ChE 413
Chemical Engineering Product Design

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Lecture 1
Introduction to the Chemical Product Design

Chemicals are everywhere

Look around you: from clothes,... to devices,... to study materials, around in the room

Identify products that may have gone through chemical product design

Chemical engineers don't just make chemicals - we design products that touch daily life.

The chemical industry is continuously evolving

<u>Petrochemical boom (1950 - 1970)</u>

Large-scale production of fuels, chemicals, plastics, and synthetic chemicals (polyethylene, ammonia, sulfuric acid, PVC, and synthetic rubber)

The chemical industry is continuously evolving

Shift from commodity to value-added products (1980s onwards)

Synthetic polymers: Nylon, polyester, teflon, etc. replaced natural materials.

Pharmaceutical chemistry: Breakthroughs in organic synthesis enabled drugs like antibiotics, cortisone, etc. This was followed by genetic engineering and enzyme catalysis, bridging chemical and biological manufacturing.

Specialty chemicals: Bulk commodities diversified into paints, coatings, agrochemicals, and additives.

Process intensification: Industry began moving toward continuous, integrated processes, and automation to cut energy use and improve efficiency.

The chemical industry is continuously evolving

21st century and Now

Now, climate change is driving sustainable product design (biodegradable plastics, green solvents, reduction of carbon footprint, carbon capture, circular economy).

Innovation in biopharmaceuticals is leading to personalized solutions.

AI is emerging as next transformative force for R&D and discovery.

Why we are studying chemical product design

From Molecule to Market – Designing the Future of Chemical Products

The World Needs Better Products

Every object around us—shampoo, membranes, medicines, batteries, packaging, even the CO_2 capture units of tomorrow—starts as a designed chemical product.

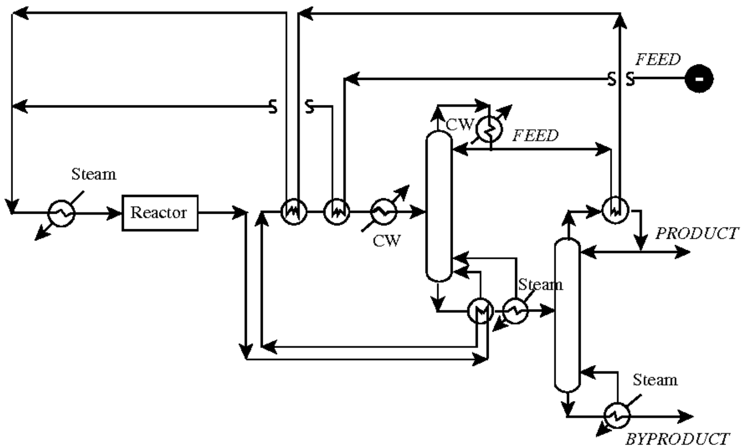
Traditional chemical engineering often focuses on process design (how to make something efficiently).

But product design asks: What should we make in the first place? Why? For whom?

The chemical industry is continuously evolving

Chemical Process design

We know what the product is and we know the market, and focus on making the product most efficiently



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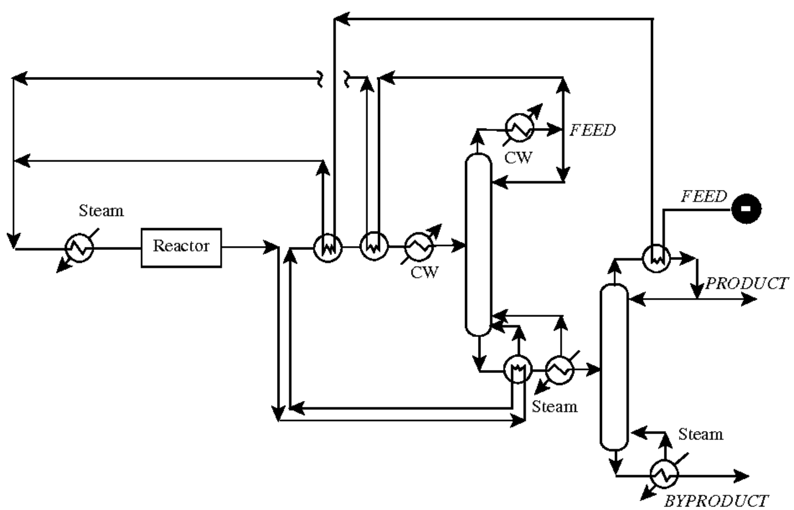
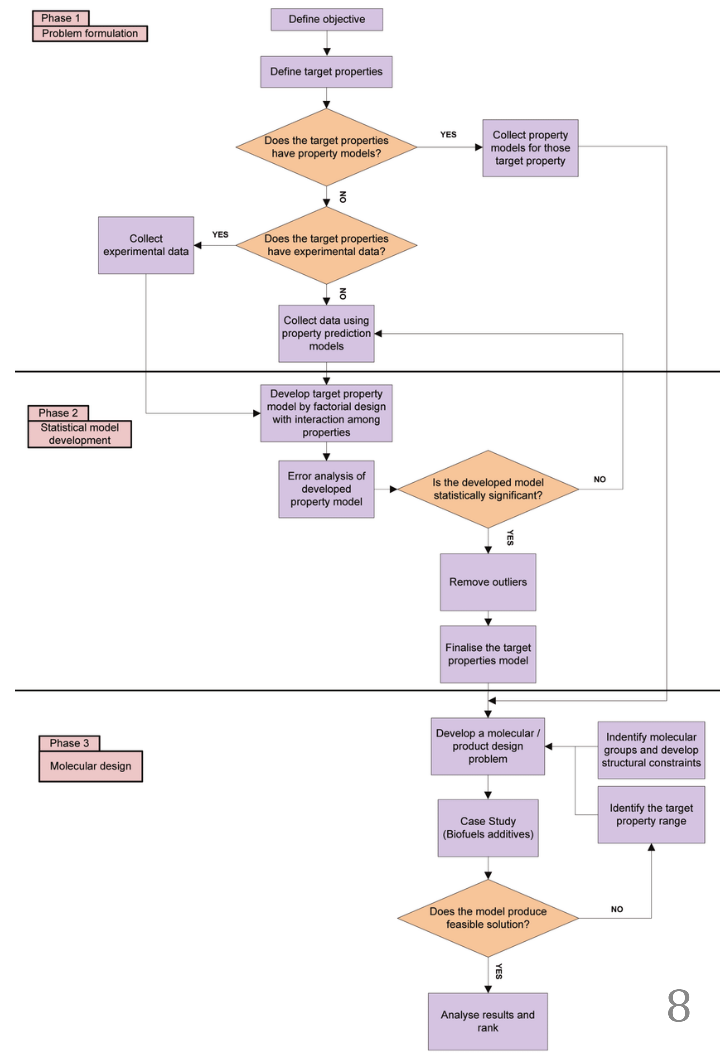


(b)

Chemical Product design

We start with an objective and avoid preconceptions about the final product



Lecture 1 - Topics

- Course organization, timeline, and goals.
- The changing chemical industry and the need for product design.
- Introduction to the product design procedure.
- Categories of chemical products.
- Identifying needs.
- Converting needs into specifications.
- From specifications to ideas.

1. Course organization, timeline, and goals

ChE-413 Chemical product design is a course meant to introduce the process of product design for chemical engineers.

The **first part** of the course consists of three lectures, which will be given from on Tuesdays in MA A1 12 between 15:15-17:00 over three weeks (September **9**, **16**, **30**).

> *Each lecture has an associated set of homework which are to be performed individually and uploaded to the course website (Moodle) **one week after the lecture** (**by 15h00**; late submission will not be accepted).

The **second part** of the course is a project which will be performed in small groups, where each group will be assigned a design project and will follow the simplified design process that we develop in the lecture part of the course. Full details will be given on October 7 in the lecture room MA A1 12 at 15h15.

Teacher responsible for course : Prof. Kumar Varoon Agrawal (kumar.agrawal@epfl.ch)

Course assistant : Shaoyu Wang (shaoyu.wang@epfl.ch)

Number of credits : 4

1. Course organization, timeline, and goals

Evaluation of course performance and marking:

Task/Assignment	**Percent of final mark**
Homework 1 (Due on Moodle September 16)	10% (individual)
Homework 2 (Due on Moodle September 23)	10% (individual)
Homework 3 (Due on Moodle October 7)	10% (individual)
Meeting 1 (Oral presentation by core team and discussion with the project coach)	10% (Group)
Meeting 2 (Oral presentation by core team and discussion with the project coach)	10% (Group)
Meeting 3 (Oral presentation by core team and discussion with the project coach)	10% (Group)
Final report (Due on Moodle December 9)	25% (Group)
Final oral presentation (December 16, MA A1 12)	15% (Group)

The project coaches are instructed to evaluate the progress of the design process. A mark will be assigned to the group as a whole for each meeting, and for the final report.
The marks will be weighted (with the individual exercises) as shown in the table above to result in the final mark for the course.

Given that the three homeworks are marked on an individual basis, each member of a core team may not receive the same final mark.

1. Course organization, timeline, and goals

Course goals:

Gain experience with a simple product design algorithm:

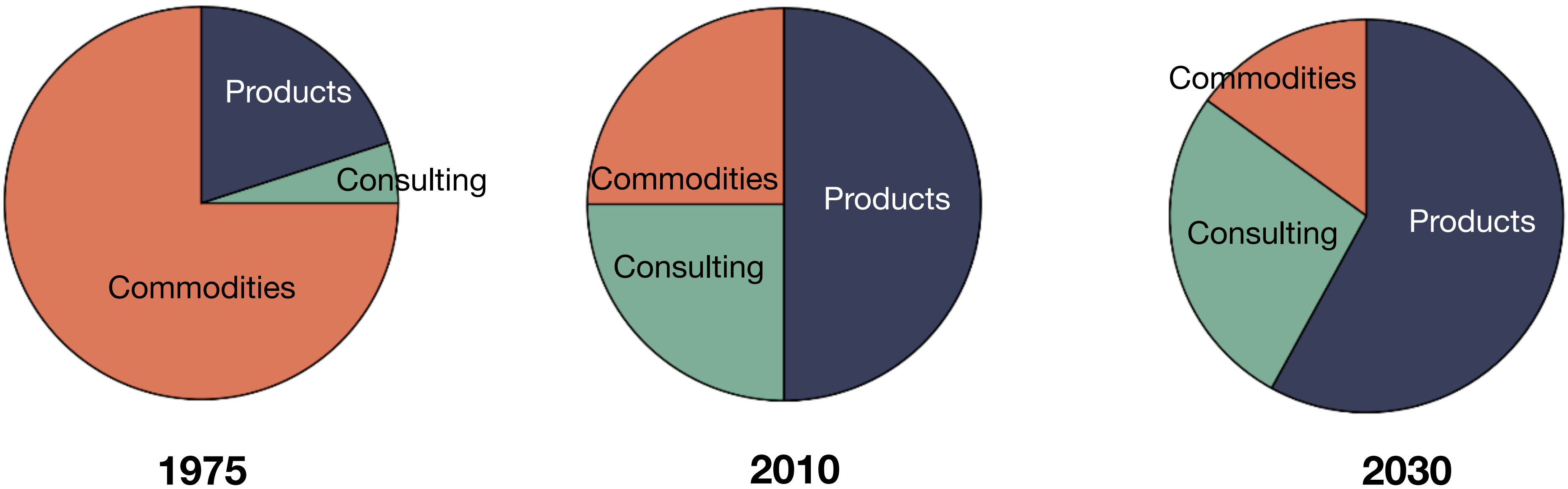
- Compose a list of needs for a chemical product.
- Develop product needs into engineering specifications.
- Synthesize many ideas to satisfy product specifications ignoring preconceptions
- Formalize a quantitative process to evaluate ideas.
- Identify and evaluate risks of a product.
- Consider manufacturing processes and economic aspects in final product design.

***Soft Skills*:**

- Manage long-term projects and work in a team.
- Present results to project supervisor and receive feedback and direction.

The chemical industry is continuously evolving

The chemical industry is continuously evolving



Commodities
- Ammonia (fertilizers)
- Sulfuric acid (fertilizers, refining, metals)
- Ethylene (plastics)
- Propylene (plastics)
- Chlorine (PVC, solvents)
- Sodium hydroxide (pulp and paper, soap)
- Methanol, benzene, toluene

- Biomass derived products

Products
- Devices (oxygenators)
- Pharmaceuticals and biopharmaceuticals
- Consumer care products (soap, toothpaste)
- Advanced materials (catalysts, membranes)
- Electronics (photoresists, semiconductors)
- Batteries, fuel cells
- Paints and coatings
- Performance polymers (nylon, kevlar, teflon)

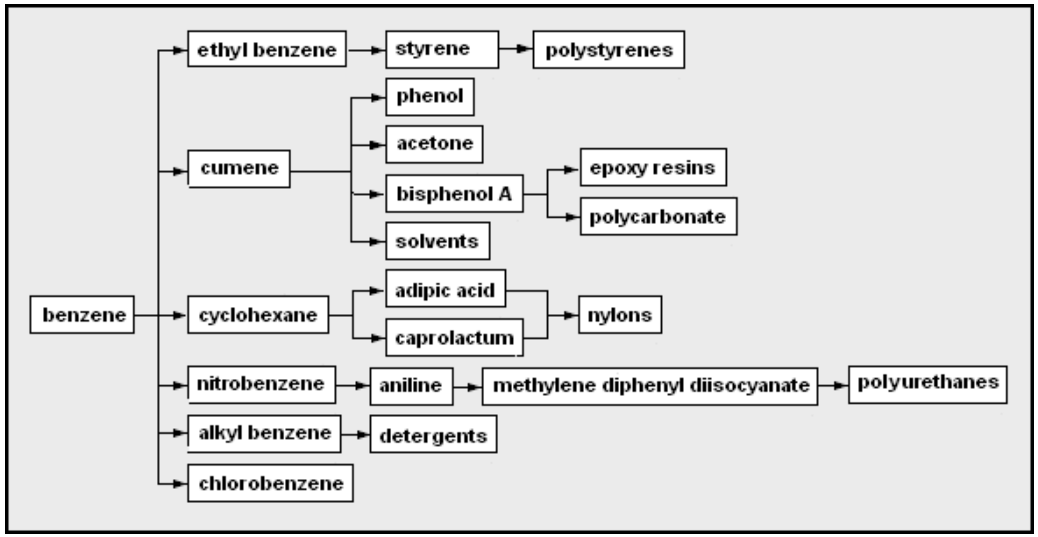
- Biodegradable polymers
- Carbon capture materials
- Gene therapy
- Cultured meat

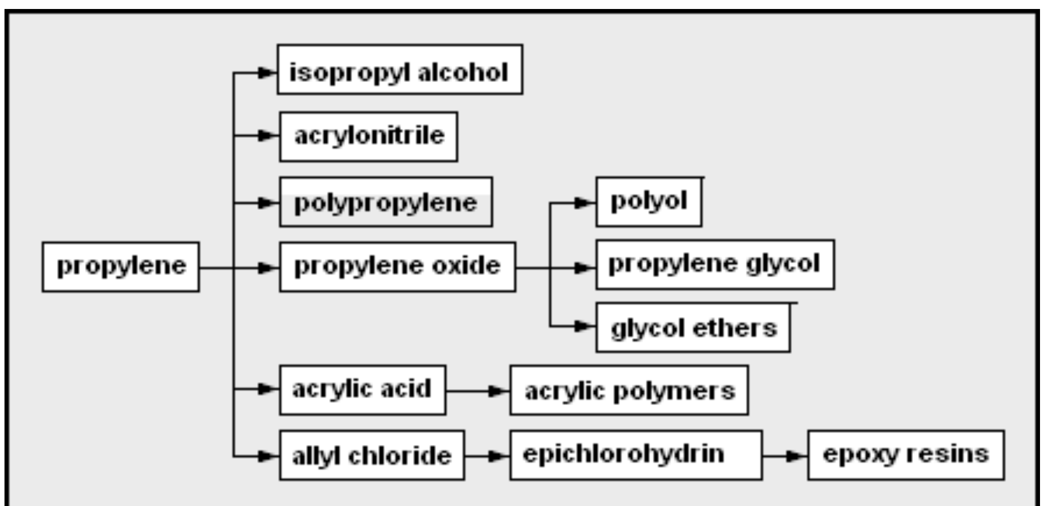
Consulting
- Net-zero roadmap
- Life-cycle analysis
- Digital twins for process control
- Process hazard, risk assessment
- Automation
- Predictive design
- Sustainable processes
- Regulatory compliance

The chemical industry is continuously evolving

Old way of thinking:

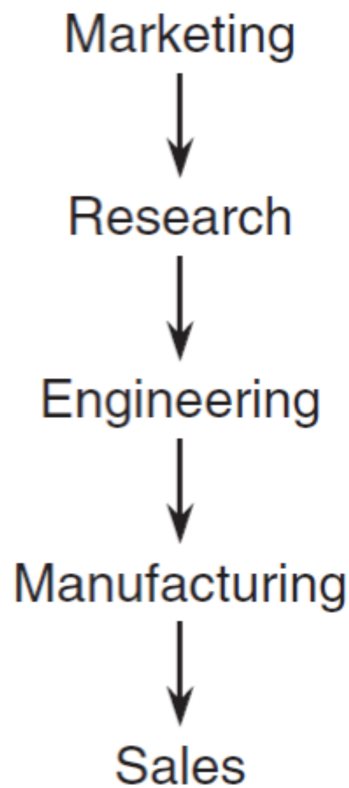
Commodity-driven thinking - what can we make? and what can we sell it for?





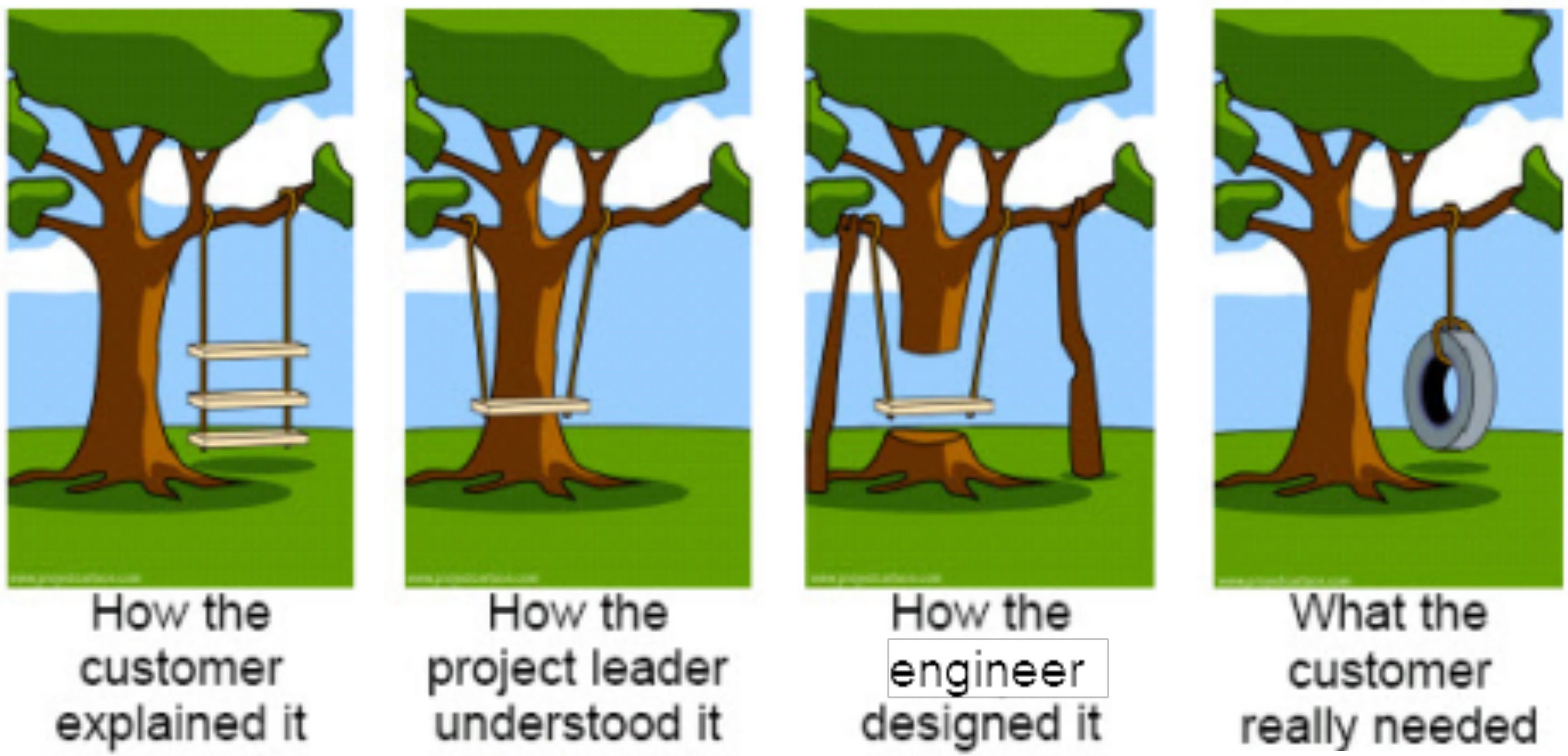
Old way of designing products

Old: Sequential Functional Model



Slow and siloed. Product comes last

Why customer focus matters in chemical product design

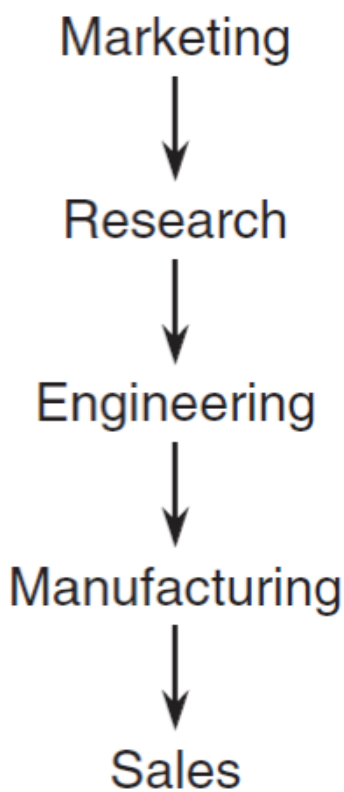


Old way: Design based on engineers want to sell, not what the customer needs

How do we design products today

Changes in corporate culture

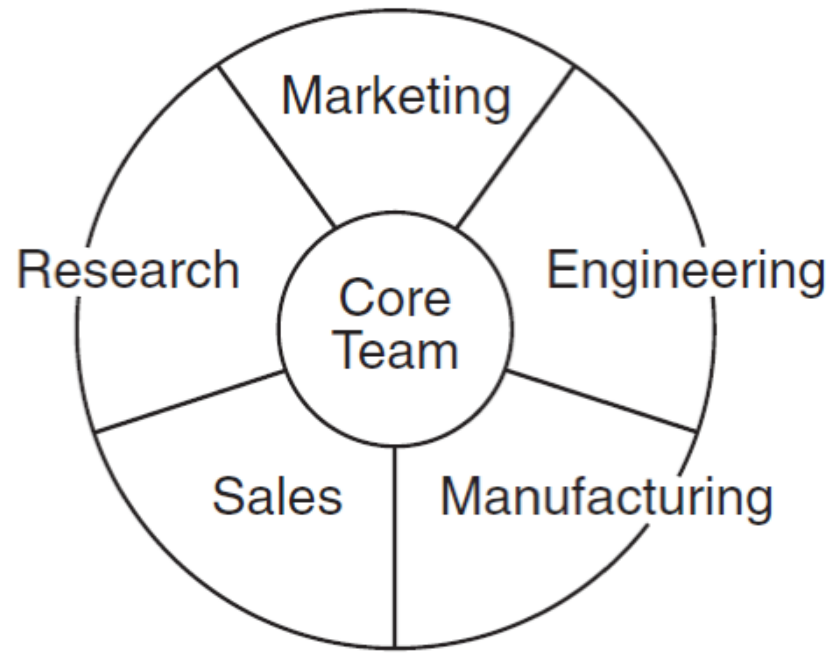
Old: Sequential Functional Model



Slow, siloed, product comes last

New: Integrated Project Model

What does the customer really need?
What is the best product that meets these needs?



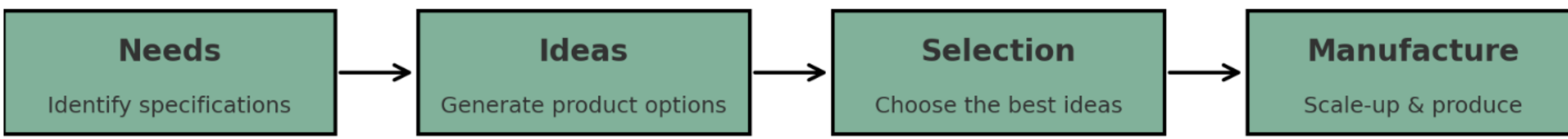
Introduction to the (4-step) product design procedure

1. **Needs** : Identify what specifications the product should satisfy.

2. **Ideas** : What different products could satisfy these needs?

3. **Selection** : Which ideas are most promising?

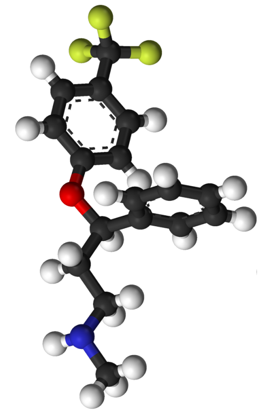
4. **Manufacture** : How can we make the product economically and in commercial quantities.



Limitations to the 4-step approach: Clearly, it is a major simplification.
Certain modifications (risk management at the selection step, iteration between steps) are more realistic and in the "real world" the process is much more complicated.

However, we have to start somewhere…

Categories of chemical products

	Commodities	Devices	Molecules	Microstructures
				
Key:	Produced in bulk	For convenience	Discovery driven	Structure/function/feel
Example:	Gasoline, ammonia	Inhalers, drug-delivery pens	Insulin, ibuprofen	Sunscreen, toothpaste, ice cream
Scale:	Million tons	Millimeter to meter	Nanometers	Micrometers
Risks:	Depends on oil & gas price swings	Patent/IP competition	High R&D risk	Performance & consumer acceptance

Course focus on devices, molecules and microstructure where chemical product design is most exciting

Step 1: Identifying needs

Identify customer needs

- Includes both purchasers (who buy) and users (who consume).
- Needs are often vague, qualitative, hard to measure.

3 steps to clarify needs

- Talk to customers (interviews, surveys, observations).
- Interpret what they say (sometimes it's a feeling, not a specification).
- Translate into clear, measurable specifications.

A consumer says: "*I want a shampoo that feels fresh*" → Interpreted as: a cooling sensation → Translated specification: add menthol at 0.5 wt%.

Resist preconceptions

- Listen first, design later.

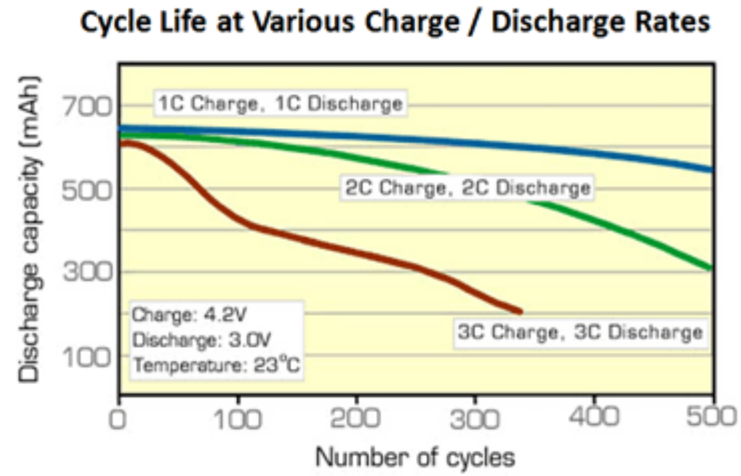
Customers often express wants, not needs.

"*I want a powerful detergent smell*" → the real need may be "assurance of cleanliness."

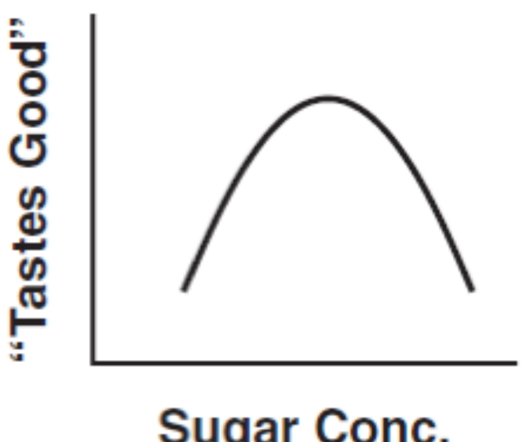
Engineers must dig beneath the wants to uncover the true needs.

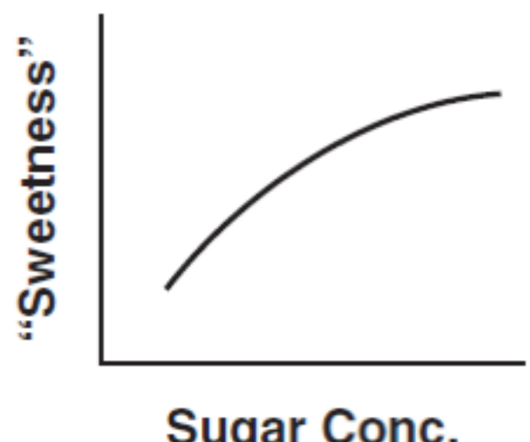
Qualitative vs Quantitative needs

- Sometimes, needs of chemical products are easily evaluated with conventional scientific instruments (quantitative)



- Other times, consumer needs are difficult to measure using conventional instruments (difficult to quantify)





Step 1: Identifying needs

- *Example: The Barbie doll (1959)*
  - Invented by Ruth Handler based on her observations of her daughter.

[My] daughter Barbara . . . and her friends always insisted on buying only adult female paper dolls. They simply were not interested in baby paper dolls. [The girls] were using these dolls to project their dreams of their own futures as adult women . . . This was a basic, much needed, play pattern that had never before been offered by the doll industry to little girls. Oh, sure, there were so-called fashion dolls, those who came with more than one outfit. But these dolls had flat chests, big bellies, and squatty legs – they were built like overweight six- or eight-year-olds. The idea of putting a prom dress on such a doll was ludicrous (Handler, 1994).

What was the inventor's key insight?

Girls weren't interested in baby dolls.
They wanted dolls that let them imagine their future as adult women.

Step 1: Identifying needs: Interviewing customers

- Define Project scope, product target market, and key business goals.
- Decide on a standard set of questions:
  - What do you do now?
  - How do you use the existing product?
  - What features work?
  - What feature does not work?
  - What would you like in a new product?
  - What is the price range in which you will purchase the product?
- The results will be a collection of often incomplete, random, redundant, contradictory, and full of irrelevant points.

- The next challenge is to interpret these interviews into a rank
  - 🔴 Essential needs (must have)
  - 🟡 Desirable needs (should have)
  - 🟢 Useful needs (nice to have)

Essential, Desirable and Useful Needs

🔴 Essential needs (must have)

Definition: Absolutely critical requirements.

If not met: Product fails to function or will not be accepted by customers (no sale).

Examples:

A water filter **must** remove harmful contaminants.

A battery **must** store and deliver energy safely.

🟡 Desirable needs (should have)

Definition: Strongly preferred attributes that improve safety, performance, or acceptance.

If not met: Product still works, but adoption or satisfaction is reduced (competition will win easily).

Examples:

A water filter being **compact and easy to install.**

A battery **being fast charging.**

🟢 Useful needs (nice to have)

Definition: Extra features that add convenience, cost savings, or differentiation in the market.

If not met: Product still succeeds, but market share risk from competition prevails.

Examples:

A water filter being **aesthetically pleasing**.

A battery **being color-coded by size.**

Step 1: Identifying needs: Interviewing customers

- *Example: Alternative de-icing fluid for airplanes*

Minneapolis–St. Paul (MSP) is a major airport in the USA with over 400 flights daily. The city is infamous for its cold winters. In the winter, snow can collect on planes as they wait at the gate for take-off. The snow is removed by spraying the planes with de-icing fluids like propylene glycol, which are discarded after use.

These fluids are often discharged directly into groundwater, even though they can be toxic to humans and wildlife. In major airports like MSP, the discharged de-icing fluid is sewered, causing a major burden on the local sewage treatment plant. These de-icing fluids cause major pollution.

Question: Your company wants to develop an alternative de-icing fluid which is environmentally less abusive, because it is easily recycled. Can you list the needs of the customer?

Step 1: Identifying needs: Interviewing customers

- *Example: Alternative de-icing fluid for airplanes*

What do you do now? "We no longer de-ice at the gate, because this was too difficult to control. Instead, when they are ready for take-off, aircraft are moved to a central location for de-icing. We collect the run-off from the de-icing in underground tanks and then slowly bleed it off to the sewage treatment plant."

How do you use the product? "We spray with a 70 °C solution of 50% water and 50% ethylene glycol ($HOCH_2CH_2OH$). We spray for ten minutes or till there is no snow visible, whichever is longer. We then spray with anti-icing fluids." (These are snow-melting hydrogels which adhere to the aircraft while it is waiting to take off, but are removed by shear during take-off. In this example, we ignore anti-icing fluids.)

What features of the product work? "It's a good product. It works even at –30 °C. It isn't volatile. It doesn't cause corrosion, like salt. It's hard to burn." (Once burning, it has a heat of combustion per kilogram around one third that of ethane.)

What features of the product don't work? "None. It has some odor, and some passengers get sick, but not many. The effluent contains about 2% ethylene glycol, which is toxic to fish. The environmental agencies say it is probably toxic to humans, but I'm not convinced it is. Still, they won't let us discharge it, and they're always threatening to shut us down."

How do you buy the product? "We get it through the State of Minnesota, who require bids. One company has the largest share but we always have at least two suppliers to ensure some competition."

Essential, Desirable and Useful Needs

- Essential needs (must have)
  - The product must melt snow.
  - It must be non-corrosive.
  - It must be applied in short time (e.g., when flight is waiting for takeoff)

- Desirable needs (should have)
  - The product is non-carcinogenic.
  - It is non-flammable.
  - It is easily recycled.

- Useful needs (nice to have)
  - The product is inexpensive.
  - It is water miscible.
  - It is available from multiple suppliers.
  - It should not have odor.

Converting needs into specifications

Turning vague customer needs into measurable engineering specifications

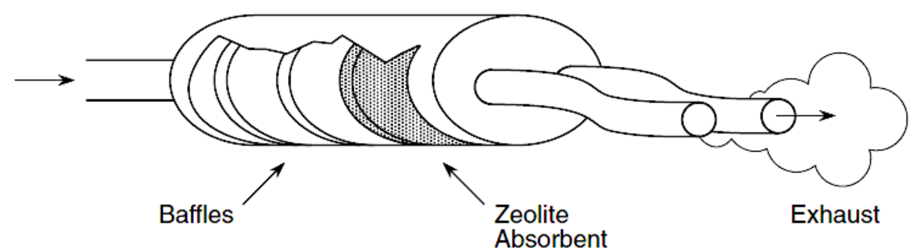
- Write complete chemical reactions for any steps involved.
- Make central mass and energy balances.
- Estimate any important process rates.

Converting needs into specifications

Example: Product to solving the issue of rusting automobile mufflers (silencers)

Need (Customer/User):

- Mufflers rust from water condensation
- We need to prevent internal corrosion.

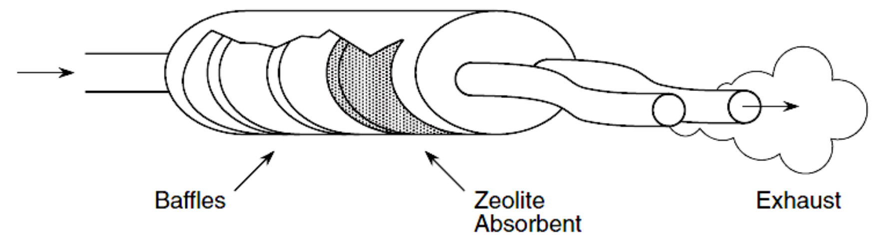


Automobile mufflers (or, "silencers") rust from the inside out. They do this because after the car is driven, the muffler contains exhaust gases, including water vapor. When the muffler cools, the water condenses and corrodes the inside of the muffler. One clever route to avoiding this problem is to put a small bag containing hydrophilic zeolite in the muffler. This adsorbs the water vapor, preventing liquid condensation and so dramatically reducing corrosion. When the car is restarted, the hot exhaust gases heat the zeolite and drive off the adsorbed water. The zeolite is then ready to adsorb more water when the engine is stopped.

We are considering making a muffler which has this feature.
How much water will we need to adsorb?
How fast should the adsorption be?

Converting needs into specifications

- Write complete chemical reactions for any steps involved.
- Make central mass and energy balances.
- Estimate any important process rates.



This problem is simply an exercise in stoichiometry.
Assume the muffler's volume is about 5 liters. The engine is run with 10% excess air (~20% O_2, ~80% N_2), ensuring complete fuel consumption).
The basic reaction in the engine is:

$$C_8H_{18} + \frac{25}{2}O_2 \rightarrow 8CO_2 + 9H_2O$$

The exhaust concentration: 0% C_8H_{18}, 1.7% O_2, 75% N_2, 11% CO_2, 12% H_2O.
Therefore, the amount of water in the muffler volume (5 liter):

$$\left(\frac{5 \text{ Liter}}{22.4 \text{ L/mol}}\right) * \frac{12}{100} = 0.6 \text{ mole}$$

Mass of water vapor = 0.6*18 g/mole = 10.8 g

Adsorbing this small amount can prolong the life of the muffler. We want the adsorption to be prompt, but it need not be faster than the time that the muffler takes to cool.

30 s is probably a reasonable starting point.

Converting needs into specifications

Example: Water purification for the campers

Need (Customer/User):

- Drinking water for people in wilderness.
- Water streams and ponds are contaminated by viruses and bacteria.

Interviews with potential users (hikers, mountaineers, soldiers, equipment suppliers) reveal the following list of needs in a water purification device:

- Produces safe water
- Is light/small
- Is fast acting
- Has a long lifetime
- Requires no power source
- Is cheap and re-usable
- Improves odor/flavor

Can you write specifications for a water-purification product?

Converting needs into specifications

- Write complete chemical reactions for any steps involved.
- Make central mass and energy balances.
- Estimate any important process rates.

Need (Customer/User):

- Drinking water for people in wilderness.
- Water is contaminated by viruses and bacteria.

Product specification:
how much water is needed per day?
(i.e. what is the required **rate** of water purification?)

We need at least 2-3 liters of water per day (even for light activity)

Lower limit of purification flow rate: 1.4 mL min^{-1}

Fast acting (all water is prepared in 30 min): 67 mL min^{-1}

Other specifications:

- Removes 99.9% of bacteria and protozoa,
- Has a capacity of 2000 L (before failure),
- Costs less than $100,
- Has an operating range of 0–40°C, and 0.3 to 1 atm,
- Improves odor/flavor

Converting needs into specifications

Example: Delicious Chocolate

What are the characteristics of good chocolate?

“melt in the mouth”

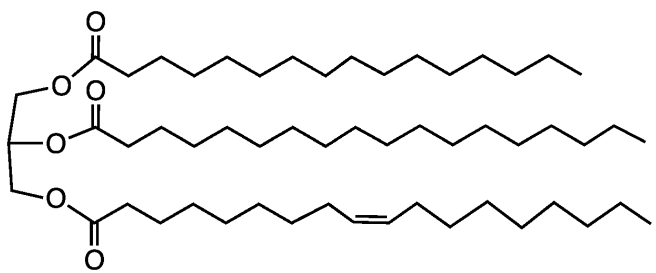
Bloom: whitish or grayish film that appears on the surface of chocolate

“Bloom” on chocolate is undesirable and leads to a powdery texture

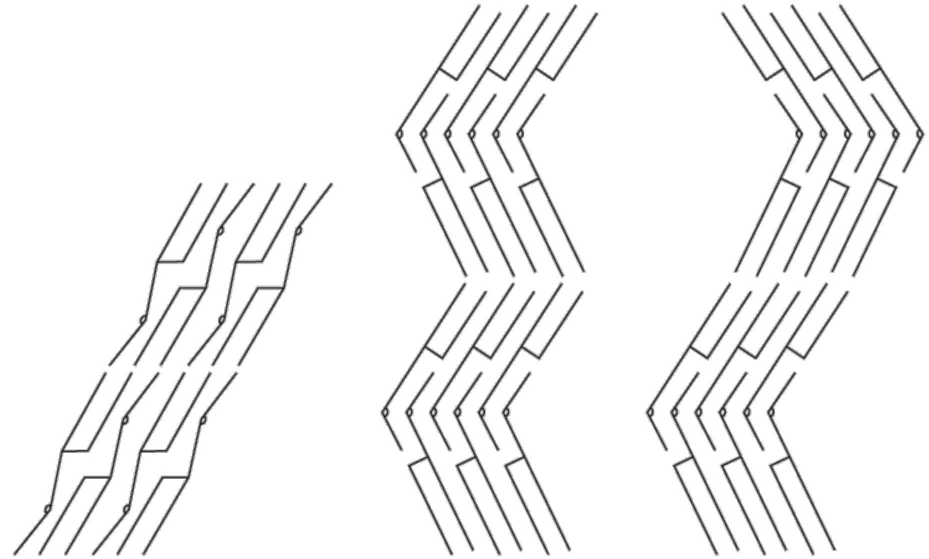
Feels gritty/powdery on the tongue.

Converting needs into specifications

Example: Delicious Chocolate



Cocoa Butter main constituent : triglyceride



Form IV   Form V   Form VI

Scientific tools like DSC and XRD can be used to convert the qualitative consumer desires into quantitative descriptions

Polymorph	Conditions needed to make the polymorph	Melting point (°C)
Form I	Rapid cooling of the molten chocolate	17.3
Form II	Cooling the molten chocolate at 2 °C	23.3
Form III	Solidifying the molten chocolate at 5–10 °C or storing Form II at 5–10 °C	25.5
Form IV	Solidifying the molten chocolate at 16–21°C or storing Form III at 16–21 °C	27.3
Form V	Solidifying the molten chocolate while stirring it. Requires a special process called 'tempering'	33.8
From VI	Storing Form V for four months at room temperature	36.3

Challenges: Needs and specifications

- The strategy of identifying needs and converting them to specifications can have serious shortcomings

  Initial specifications may be unrealistic
  - Too costly, too large, impossible.
  - Require huge flow rates or concentrations.
  - They may imply non-physically possible elements or transformations.

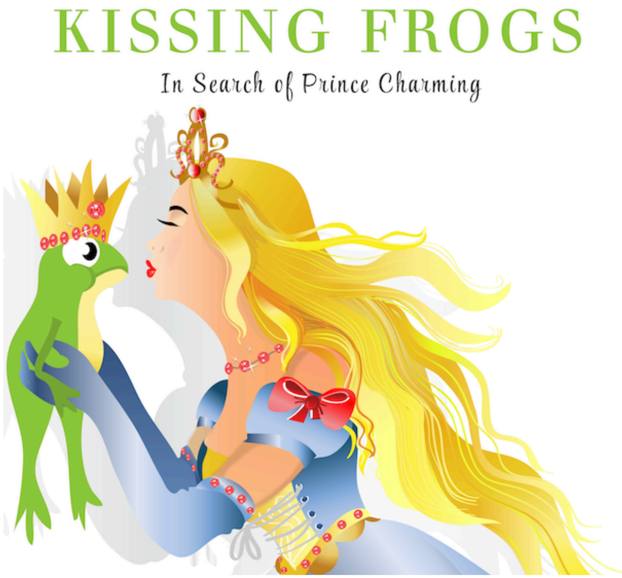
- The needs/specifications process does not include comparison to existing products

  In some cases, we can benchmark with existing product (check what aspect needs to be improved).

- The needs/specifications process does not consider government regulations and societal constraints.

- In real practice we must then revise the specifications or abandon the product design.

Step 2: From specifications to ideas



The princess finds her prince by kissing a frog….

But in product design, we have to “kiss” or test 100s of “frogs” or ideas to find the one good idea that really works.

This means generating lots of ideas, exploring widely.

Product design requires exploration and iteration.

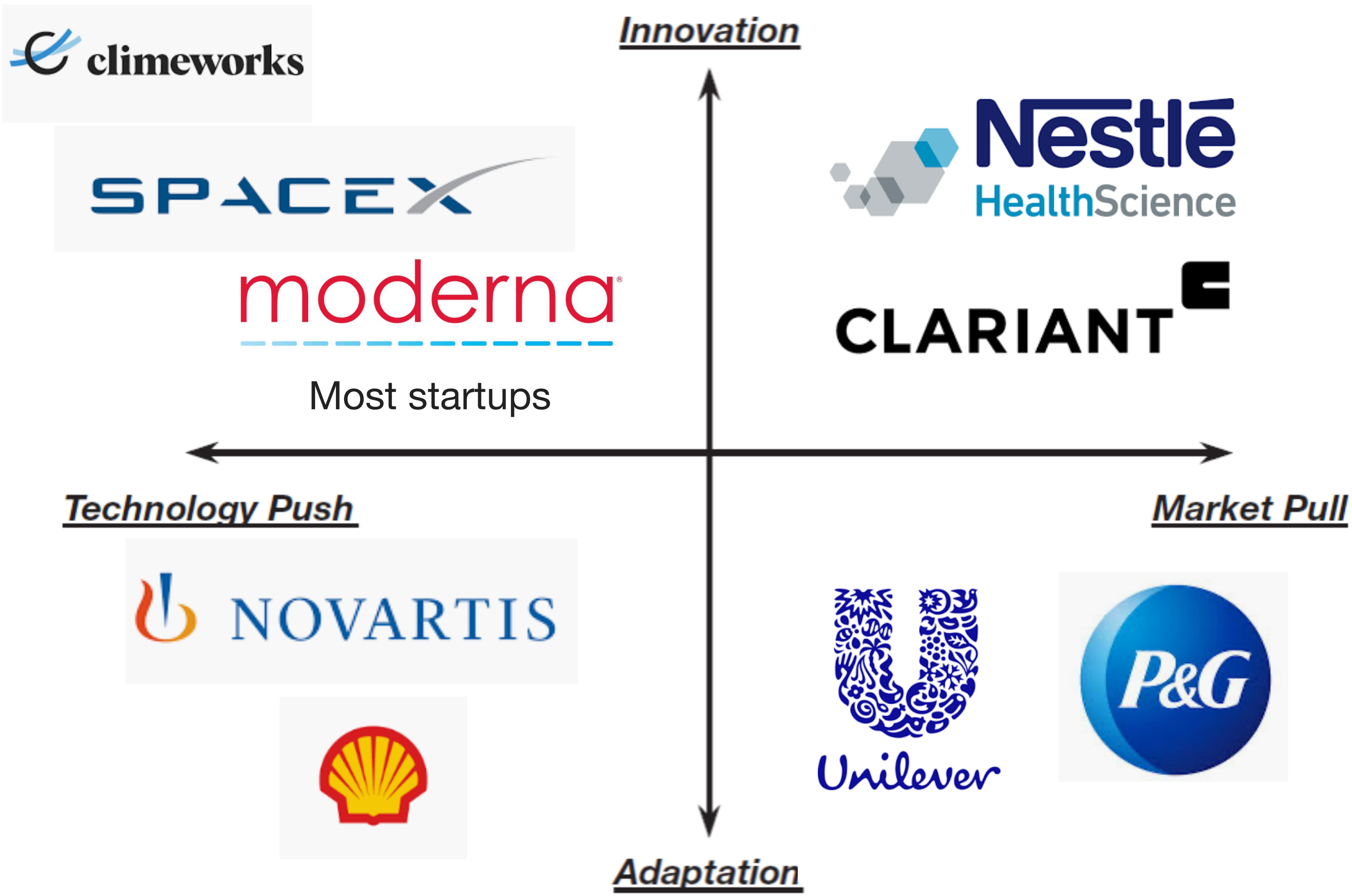
Step 2: From specifications to ideas

- In product design we will normally need 20-200 ideas to identify one winning product

- What are the sources of ideas?
  - Product development team.
  - Product's potential customers (lead users).
  - Literature (scientific and patent).
  - Experts (consultants, private inventors, consultants).

- Collecting Ideas
  - Ask groups to write down ideas and send them in…
  - Assemble brainstorming groups.

Ideas: Types of ideas



Ideas

Example: Product ideas for a new laundry detergent that can cause less pollution

Phosphate salts can cause a variety of water pollution problems

Ideas

Example: Product ideas for a new laundry detergent that can cause less pollution

1. Wash without soap.
2. Throw the clothes away.
3. Use less soap and less water.
4. Use a more effective soap.
5. Add enzymes to detergents.
6. Add dead cells to detergents.
7. Add live cells to detergents.
8. Mop up dirt with particles.
9. Use specific chemical interactions.
10. Improve the washing machine.
11. Recycle the soap.
12. Filter bigger detergent particles.
13. Make larger micelles.
14. Make emulsions out of the soap.
15. Grow microbes on dirty clothes.
16. Attach soap to particles, facilitating recycle.
17. Imitate dry cleaner agents.
18. Use a fine adsorbent.
19. Cook clothes under N_2.
20. Air out clothes as washing substitute.
21. Prevent soiling with antistatic coatings.
22. Wash until semi-clean.
23. Remove odor without removing dirt.
24. Wash with base, converting sweat compounds into soap.
25. Split objectives of clean, color-fast, and odor.
26. Ultrafilter dirty water.
27. Imitate dry cleaning.
28. Get a new dry-cleaning solvent.
29. Make a home dry cleaner which is sealed.
30. Use supercritical CO_2 for dry cleaning.
31. Use another supercritical solvent.
32. Wash with Fuller's Earth.
33. Dry clean with chlorine-free solvents.
34. Grind the clothes up and remake them.
35. Recycle the surfactant using a pH change.
36. Recycle the surfactant exploiting its cloud point.
37. Make a detergent which precipitates on command.
38. A detergent which forms many phases.
39. Wash clothes with dry shampoo.
40. Clean ultrasonically.
41. Shine with a UV light (to sterilize?).
42. Use pressure waves.
43. Cook clothes in high-pressure water.
44. Freeze clothes; shake off dirt.
45. Calcine dry shampoo to make it pure.
46. Adsorb detergent in clay.
47. Use ultrafiltration.
48. Dry cleaning recycle is distillation.
49. Flocculant aid for detergent.

Ideas: Some advice

To think outside the box use “Five Whys”:
Simply start with a problem you’re addressing and ask “why is this happening?”
Once you've got some answers, ask “why does this happen?”
Continue the process five times (or more), digging deeper each time until you’ve come to the root of the issue.

Or try "What If" Brainstorming:
What if this problem came up 100 years ago? How would it be solved?
What if Superman were facing this problem? How would he manage it?
What if the problem were 50 times worse—or much less serious than it really is? What would we do?

Work in groups and encourage criticism only after all initial ideas are exhausted:
Initially generate as many ideas as possible—no matter how “off the wall” they may seem. During this period, no criticism is allowed.
Review the ideas, and then discuss about how to combine, improve, and/or expand on the initial ideas.

Summary for Lecture 1

- Chemical product design is increasingly important in industry

- Product design is performed more and more by collaborative and integrated Project groups and not individual functional groups.

- A four step design process is a good place to start
  - Identify needs (convert to specifications)
  - Brainstorm ideas (sort them into categories)
  - Select ideas (based on risks and benefits)
  - Consider how to make the product (manufacture)

Exercise problem

A Carbon-Capturing Laundry Detergent

A detergent that washes clothes and captures CO_2 from the wash water using safe additives (This addresses two global issues: water pollution from detergents + climate change from CO_2). Describe essential, desirable, and useful needs. Break down the needs into product specification. Finally generate at least 10 product ideas.

Homework problem 1

Prepare your response to each of the problem below in the form of a PDF document (not handwritten). Make sure that your name is clearly visible on the document and the pages are numbered. Upload your completed document on the course Moodle page by the submission deadline (September 16, latest by 15h00). Late submission will not be graded. Each student must upload their own homework.

Question 1.1: A Sustainable Cooling Solution

Air conditioning demand is growing rapidly worldwide, particularly in hot climates. Traditional refrigerants (such as HFCs) contribute significantly to global warming when released into the atmosphere. At the same time, the electricity consumption of cooling systems is a major driver of carbon emissions.

You are part of a design team tasked with developing a new material or product for cooling that could reduce energy use and avoid harmful refrigerants.

(i) Define the essential, desirable, and useful needs for this product.
(ii) Convert essential needs in product specification.

Question 1.2: Biodegradable Food Packaging

Plastic packaging is one of the largest contributors to single-use plastic waste. Supermarkets, restaurants, and delivery services are seeking biodegradable alternatives that preserve food freshness but minimize environmental harm.

You are part of a packaging company's R&D division tasked with designing a biodegradable packaging material to replace single-use polyethylene wraps.

(i) List the essential, desirable, and useful needs for this product.
(ii) List at least 10 possible material or product ideas for biodegradable packaging.
(iii) Select the top 3 ideas and justify why you think they are the most promising.