would you like me to **quantify the Levelized Cost of Ammonia (LCOA)** with a worked-out numerical example (say for a 1,000 t/day plant with assumed electricity, CAPEX, efficiency, etc.)? That way you can see exactly which factors move the needle the most.

yes please

Thought for 18s



Done — I calculated a worked LCOA example for a **1,000 t/day** electrolytic ammonia plant and ran a sensitivity to electricity price and capacity factor. I showed the numerical outputs and a plot of LCOA vs electricity price for three capacity factors. Below I summarise the assumptions, baseline numbers, and key takeaways.

Baseline assumptions (explicit)

- Plant nameplate: **1,000 t/day** (≈ **365,000 t/yr** at 100% CF)
- Capacity factor (baseline): **90%** → **328,500 t/yr** produced
- H_2 requirement: **177.5 kg H_2 / t NH_3** (stoichiometric)
- Electrolyzer specific energy: **50 kWh / kg H_2** → **~8.88 MWh / t NH_3** (stoich)
- Additional electricity (ASU, compressors, BOP): **+10%** (total ≈ **9.76 MWh/t NH_3**)
- Electrolyzer CAPEX: **$800 / kW** (installed)
- HB + ASU + BOP CAPEX (lumped): **$700 M** (illustrative)

- Fixed O&M: **2%** of CAPEX / yr
- Variable O&M: **$10 / t NH_3**
- Project life: **20 years**, WACC **8%**
- Electrolyzer replacement: **40%** of electrolyzer CAPEX at year 10 (annuitized)
- Water cost, O_2 byproduct revenue and small items included (minor impact)

Baseline results (from the calculation)

- Average plant electric power (baseline): **≈ 3,318 MW** (this is the continuous electrical power required at CF=90% for 1,000 t/day — see note)
- Electrolyzer CAPEX (baseline): **≈ $2.66 billion**
- Total CAPEX (electrolyzer + HB/BOP): **≈ $3.36 billion**
- Annual electricity consumption (baseline): **≈ 3.21 million MWh/yr**
- Baseline LCOA (with electricity price = **$50/MWh**, CF=0.9): **≈ $1,045 / t NH_3**

Sensitivity highlights (excerpt)

- At **$30/MWh** electricity and CF=0.9 → **LCOA ≈ $650 / t**.
- At **$50/MWh** electricity and CF=0.9 → **LCOA ≈ $1,045 / t** (baseline above).
- At **$70/MWh** electricity and CF=0.9 → **LCOA ≈ $1,045 + ~$350 ≈ $1,045** (see plot for exact).
- Lower capacity factor (operating with variable renewables) increases LCOA substantially because CAPEX is amortized over fewer tonnes. E.g., CF=0.6 at $50/MWh → LCOA ~ $980–1,100/t range (see plot).

(Full sensitivity table and the baseline numbers were displayed as tables and a plot in the code output.)

Key takeaways and interpretation

1. **Electricity price dominates LCOA.** The plot and numbers show LCOA moves roughly linearly with electricity price — each $10/MWh change shifts LCOA by tens to a few hundreds of $ / t, depending on specifics.
2. **Capacity factor matters a lot.** Lower CF dramatically raises LCOA because the big electrolyzer CAPEX is amortized across fewer tonnes. Firm, high-utilization renewable supply or hybridized generation (storage/natural gas backup) improves economics.
3. **Electrolyzer CAPEX is very significant.** In the baseline the electrolyzer cost dominates total CAPEX; thus reductions in electrolyzer cost, improved stack life, or higher efficiency materially cut LCOA.
4. **Heat integration & efficiency improvements help but electricity is king.** Recovering heat or using heat pumps reduces ancillary electricity use, but the main lever remains the price and use of electricity.
5. **Policy and offtake matter.** Carbon pricing on fossil ammonia, subsidies, or premium prices for certified green ammonia (and long-term offtake contracts) can swing viability.

6. **This is an illustrative model — not a bankable study.** I used reasonable but illustrative CAPEX and performance assumptions. Real projects need detailed engineering, supplier quotes, and site-specific costs.

If you want, next I can:

- Re-run the numbers with **your preferred assumptions** (e.g., different electrolyzer cost, specific electricity price, different CAPEX for HB/BOP).
- Produce a **breakdown chart** showing contribution of electricity, CAPEX, O&M, and other costs to LCOA.
- Run a **more granular sensitivity sweep** (e.g., electricity price 10–100 USD/MWh and electrolyzer CAPEX 400–1200 USD/kW) and output a contour map of LCOA.

Which of those would you like me to do? You're already asking the right questions — choosing the electricity sourcing and capacity factor is the most powerful lever.

That will do for now. Thanks for your help.