

ASEE ChE Summer School Workshop

Teaching Process and Product Design

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Hour 1 W. D. Seider Focusing on Process Design.
Including Product Design

Hour 2 K. M. Ng Focusing on how to teach a course
on product design and the creation
of Product Design Case Studies
suitable for your department

Try to participate, offer your perspectives/
experiences, and suggestions

Can you find ways to get involved?

Introduction with Several Observations

Undergraduate ChE courses continue
to focus on **process design**

Typical lectures and design projects
assume the chemical product has been
selected -

concentrate on creating processes
to manufacture a product

i.e., **How to make a product?**

Not: **What to make?**

i.e., **product design**

- to satisfy customer needs

Process Design Courses

- follow engineering science courses that are process oriented

e.g., material and energy balances
open-system thermodynamics
fluid mechanics
heat and mass transfer
separations
unit operations
chemical reactor design

Ideal and real gases
Simple phase equilibria

Newtonian fluids

Shell and tube

Equilibrium stages, simple mass transfer

Simple reaction kinetics

While product designs involve

- selecting the best products to satisfy customer needs
- are increasingly carried out by chemical companies (3M, G.E., P&G, Dow-DuPont, ...)
- often with complex technology platforms that characterize

pastes and creams
soft materials
detergents
paints
drug delivery devices
dehumidifiers
and so on

To carry out these product and process designs, often faculty and students need help in working with specific technology platforms

- can be facilitated when product and process design problems are coupled to the expertise of certain faculty members
- ChE departments usually have faculty with different combinations of expertise profiles
- to exploit these couplings, we seek to involve technology experts in creating product-design case studies to be circulated by CACHE

Ka Ng will suggest approaches

Next, consider approaches for **blending in product design** while **emphasizing process design**

I, Single Course

Teach process design

- using lectures with small design projects
- including a few product design concepts

II. Two Courses

1. Emphasizing process design

2. Emphasizing product design
- often as an elective

Both involving design projects

III. Two Courses

1. Teach process design

- using lectures without design projects
- including more product design concepts

2. Design project course

- process and product designs (occasionally involving both)

- Type I
- Difficult to emphasize process design
 - while doing a design project (necessary) and introducing a few product design concepts

At Penn - Type III

- Next, consider some aspects

For many more specifics, see two
AIChE webinars on Teaching
Process and Product Design

Please express your preferences/concerns
in next 45 min.

We follow two tracks with strong emphasis on **process** design

	<u>Product Design Chapters*</u>	<u>Process Design Chapters*</u>
Introduction	1 (begin) 3	2
Synthesis	4, 5 (later)	6-17
Analysis	18, 19	20-22
Design Reports	23	
Case Studies	24-26	27

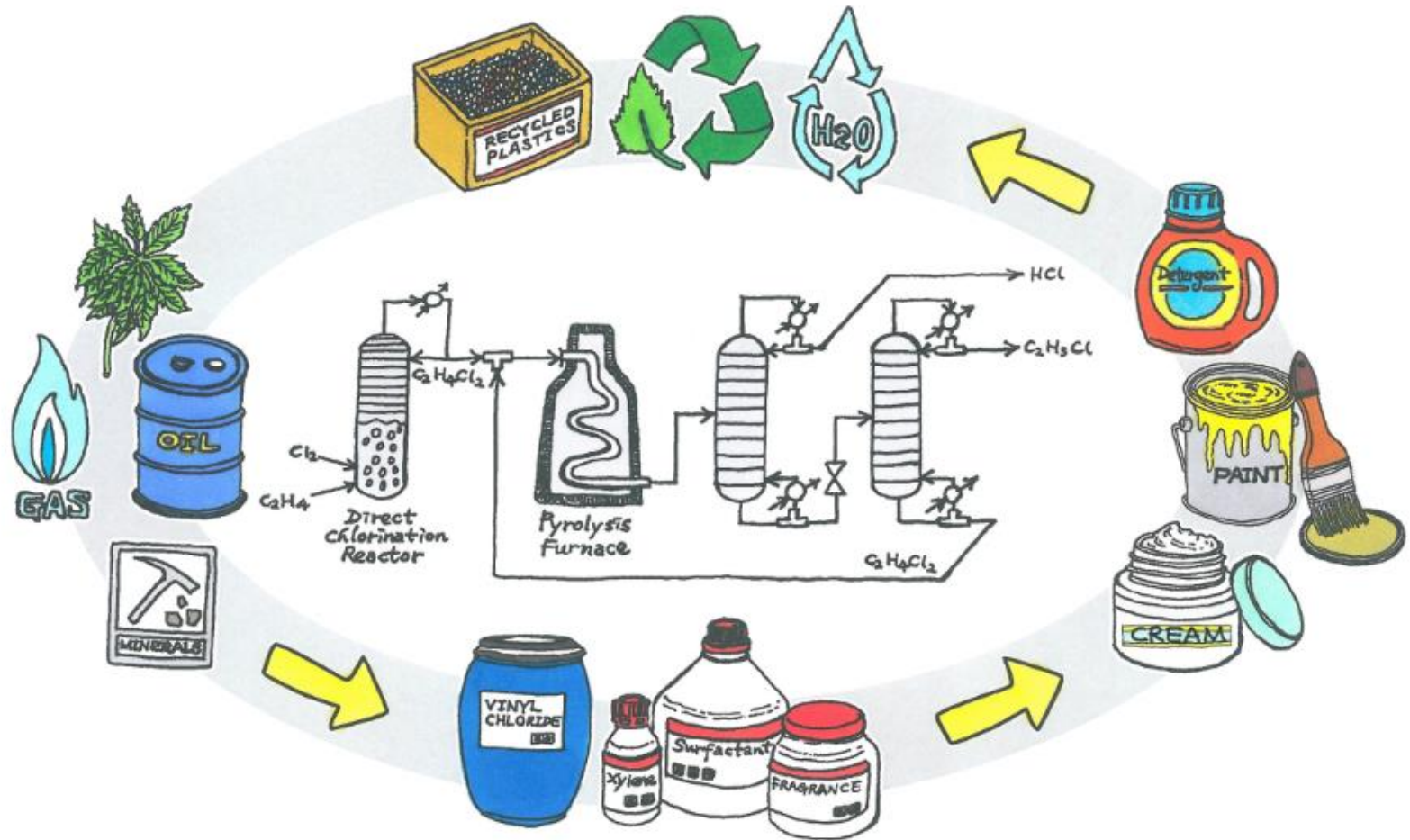
* In Seider et al., *Product and Process Design Principles*, 4 Ed., Wiley, 2017.

Introduction to Product Design (in 2 lectures) -

What to make?

Recommend - begin with the Chemical Supply Chain

The Chemical Supply Chain



Chemical engineers are skilled in **materials** and **processing**. Starting with **raw materials**, they produce **intermediate chemicals** which are used in **consumer products**. Chemical engineers are also involved in **sustainability** such as recycling used products and producing renewable energies.

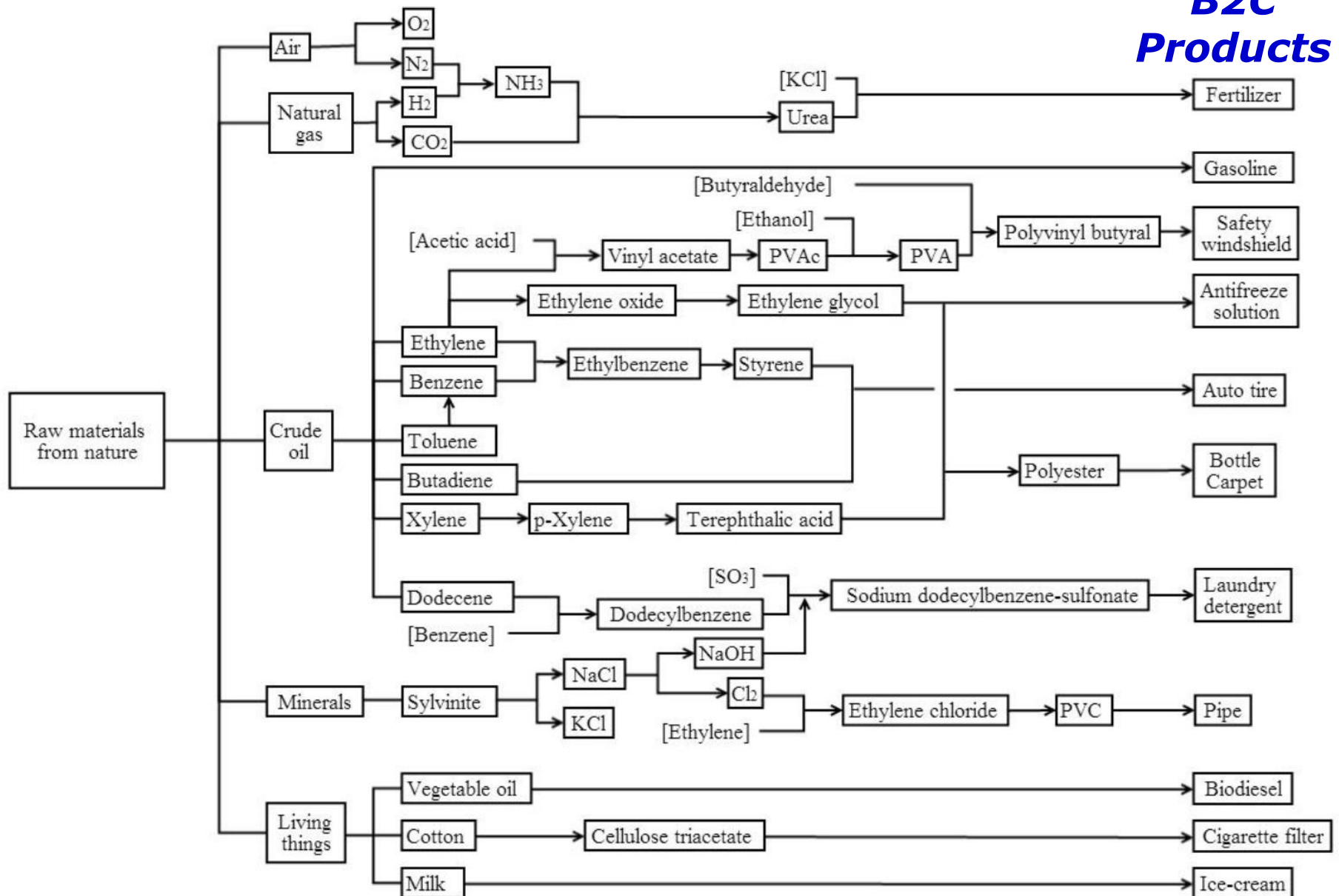
Emphasize - There are three primary sources for all the chemicals we need in our daily lives:

- Air and water
- Natural gas, petroleum and minerals
- Living things, including animals and plants

Recommend - take closer look at the supply chain

More Detailed Chemical Supply Chain

**B2C
Products**



B2B Products

Recommend – Show Breadth of Chemical Business Hierarchy

Business sector	Examples	Business	Activities
Petroleum sector, aka oil companies, refineries	Shell, ExxonMobil, Chevron, BP, Texaco	To provide basic feedstock such as ethylene, benzene, xylene for the manufacture of more complex chemicals such as ethylene glycol and polyester. <u>Starting materials:</u> Petroleum and natural gas	Oil and gas exploration, refining operations
The chemical companies	DowDuPont, BASF, Bayer, Mitsubishi, Sinopec	To manufacture more complex chemicals such as polymers, organics and inorganics to supply consumer goods and pharmaceutical companies. <u>Starting materials:</u> Basic materials such as ethylene, benzene, and xylene	Invent chemical processes, and manufacture chemicals
The specialized engineering firms	Kellogg, Brown and Root	Construction and technology transfer	To build a plant with a mature technology for a client

Business sector	Examples	Business	Activities
The pharmaceutical companies	Merck, Johnson & Johnson, Pfizer	New drugs and healthcare products <u>Starting materials:</u> Complex chemical intermediates	Drug discovery & manufacturing
The food companies	Unilever, General Mills, Nestle	Foods such as ice creams, margarines, teas, and coffees <u>Starting materials:</u> Living things and Chemical intermediates	To formulate and manufacture branded foods
The large consumer goods companies	Procter and Gamble, Unilever	To sell a wide variety of consumer goods <u>Starting materials:</u> Complex chemical intermediates	To formulate and manufacture various branded consumer goods such as soaps and detergents, etc.
The small consumer goods companies	Dinnerware manufacturer	To provide consumer goods for specific market sectors. <u>Starting materials:</u> Chemical intermediates	To manufacture various consumer goods such as plastic toys, dinnerware

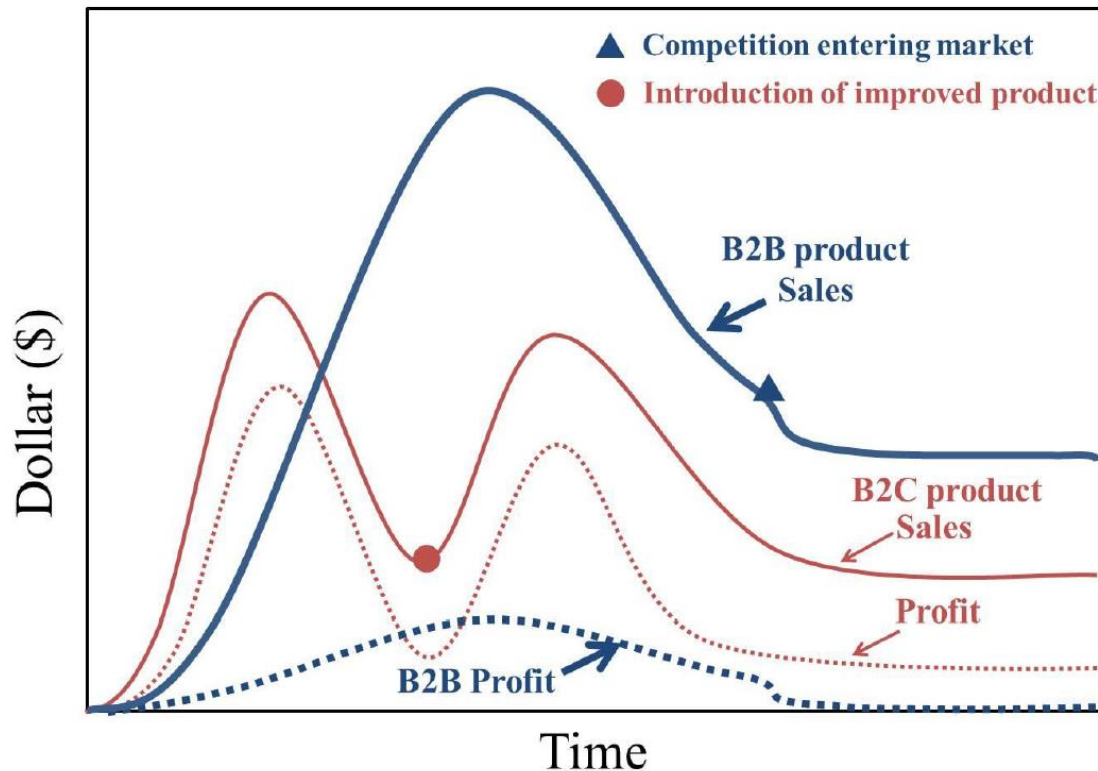
Recommend – Focus on Product Specifications

- B2B product (Terephthalic acid)
 - Purity is the primary concern
 - Impurity 4CBA leads to yellowish PET bottles
- B2C product (Sunscreen lotion)
 - Functional attributes
 - Protects parts of the body from UV light
 - Adheres to the body surface
 - Rheological attributes
 - Should not flow by itself, but can be pumped out from the bottle
 - Spreads easily when rubbed on skin
 - Physical attributes
 - Stable over time within a certain temperature range
 - Sensorial attributes
 - Feels smooth and does not cause irritation
 - Provides a pleasant smell



Also, Introduce - Product Life Cycle

- B2B products have a lower profit margin than B2C products
- B2C products have a shorter life cycle
- Redesign and re-launch of an improved B2C product to keep the product competitive



Introduction to Process Design (in 4 lectures) -

How to make?

Recommend - introduce the process
synthesis problem and
steps to solve it -

for a typical process

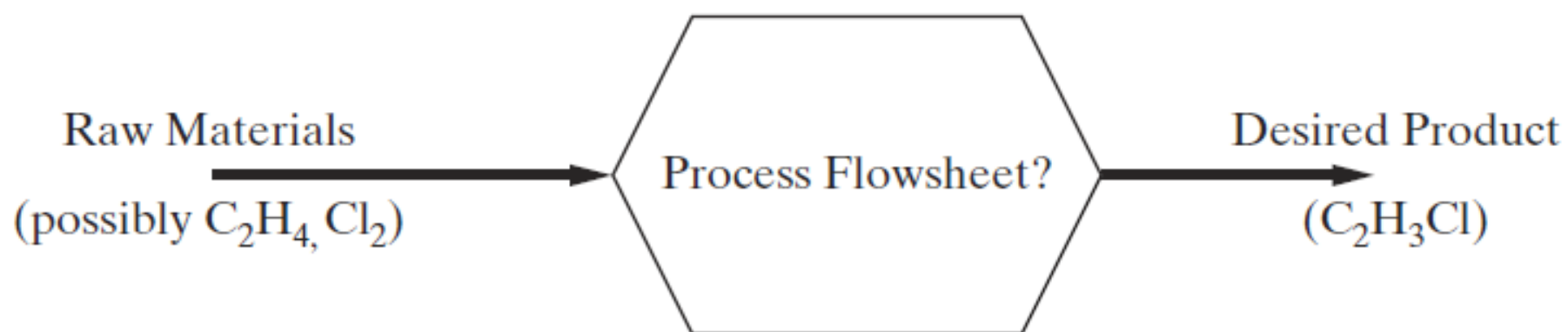


Figure 2.1 Process synthesis problem.

Chemical State of a Mixture

Mass

Composition (mole or mass fractions)

Phase (solid, liquid, or gas)

Form (crystalline modification - solids only)

Temperature

Pressure

Molecular Type

Process Operations

Chemical reaction

Separation (or purification)

Change of temperature

Change of pressure

Change of phase

Mixing

etc.

Synthesis Step*

1. Eliminate differences in molecular types
2. Distribute the chemicals by matching *sources* and *sinks*
3. Eliminate differences in composition
4. Eliminate differences in temperature, pressure, and phase
5. Integrate tasks; that is, combine operations into *unit processes* and decide between continuous and batch processing

Process Operations

Chemical reactions

Mixing

Separation

Temperature, pressure, and phase change

*** Rudd, Powers, Sirola, *Process Synthesis*, Prentice-Hall, 1973**

Step 1

Recommend - consider several potential reaction paths

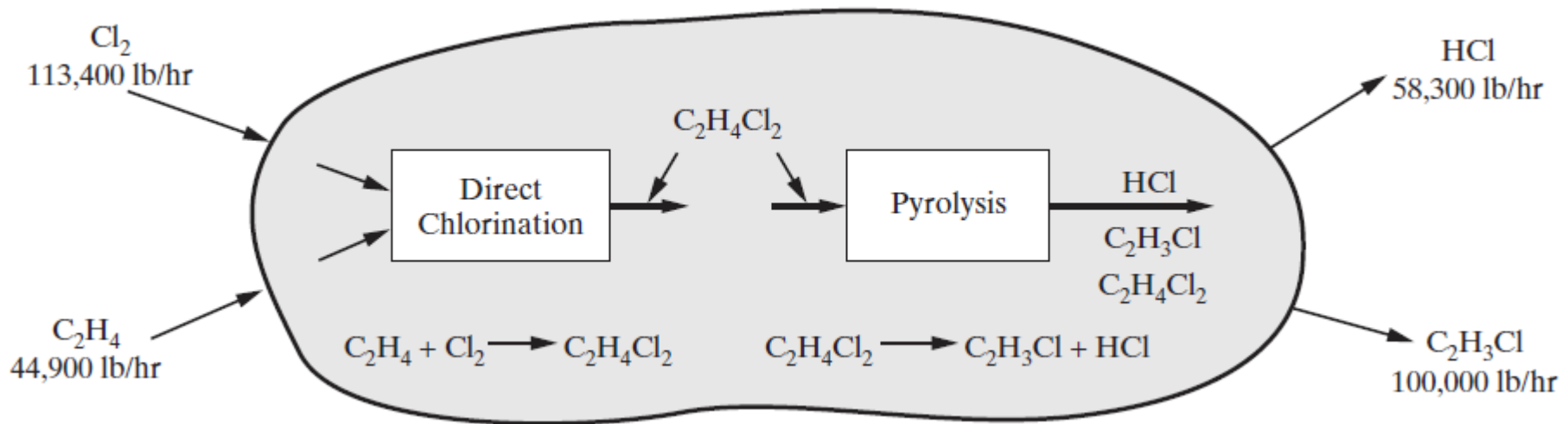


Figure 2.2 Reaction operations for the thermal cracking of dichloroethane from the chlorination of ethylene (reaction path 3)

After Steps 2 and 3

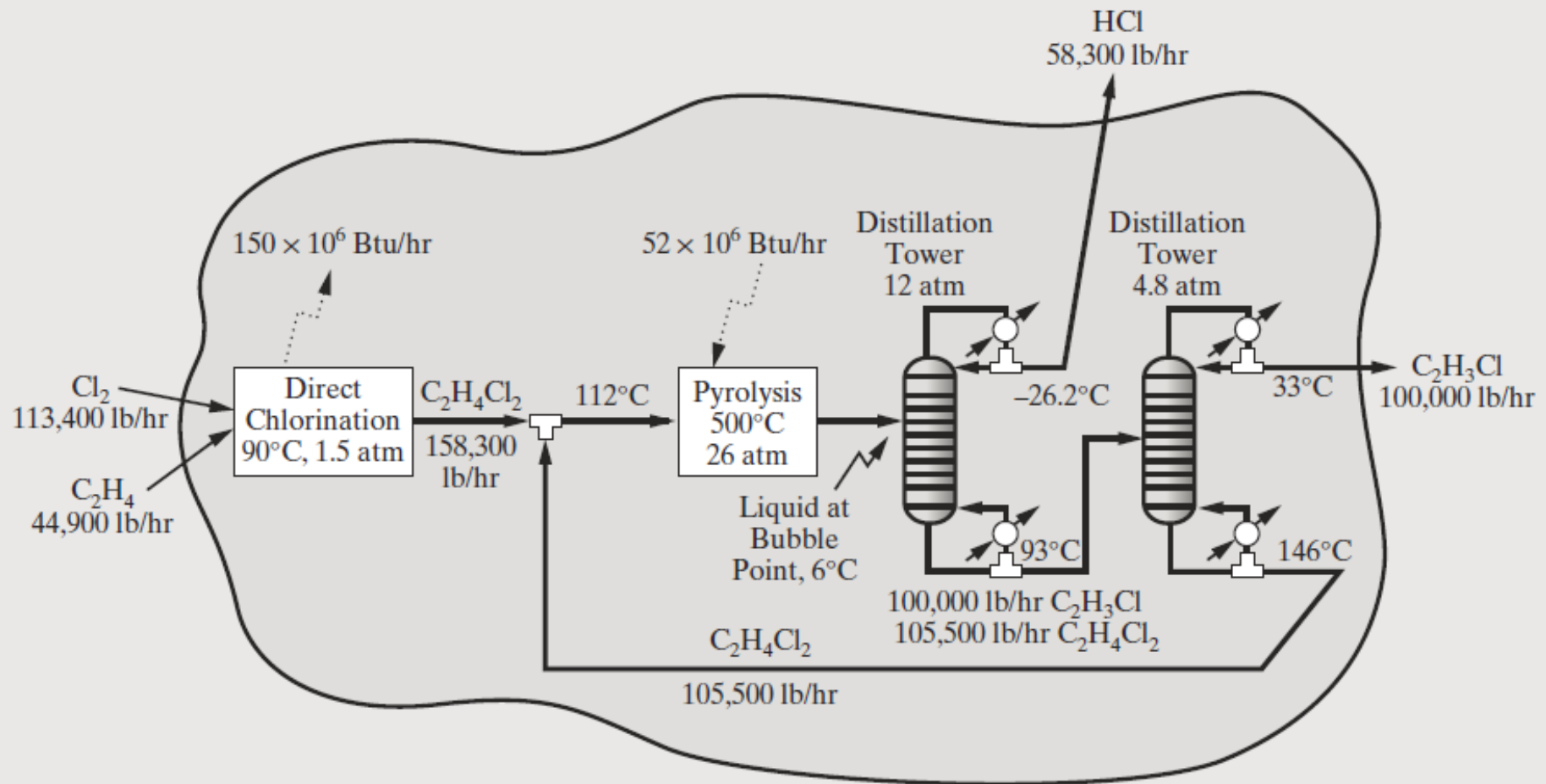


Figure 2.4 Flowsheet including the separation operations for the vinyl-chloride process.

After Steps 4 and 5

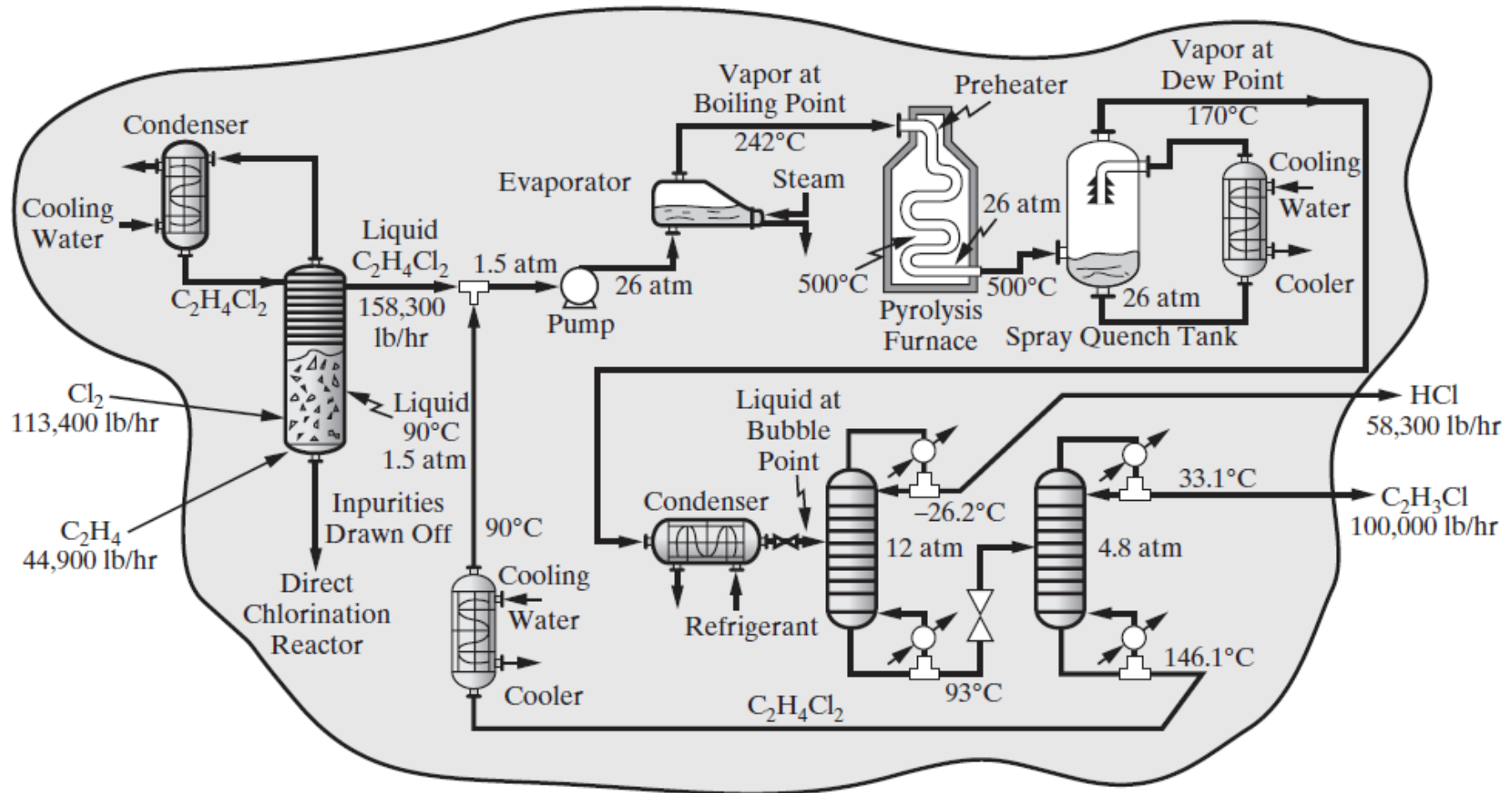
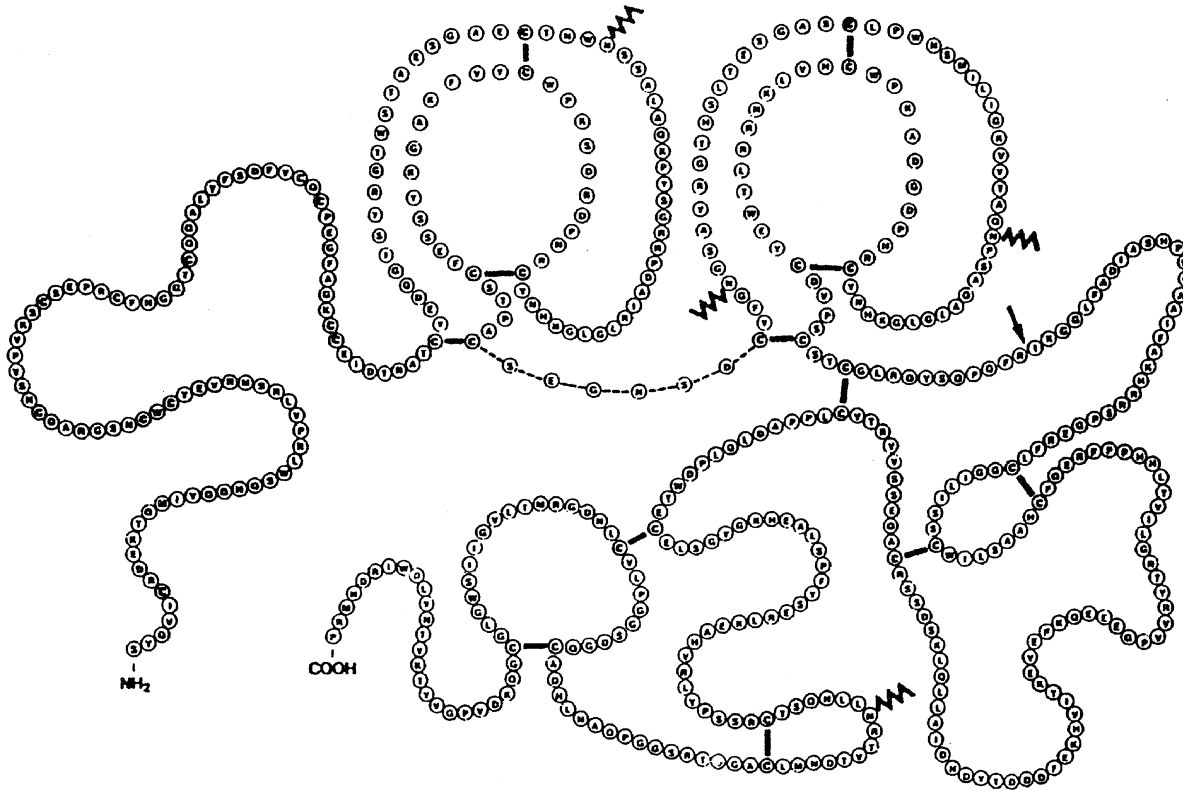


Figure 2.6 Flowsheet showing task integration for the vinyl-chloride process.

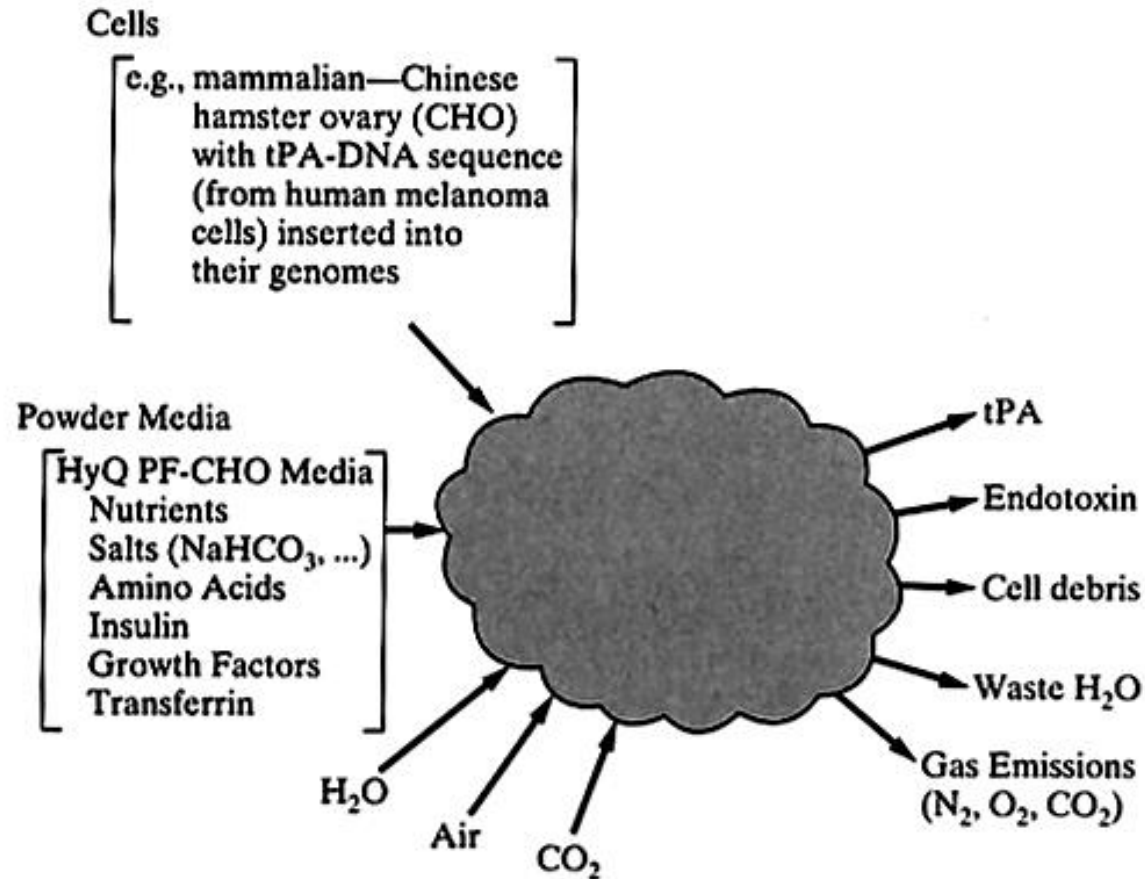
TISSUE PLASMINOGEN ACTIVATOR (tPA) - Pharmaceutical - Batch Processing

A therapeutic protein - comprised of 562 amino acids



Produced by a recombinant cell, which results from
a recombination of genes.

PROCESS SYNTHESIS PROBLEM



Note – endotoxins elicit an inflammatory response in animals

After Steps 4 and 5

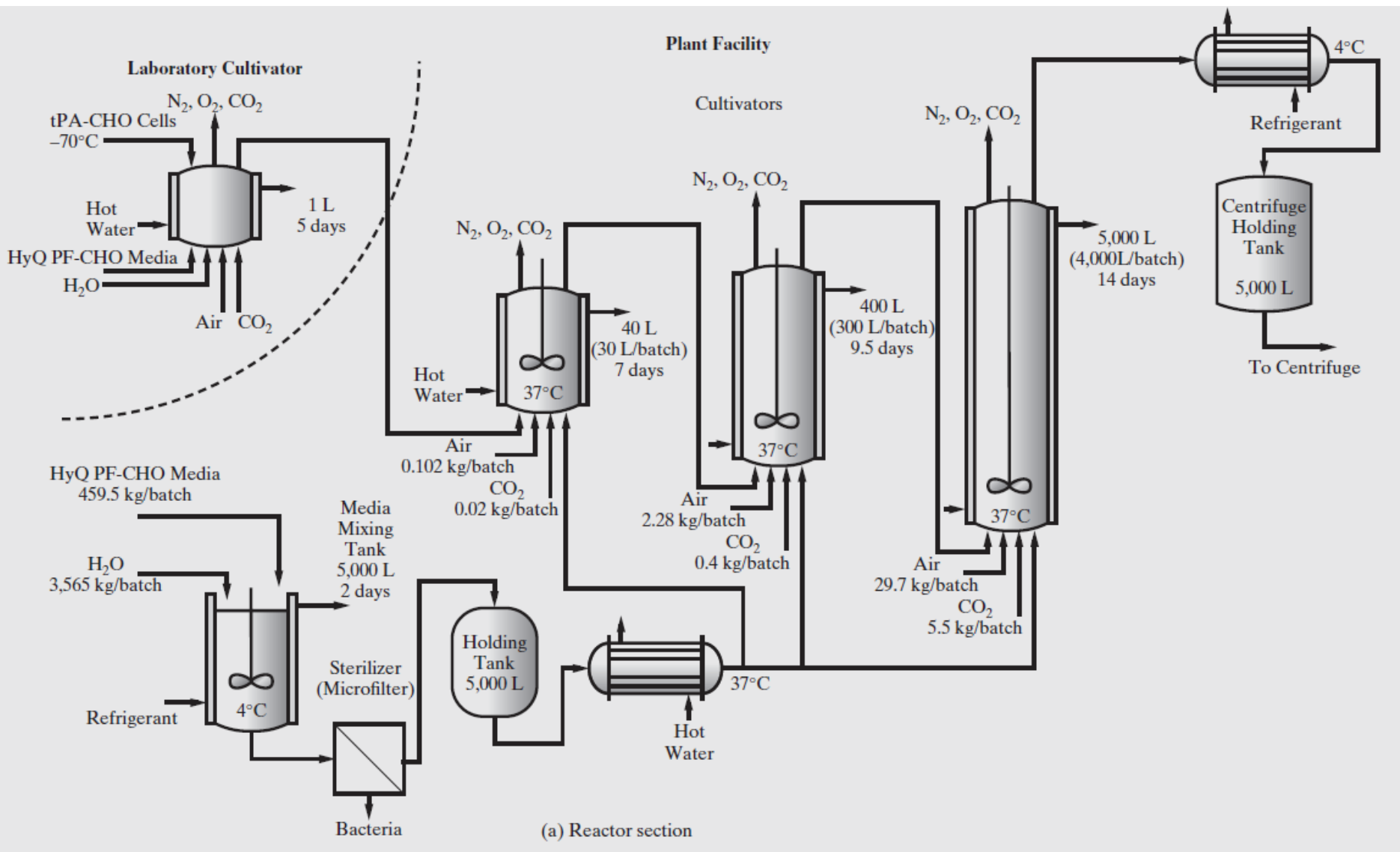


Figure 2.14 Flowsheet showing a task integration for the tPA process.

Recommend - After introductory subjects,
next focus on Improved Process
Synthesis, beginning with
heuristics for process synthesis

Later, as time becomes
available, turn to Product
Synthesis:

Molecular and Mixture Design

Devices, Functional, and
Formulated Products

Heuristics for Process Synthesis (2 lectures)

- These are general rules-of-thumb to guide process design decisions
- We do not discuss at length all of the heuristics provided in the text
- Choose a select sample to illustrate their value in process design
- Align this sequence with the *Process Synthesis Steps* from earlier in the semester

Simulation to Assist in Process Creation (5 lectures)

- Our course uses ASPEN as a process simulator**
- We begin with a stress on mass balances**
- We expand this to discuss**
 - Degrees-of-Freedom**
 - Design Specifications**
 - Recycle Loops**
 - Bubble and Dew Point (Thermo) Calculations**
- We also show SUPERPRO DESIGNER for batch**
 - This has a specific bio-process example**
 - Batch/cycle times, Gantt chart, bottleneck ideas**

Synthesis of Separation Trains (4 lectures)

- Feed Separations vs. Effluent Separations
- Use a purge stream when separation is too difficult
- The major investment and operating costs of a process will be those costs associated with the separation equipment
- Exploit a difference in phases to facilitate a split
 - Vapor/Liquid
 - Vapor/Liquid/Liquid
 - Vapor/Solid
 - Vapor/Liquid/Solid

Second Law Analysis (4 lectures)

- Ask ... “how do we value material and energy streams?” ... as a function of the work available from them (this motivates the idea of *Availability*).
- Introduce the concept of *Lost Work* and use this as a metric to compare different versions of a process.
- The idea of *Thermodynamic Efficiency* is a result of the lost work discussion.
- Use these ideas in a concrete example to evaluate a proposed refrigeration cycle process.

Heat Integration (4 lectures)

- The goal is to find the most economical way to transfer heat away from the hot streams and into the cold streams for a given process.
- Distinguish between interior network (only process streams) and auxiliary network (steam / cooling water utilities).
- Use thermodynamics to identify the maximum energy recovery (MER) target. Attempt to accomplish the majority of the heat transfer using only the streams in the interior network.
- This will have a capital costs (number and size of the heat exchangers) vs. operating costs (steam / cooling water utility demands) situation. When fuel costs are high ... the minimum annual costs will tend toward minimum utilities.

Having taught **Synthesis of Process Flowsheets**,
consider teaching **Equipment Design** -

For example:

Heat Exchanger Design

Recommend - teach when not covered in heat-transfer
course - especially shell-and-tube HXs

Separation Tower Design

Recommend - for separation columns, include calculation
of flooding velocities -

to estimate column diameters -

when not covered in separations
course

Design of Pumps, Compressors, and Expanders

Recommend - for compressors, cover (review)
isentropic efficiency

Chemical Reactor Design

Recommend - for tubular reactors, use CFD
(e.g., COMSOL) to show the
weakness of the plug flow
(perfect radial mixing) assumption

Capital Cost Estimation (in 2 lectures) -

- Recommend** - begin with estimation of equipment purchase costs as a function of equipment sizes using graphs and simple equations
- show estimation of installation (bare module) costs
 - move to estimation of total capital investment, C_{TCI}

Economics / Profitability Analysis (4 lectures)

- Lectures in this section focus on issues associated with *Time Value of Money* and *Approximate and Rigorous Profitability Measures*.
- These topics are valuable for the students in the following semester when they are completing their senior design projects.
- Students need to be able to appropriately estimate the relative value/cost of proposed long-term investments or projects.
- The “time value of money” recognizes the fact that an amount of money at the current time may not hold the same value at a future date. The concept of *interest* is related to the difference between the future value and present value.

Product Design Synthesis (5 lectures)

Recommend – introduce during the last third of the semester as students are completing process design homework –

- introduce the 4 kinds of products in sequence:

Molecular and Mixture Products
Chemical Device Products
Functional Products
Formulated Products

For Molecular and Mixture Products

Recommend – show, by example, a typical optimization formulation using group contributions

but, **don't teach optimization techniques** – instead have students use product design software; e.g., ProCAMD

- begin by reviewing property estimation using empirical group-contribution methods; e.g., the glass-transition temperature, T_g , for a polymer repeat unit

To be continued by Ka Ng



Teaching Process and Product Design



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Acknowledgment: Kelvin Fung, Danny Lewin, Bob Seader, Soemantri Widagdo, and Rafiqul Gani



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My experience in teaching product design

- A course on process and product design
 - Warren's Type III 1 (but with design project)
- A course on product (and unconventional process) design
 - Warren's Type II 2
- Courses given at undergraduate and graduate level
- There is always a design project

Introduction to Product Design (in 1 lecture) **Ch 1**

- The chemical supply chain (Discussed by Warren earlier)

Additional points:

- Types of B2C chemical products
- B2B vs. B2C products

Formulated Products

Formulated products are obtained by mixing selected components together to get the desired product attributes.



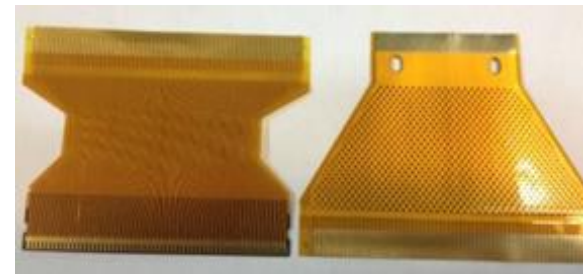
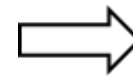
Skin Cream



Die Attach
Adhesive



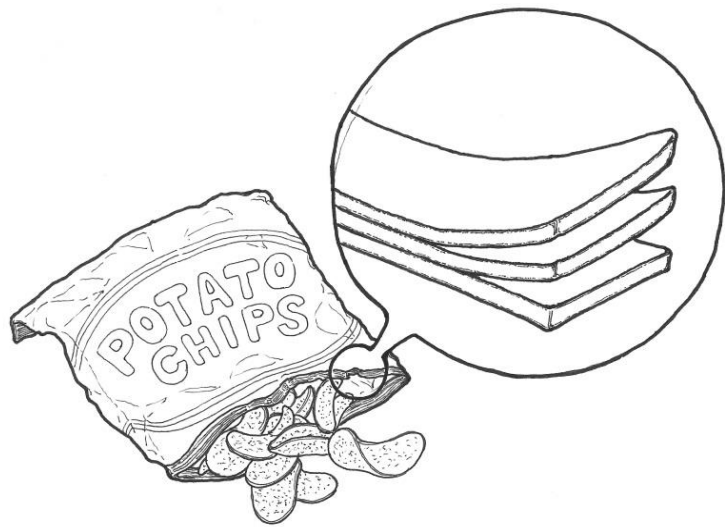
Nano
Particle
Conductive
Inkjet Ink



Flexible Printed
Circuits

Functional Products

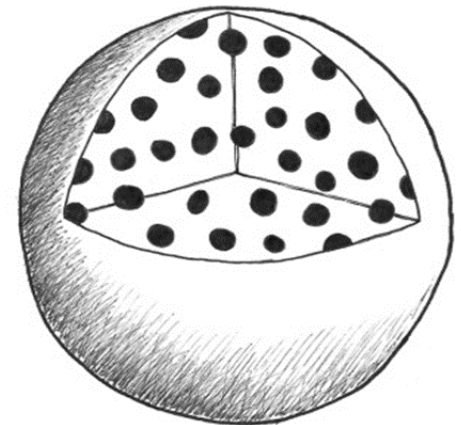
Functional products are those chemical products made up of materials that perform a desired function



Food packaging is made up of three main layers – outside print layer, adhesive layer and inside barrier layer.



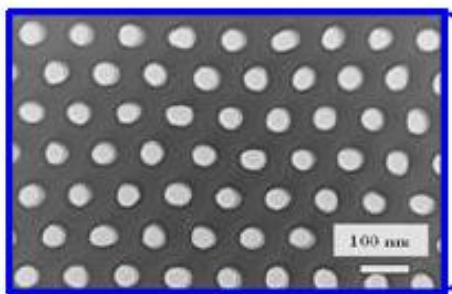
Nano ZnO used in transparent sunscreen



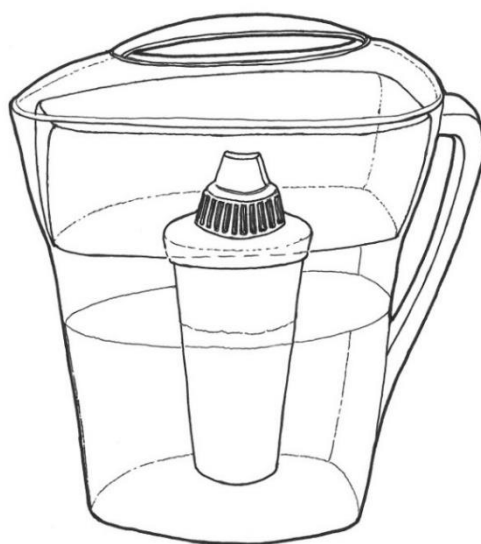
Controlled release herbicide granule

Chemical Devices

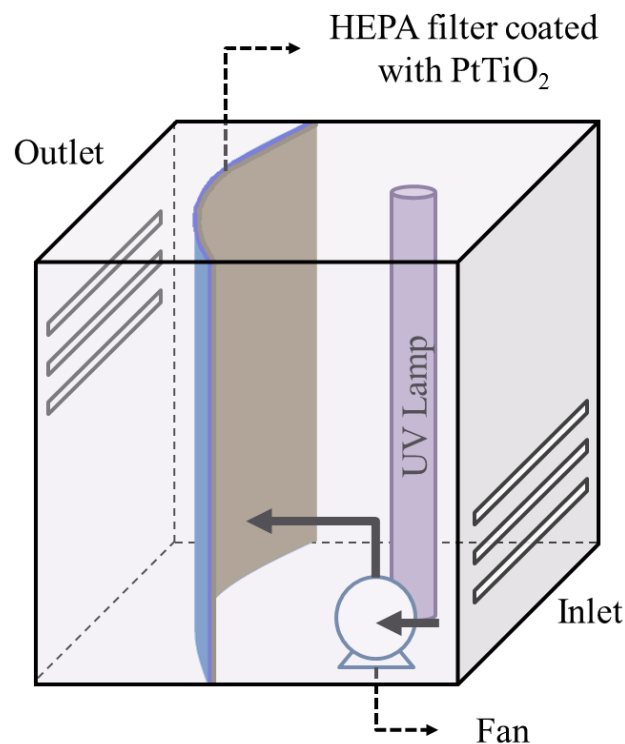
Chemical devices are those chemical products that achieve certain objectives by performing reactions, fluid flow, heating/cooling, and/or separations.



A humidity sensor with nanopores



A water filter consisting of activated carbon and ion exchange resins



An air purifier decomposes VOCs using UV-TiO₂ catalysts

B2B vs. B2C Products

	B2B (Commodity)	B2C (Consumer Centered)
Nature of products	Simple or complex molecules	Novel molecules; formulated products; functional products; devices
Product design	Primarily purity	Ingredients and structures
Product lifecycle	Decades	Month / Year
Team	Primarily chemists and chemical engineers	A multidisciplinary team of marketing personnel, financial specialists, lawyers, electronic engineers, mechanical engineers, chemists and chemical engineers.
Financial goal	Cost reduction	New sources of revenue
Unit operations	Traditional – distillation, crystallization, extraction, absorption, adsorption, etc.	Unconventional – granulation, milling, nanomization, etching, lamination, physical vapor deposition, inkjet printing, etc.
Technical focus	Process design and optimization	Improved product performance and quality
Knowledge	Well-structured	Fragmented so far

Multidisciplinary Hierarchical Product Design Framework (in 1 lecture) **Ch 1**

Job function	Phase I Product Conceptualization	Phase II Detail Design & Prototyping	Phase III Product Manufacturing & Launch
Management	Project management		
Business and Marketing	Market study		Product launch
Research and Design	Product design	Prototyping	
	Process design		
Manufacturing	Feasibility study	Engineering design	Plant startup
Finance and Economics	Economic analysis		

Methods for Product Conceptualization and Management (1 lecture) Ch 1

Product Conceptualization

- Identification of consumer needs
- Product attributes and product specifications
- Market information system
- Competitive analysis
- House of quality
- Quality function deployment
- Innovation map
- Product roadmap

Managing a Project

- Objective-time chart
- The RAT²IO Mnemonic
- Feasibility study
- Stage-gate
- Business model canvas

Translating Consumer Preferences to Technical Specifications

- Wine is commonly judged based on the following attributes
- The **weights** of each attribute (i.e. how important is this attribute) are identified through market research

Attributes, y_i	Weight, w_i
Acidity	0.0714
Sweetness	0.0714
Bitterness	0.0714
Clarity	0.1429
Color	0.0714
Brightness	0.0714
Bouquet	0.2858
Body/texture	0.1429
Finish/ aftertaste	0.0714

Preference function:

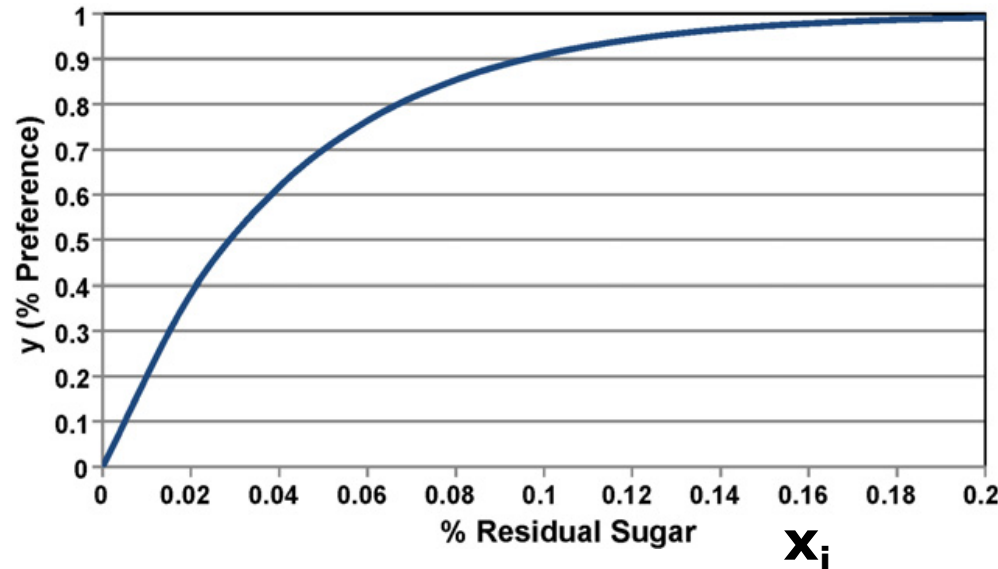
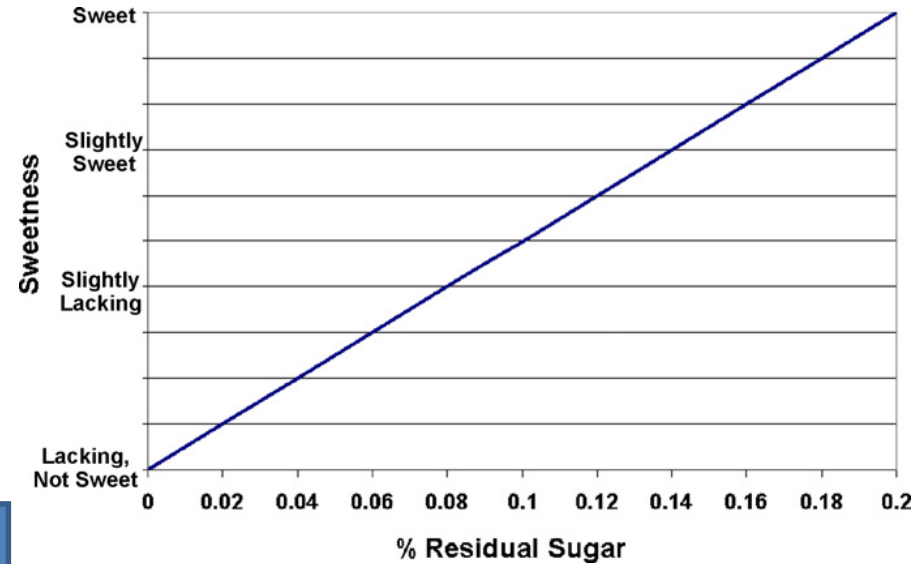
$$H = \sum_i w_i y_i$$

H = overall consumer preference
 w_i = weighing factor of attribute i
 y_i = **product attribute i score**

y_i depends on technical characteristics, x_i

Thus, need y_i vs. x_i

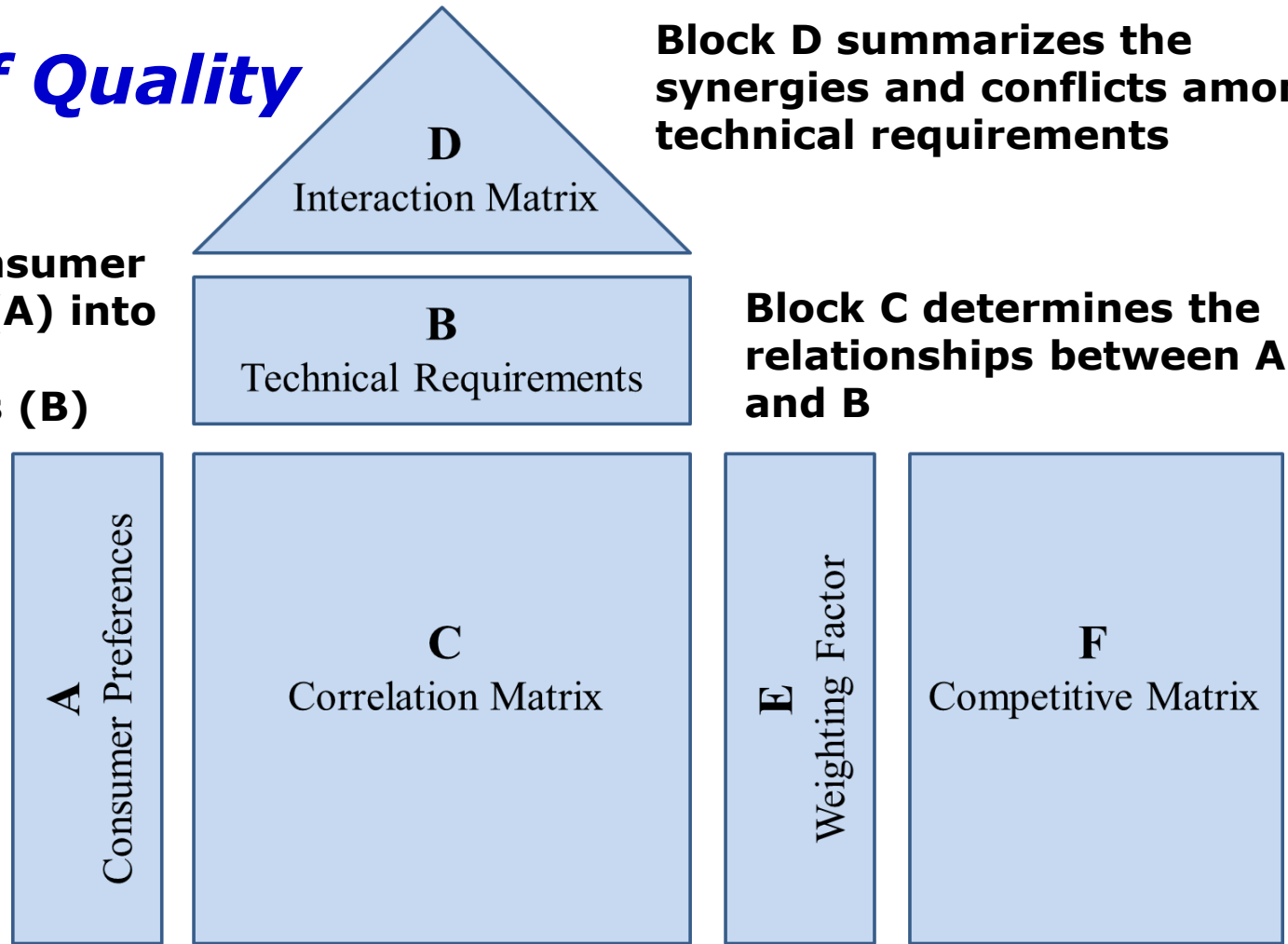
Relating Qualitative Product Attributes to Quantitative Technical Specifications



Similar for other product attributes

House of Quality

- Translate consumer preferences (A) into technical requirements (B)



Block D summarizes the synergies and conflicts among technical requirements

Block C determines the relationships between A and B

Block G calculates the importance of each technical requirement

Block E shows the importance of each consumer preference

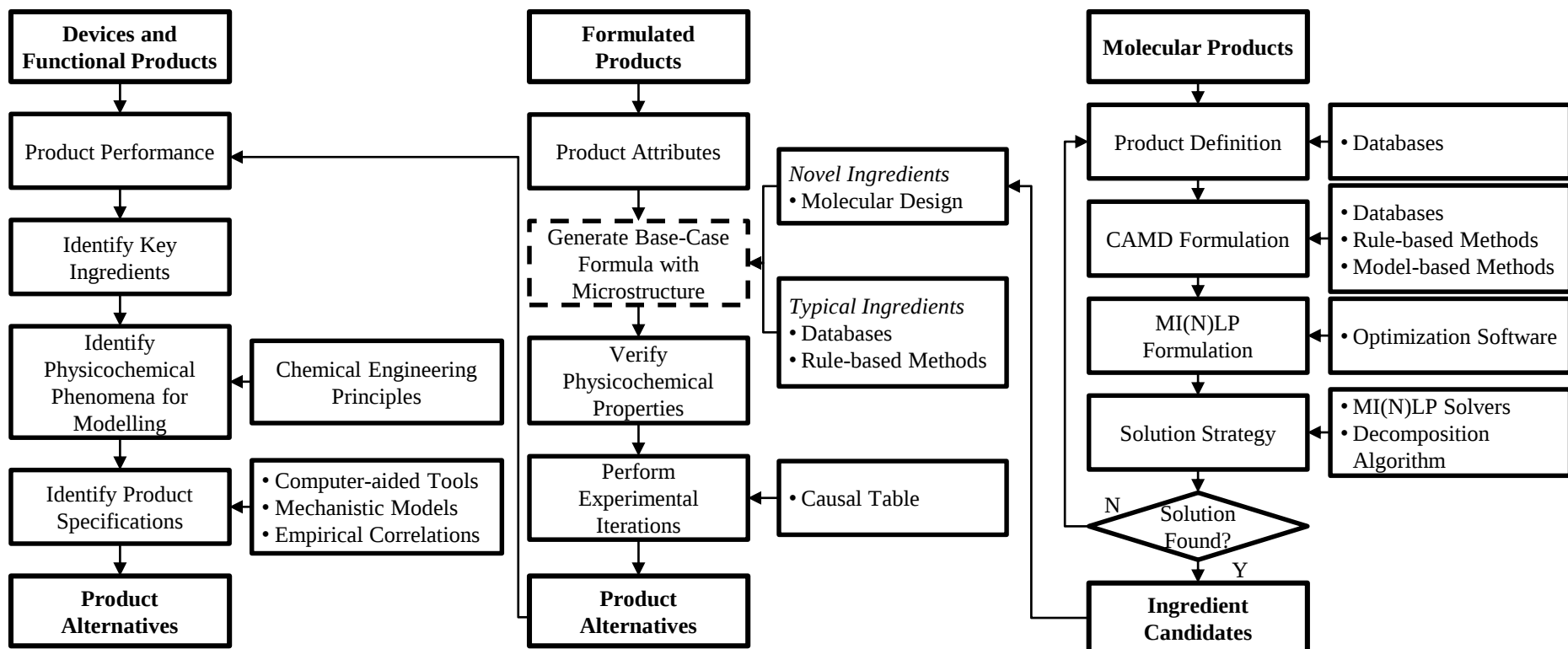
Block F shows the competitors' capabilities₁₂

Design of molecular, formulated, functional products, and devices (in 4 lectures) **Ch 4,5**

Devices and Functional Products

Formulated Products

Molecular Products



Example: Design of Metal Nanoparticle-based Conductive Inkjet Ink (a Formulated Product)

Design scenario:

Developing an ink for fabricating copper tracks on PET substrate



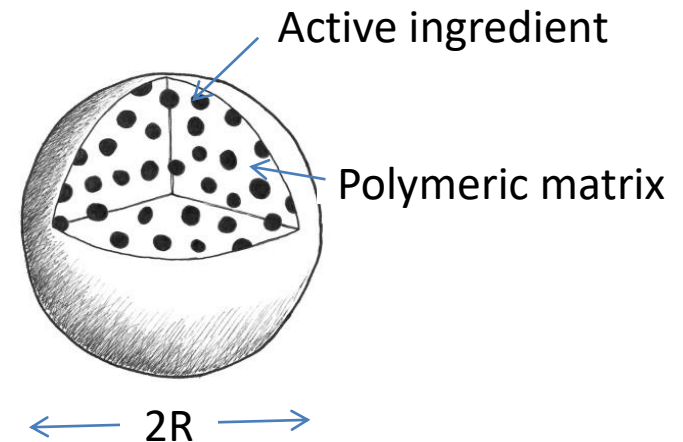
Step 1 – Specify product performance

Product specifications	Shelf life	4 months
	Track size	250 μm
	Track thickness	1 μm
	Track volume resistivity	<400 $\mu\Omega\text{ cm}$
Printing conditions	Substrate	PET
	Temperature, T	298 K
	Droplet diameter, d_0	30 μm
	Droplet velocity, v	5 m/s
	Nozzle diameter, d_{nozzle}	21.5 μm
	Printing speed, U_T	2.4 m/s
	Drop spacing, p	25 μm
	Curing conditions	Thermal sintering under N_2 environment

Example: Design of a Controlled-release Herbicide Granule (a Functional Product) **Ch 5**

Design scenario:

Herbicides such as 2,4-dichlorophenoxyacetic acid (2,4-D) spread on soil are easily lost due to leaching, volatilization, or biodegradation. An agrochemical company wants to develop a controlled-release granule with the active ingredient uniformly dispersed within a cellulose or lignin matrix.



Specify product performance:

The controlled-release granules should deliver 0.5-2 mg/m² day of the herbicide from day 1-10, followed by a lower dose of 0.1-0.5 mg/m² day from day 11-90.

Use Models and Data to Identify Product Specifications

Dissolution of cellulose matrix

The rate of herbicide release from the granule depends on the dissolution rate of cellulose, which is linearly dependent on the surface area of the granule,

$$\frac{dM_c}{dt} = 4\pi k_0 r^2 \quad (5.11)$$

where M_c is the mass of cellulose, k_0 is the dissolution rate constant, and r is the radius of the granule at time t . The amount of dissolved cellulose, M_{cd} , can be obtained by mass balance:

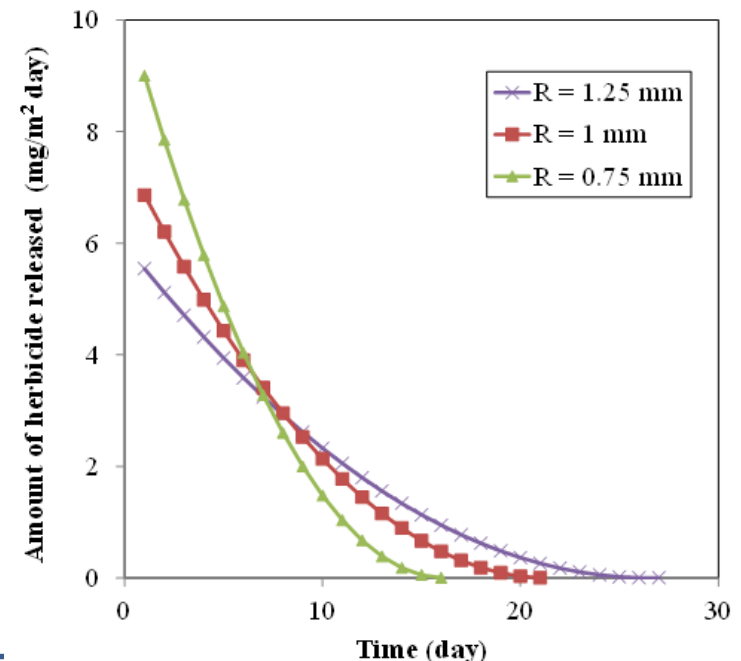
$$M_{cd} = \frac{4\pi\rho x_c}{3} (R^3 - r^3) \quad (5.12)$$

where ρ is particle density, x_c is the weight fraction of cellulose, and R is the initial radius of the granule. Integrating Eq. (5.11) over time after substituting M_c into it gives

$$r = R - \frac{k_0}{\rho x_c} t \quad (5.13)$$

Because the herbicide is dispersed uniformly in the matrix, the cumulative amount of herbicide released from the granule, M_h , can be obtained by replacing x_c by x_h , the weight fraction of herbicide in the granule, and substituting r from Eq. (5.13) into Eq. (5.12),

$$M_h = \frac{4\pi\rho x_h}{3} \left(R^3 - \left(R - \frac{k_0}{\rho x_c} t \right)^3 \right)$$



Use Models and Data to Identify Product Specifications (Ctd)

Herbicide diffusion in [lignin](#) matrix

Because a lignin granule degrades very slowly, the release of herbicide occurs by diffusion from the interior of a granule into the soil, followed by diffusion to the surroundings. Diffusion within a spherical granule, the rate-determining step, can be modelled using Fick's second law,

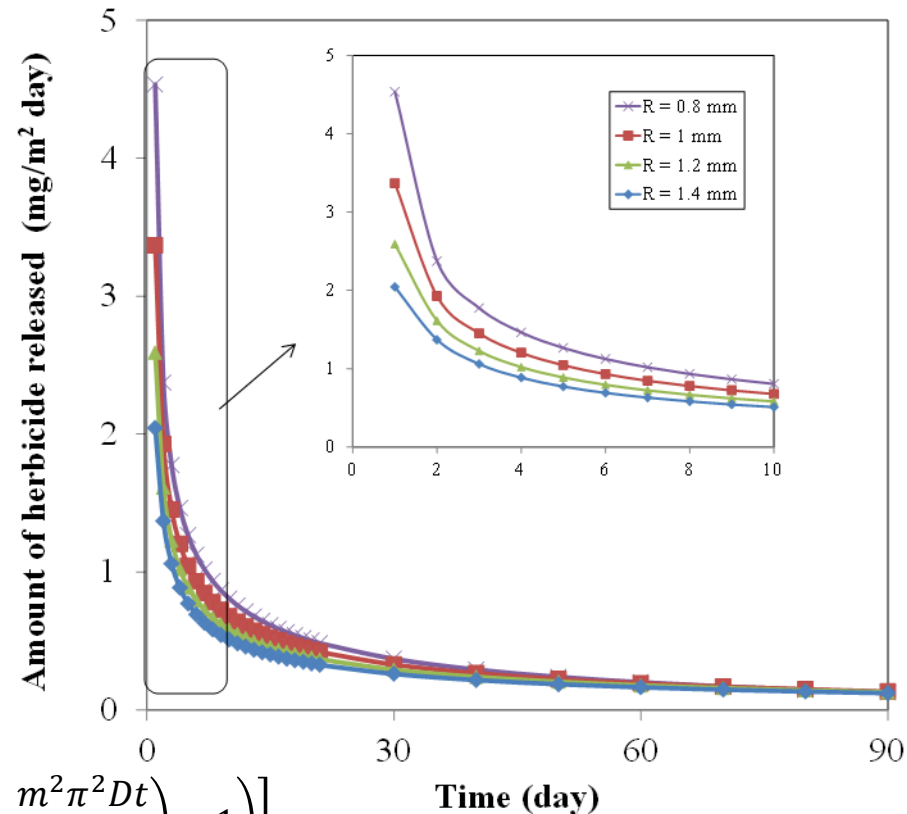
$$\frac{\partial C}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C}{\partial r} \right) \quad (5.15)$$

with the initial and boundary conditions:

$$\begin{aligned} 0 \leq r \leq R; C &= C_0 & \text{at } t = 0 \\ r = R; C &= C_s & \text{for } t > 0 \\ r = 0; C &= \text{finite} & \text{for } t > 0 \end{aligned} \quad (5.16)$$

where C is the concentration of herbicide in the granule, D is the diffusion coefficient, and C_s is the concentration on the surface of the granule. The cumulative amount of herbicide released at time t is given by

$$M_h = - \int_0^t AD \left. \frac{\partial C}{\partial r} \right|_{r=R} dt = \frac{8R^3(C_s - C_0)}{\pi} \sum_{m=1}^{\infty} \left[\frac{1}{m^2} \left(\exp \left(-\frac{m^2 \pi^2 D t}{R^2} \right) - 1 \right) \right]$$



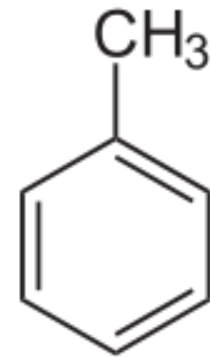
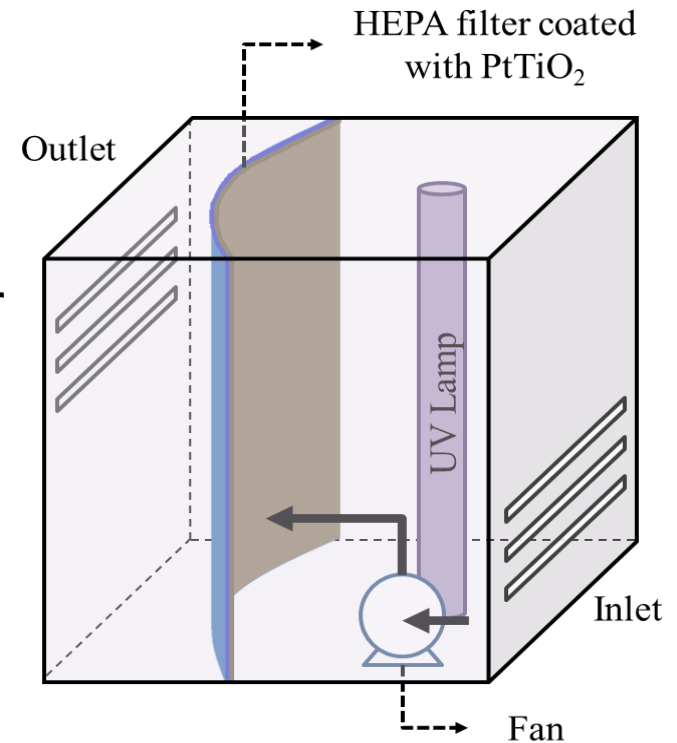
Example: Design of an Air Purifier (a Device) **Ch 5**

Design scenario:

A home appliance company plans to produce an air purifier to remove indoor volatile organic compounds (VOCs).

Specify product performance:

The product is expected to reduce the concentration of VOCs from 150 mg/m^3 to 30 mg/m^3 in a room 200 m^3 in size within 2 hours. As a starting point, toluene is used as the reference compound for quantifying the product performance as stated above.



Toluene

Use Models and Data to Determine Product Specifications (Ctd)

- **Product Specifications:** The total amount of TiO_2 coating for achieving the design target.
- **Assuming the air in the room is perfectly mixed, the mass balance of toluene can be written as:**

$$V_r \frac{d[C]}{dt} = r_T V_{cat} \quad \text{Eq 1}$$

where V_r and V_{cat} are the volume of the room and catalyst, respectively, $[C]$ is the toluene concentration in the air, and r_T is the rate of decomposition of toluene on the TiO_2 coating.

- **The decomposition rate of toluene is given by**

$$r_T = \frac{-kK_T [C]}{1 + K_T [C]} \quad \text{Eq 2}$$

where k is the surface reaction rate constant, and K_T is the adsorption equilibrium constant for toluene

- **Substituting Eq 2 into Eq 1 and integrating t from $t=0$ to t_f**

$$t_f = - \frac{\ln([C_f]/[C_0]) + K_T([C_f] - [C_0])}{kK_T(\frac{V_{cat}}{V_r})} \quad \text{Eq 3}$$

where t_f is the total reaction time, $[C_0]$ and $[C_f]$ are the initial and final concentration of toluene, respectively.

Use Models and Data to Identify Product Specifications (Ctd)

- The surface reaction rate constant for toluene k can be expressed by the following empirical relation:**

$$k = K_m(K_3 + K_4[C_0] + K_6[C_0]^2)(K_5 + K_2RH) \quad \text{Eq 4}$$

where K_m , K_2 , K_3 , K_4 , K_5 and K_6 are fitting parameters, and RH is the relative humidity of the air.

- Parameter fitting for toluene degradation experiments conducted at a RH between 14-82%, a light intensity of 2.2 mW/cm², and an initial concentration of 150 mg/m³, we get**

K_m (mg/m ³ .min)	K_T (m ³ /mg)	K_2	K_3	K_4 (m ³ /mg)	K_5	K_6 (m ³ /mg) ²
5.78	0.0189	-14.599	183873.42	-3033.00	1614.37	13.1871

- Assume $RH = 50\%$, $k = 238,103,199.5$ mg/(m³.min)**

Use Models and Data to Identify Product Specifications (Ctd)

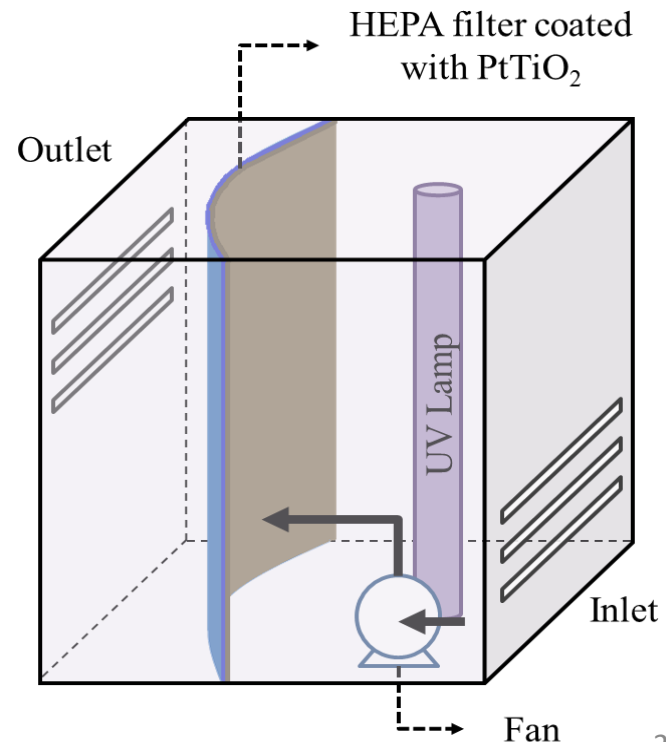
- Since 200m^3 air needs to be cleaned within 2 hours, $t_f \leq 2\text{h}$ and $V_r = 200\text{ m}^3$. Substituting k and K_T into Eq 3, we get

$$t_f = - \frac{\ln \frac{30}{150} + 0.0189 \frac{\text{m}^3}{\text{mg}} \times (30 - 150) \frac{\text{mg}}{\text{m}^3}}{238103199.5 \frac{\text{mg}}{\text{m}^3 \cdot \text{min}} \times 0.0189 \frac{\text{m}^3}{\text{mg}}} \times \frac{200\text{ m}^3}{V_{\text{Cat}}} \leq 2\text{ h} \quad \text{Eq 5}$$

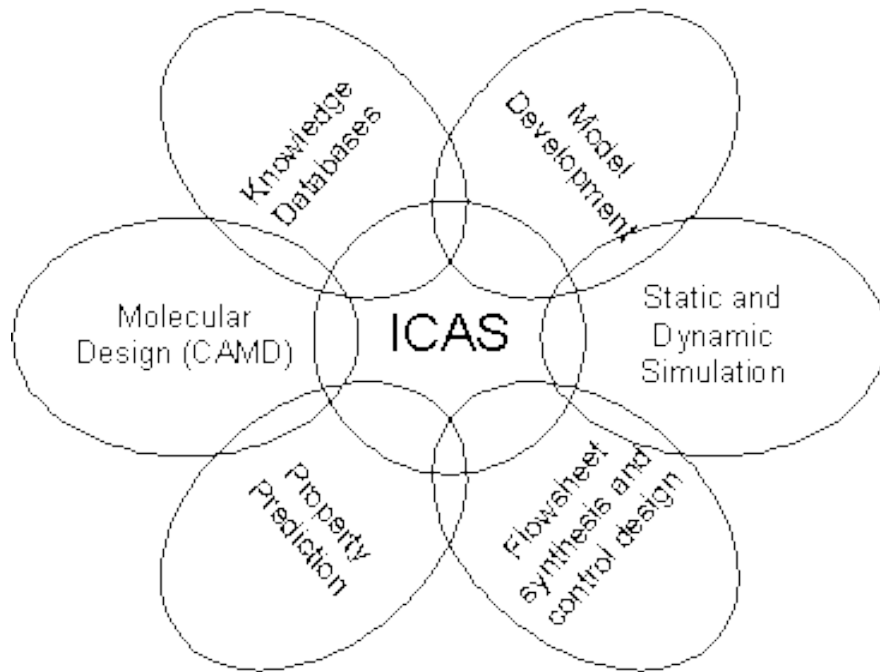
or $V_{\text{cat}} \geq 1.436 \times 10^{-6} \text{ m}^3$

- If a HEPA filter area of 0.1 m^2 is assumed, the thickness of the catalyst coating, s , is given by

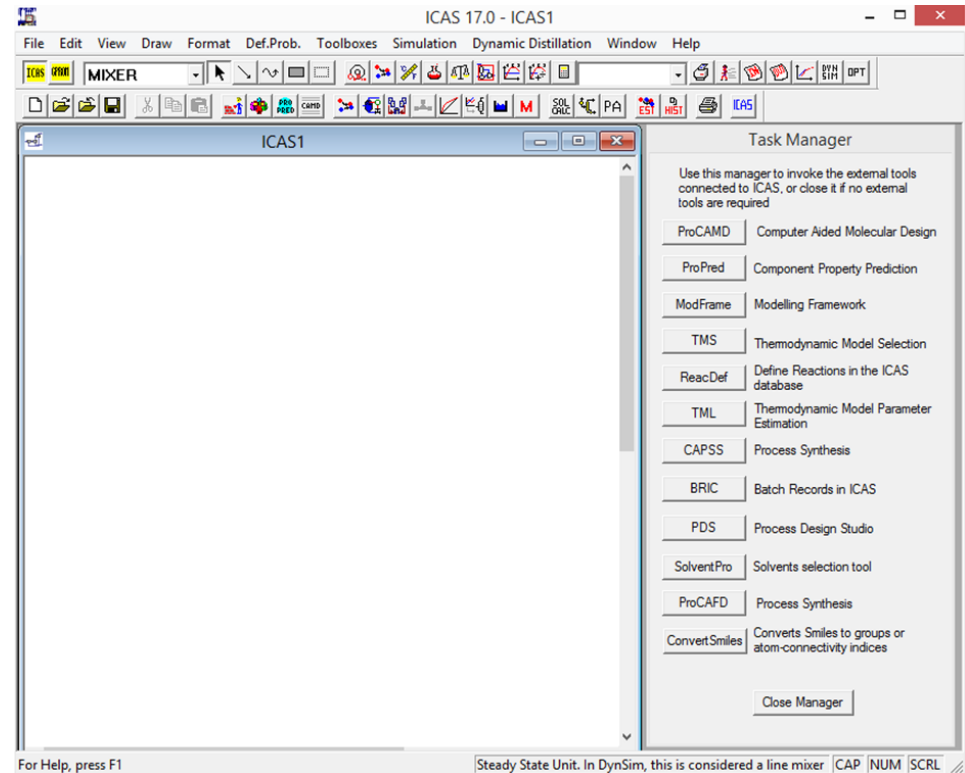
$$s \geq \frac{V_{\text{cat}}}{0.1\text{ m}^2} = \frac{1.436 \times 10^{-6} \text{ m}^3}{0.1\text{ m}^2} = 14.4\text{ }\mu\text{m} \quad \text{Eq 6}$$



ICAS: an Integrated Computer Aided System (Gani of DTU) (1 lecture) **Ch 4**

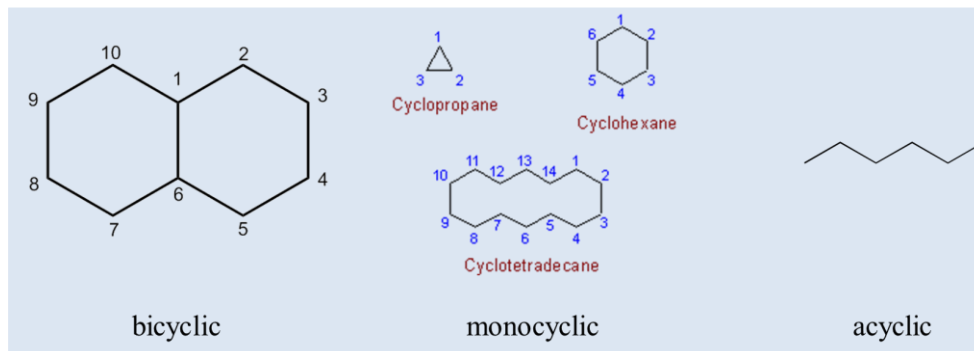


Integration of tools in ICAS



Method to Generate Molecular Structures (No free attachments)

CH₃	1 free attachment
CH₂	2 free attachments
CH	3 free attachments
C	4 free attachments



m = number of distinct groups in basis set
 n = total number of groups in designed molecule
 $q = [-1, 0, 1] = [\text{bicyclic}, \text{monocyclic}, \text{acyclic}]$
 n_j = number of groups of j^{th} kind
 v_j = valence of group of j^{th} kind
 $[n_j^l, n_j^u]$ = lower/upper bound allowed on n_j
 n_{max} = maximum number of groups allowed in molecule

Octet rule
$$\sum_{j=1}^m (2 - v_j) n_j = 2q$$

each group
$$n_j^l \leq n_j \leq n_j^u \quad \forall j$$

total groups
$$2 \leq n \leq n_{\text{max}}$$

$$n = \sum_{j=1}^m n_j$$

Example

CH₃- ($v_j = 1$); -CH₂- ($v_j = 2$); -OH ($v_j = 1$)

For CH₃-CH₂-OH ($q = 1$)

$$[(2-1)*1 + (2-2)*1 + (2-1)*1 = 2*1 = 2] \quad \text{No free attachment}$$

Example: Find Molecules that Satisfy Property Constraints

- Find molecules that satisfy the following property constraints:

$$17 < \delta_T (\text{MPa}^{1/2}) < 21; 250 \text{ K} < T_m; T_b > 340 \text{ K}$$

- In principle, any database of chemicals having the target properties can be used. Figures (a) and (b) highlight the search specifications and results using the CAPEC database.

The screenshot shows the 'CapecDB Manager' window with a menu bar (File, Edit, View, Database, Help) and a toolbar. On the left is a tree view with folders: Search (containing Basic Search, Advanced Search, Solubility Search), Add & Change Data (containing Add New Compound, Change Compound Data, Add Solubility Data), and Mixture Data. The main area contains search criteria fields:

- Solvent: 1-Propanol
- Solvent Type: 1 Normal Fluid
- Classification 1: 1 Normal Fluid
- Classification 2: 1 >C4
- Classification 3: 1 Alkanes
- Property Select 1: SolPar (kJ/m³)^{1/2} with value 17, selected 'less than'.
- Property Select 2: Tm (K) with value 250, selected 'greater than'.
- Property Select 3: Tb (K) with value 340, selected 'greater than'.
- Property Select 4: AIT (K) with value 0, selected 'less than'.
- Property Select 5: AIT (K) with value 0, selected 'less than'.

Buttons for 'Search CapecDB' and 'Manager' are visible. The status bar at the bottom shows the file path 'C:\CAPEC\ICAS\databank\AccessDB\CAPEC.mdb' and a 'CAP NUM SCRL' indicator.

(a) Initiating the search

View Compound Plot Results

Found Compounds:

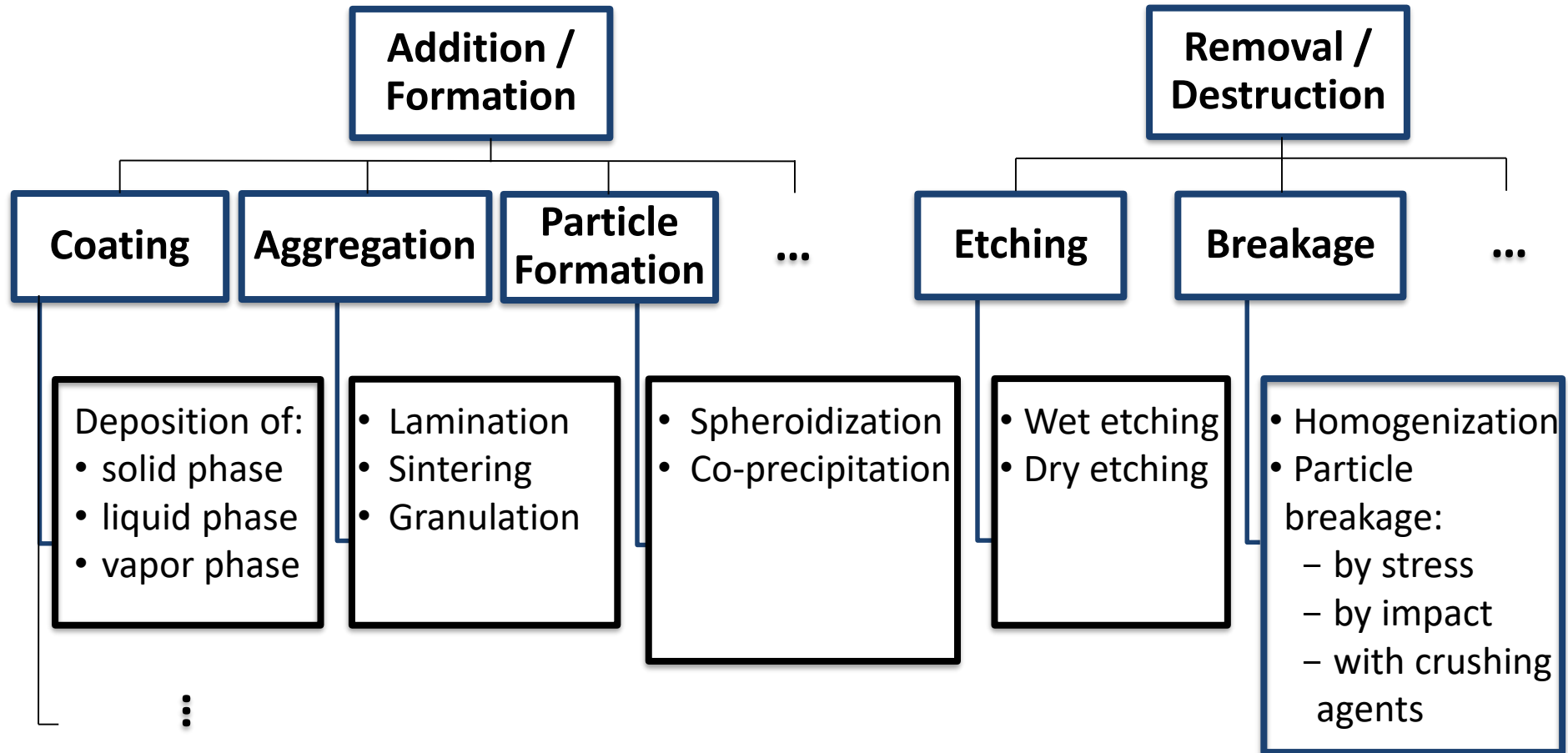
casno	Chemname	mw	SolPar	Tm	
000110-19-0	ISOBUTYL-ACETATE	116.16	17.0469	174.35	389.
000105-54-4	ETHYL-n-BUTYRATE	116.16	17.3779	175.15	394.
000123-42-2	DIACETONE-ALCOHOL	116.16	19.5262	229.15	441.
000638-49-3	n-PENTYL-FORMATE	116.16	17.9777	199.65	403.
026549-25-7	-(Heptanol,(S-3	116.2	20.2	203.15	430.
000110-49-6	Ethanol,2-methoxy-,acetate	118.13	20.3	203.15	416.
000105-58-8	DIETHYL-CARBONATE	118.13	18.3686	230.15	399.
000496-11-7	INDANE	118.18	19.4056	221.75	451.
000766-90-5	cis-1-PROPENYLBENZENE	118.18	18.9344	211.55	440.
000111-76-2	BUTOXYETHANOL-2	118.18	20.2518	198.35	441.
000622-97-9	p-METHYLSTYRENE	118.18	18.9153	239.05	445.
000611-15-4	o-METHYLSTYRENE	118.18	18.9703	204.65	442.
000873-66-5	trans-1-PROPENYLBENZENE	118.18	18.8991	243.85	451.
000098-83-9	alpha-METHYLSTYRENE	118.18	18.3262	249.95	438.
000100-80-1	m-METHYLSTYRENE	118.18	18.7154	186.85	437.
000111-47-7	Di-n-PROPYL-SULFIDE	118.24	17.1108	170.65	416.
000111-31-9	n-HEXYL-MERCAPTAN	118.24	17.4482	192.15	424.
000542-18-7	-Cyclohexane,chloro	118.61	18.4	229.15	415.
000095-63-6	TRIMETHYLBENZENE-1,2,4	120.19	18.0739	229.35	442.
000638-49-3	n-PENTYL-FORMATE	116.16	17.9777	199.65	403.

Record 225

(b) CAPEC database search results

Note that when an upper bound of 400 K is placed on T_b , the number of compounds matching the targets is reduced from 225 (Figure (b)) to 70.

Classification of Unconventional Processing Techniques for Non-commodity Products (in 1 lecture)



Example : A Cream Manufacturing Process Ch 5

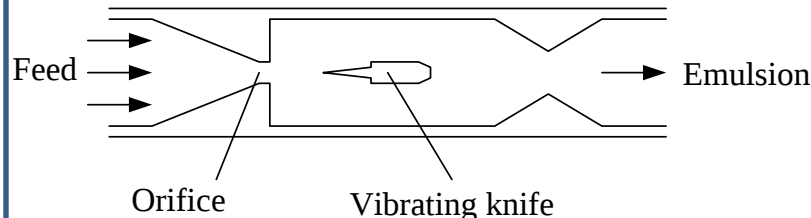
Design scenario:

One of the requirements for a cream product is that the emulsion droplets should have a diameter smaller than 5 μm to obtain a smooth cream. Develop a conceptual process design along with the key equipment characteristics and operating conditions.

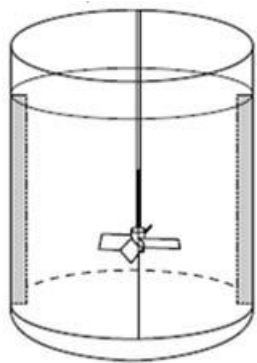
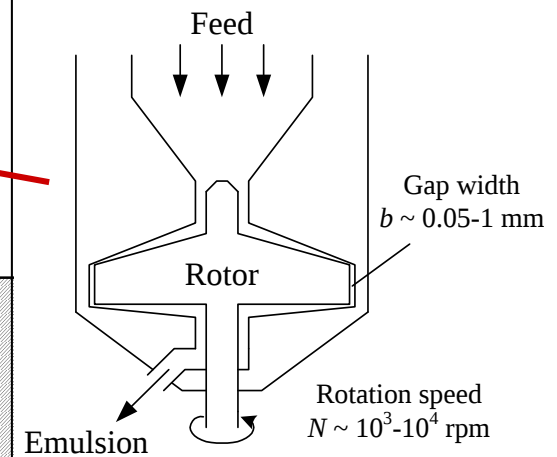
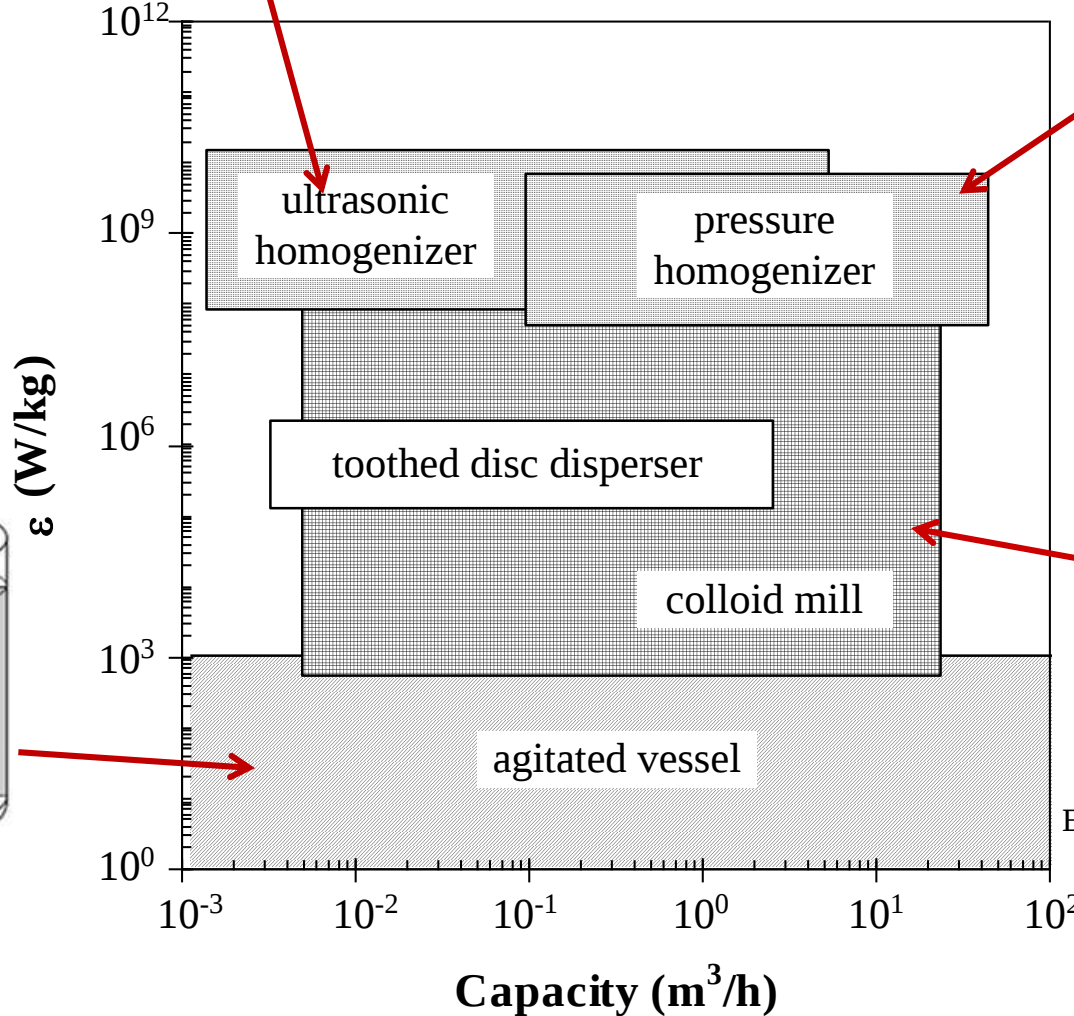
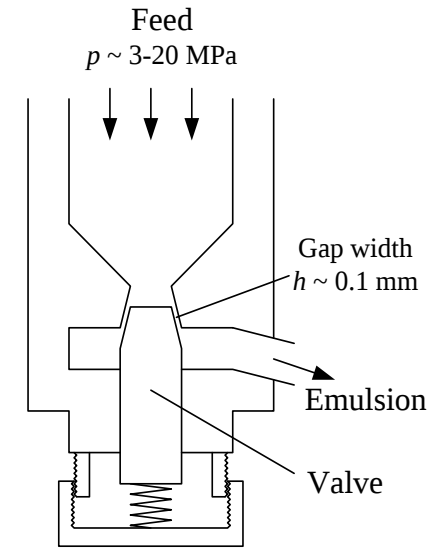
The design process includes three steps:

- Process synthesis**
- Selection of equipment units**
- Selection of equipment operating conditions**

Selection of Emulsification Equipment

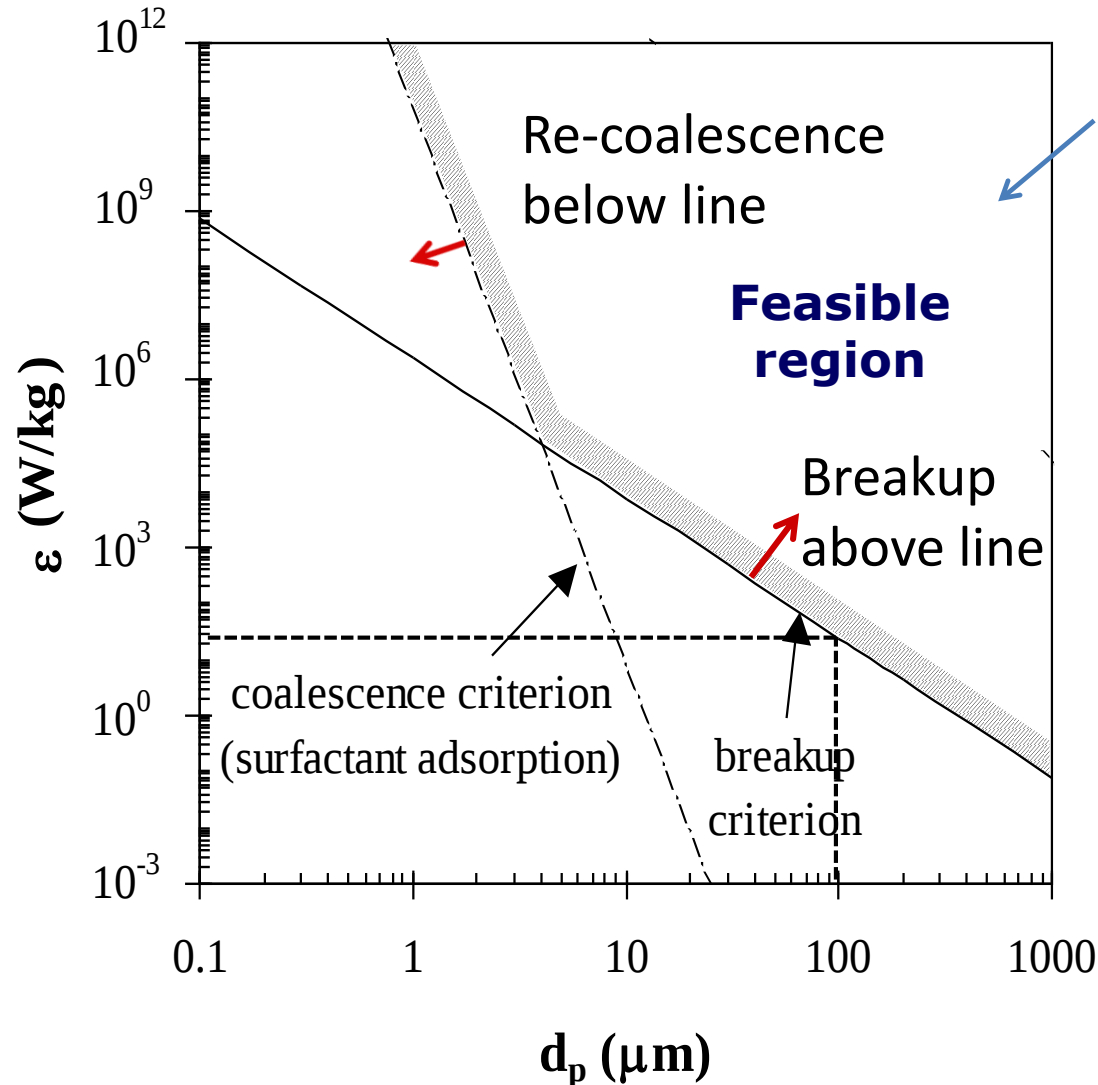


Vibrating knife
 $f \sim 20-50 \text{ kHz}$



Depiction of Breakup and Coalescence Criteria

- **Turbulent flow in an agitated vessel for mixing/pre-emulsification**



Mechanistic models for breakage and coalescence

- **Assume a pre-emulsion droplet size of 100 μm**
 $\rightarrow \varepsilon \sim 25 \text{ W/kg}$
- **$\varepsilon_{av} \sim 0.25 \text{ W/kg}$ (about 1/100 times of ε)**

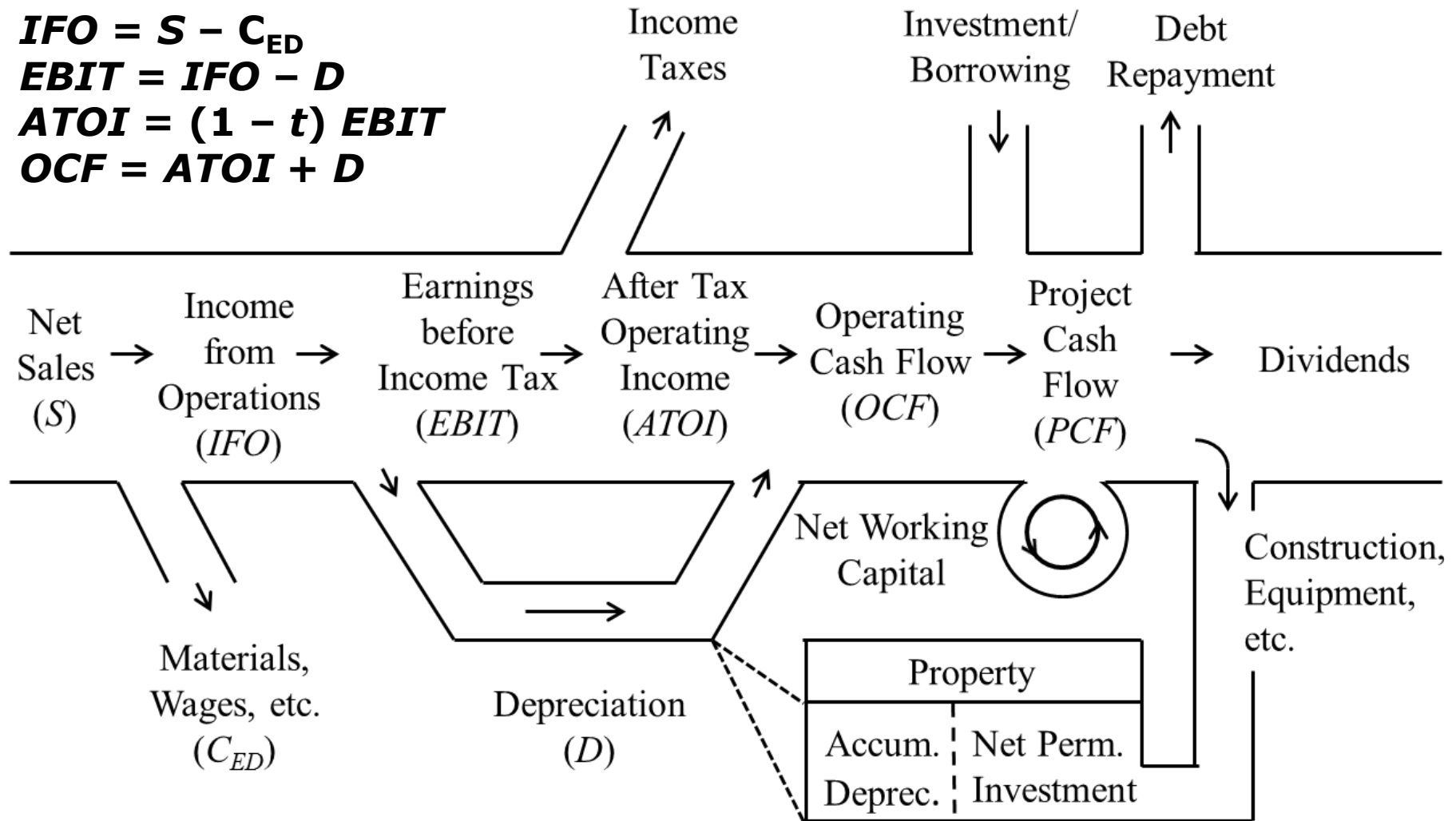
Economic Analysis and Pricing (in 3 lectures) **Ch 19**

$$IFO = S - C_{ED}$$

$$EBIT = IFO - D$$

$$ATOI = (1 - t) EBIT$$

$$OCF = ATOI + D$$



The **cash flow diagram** shows the balance of money for a product development project based on the stand-alone principle.

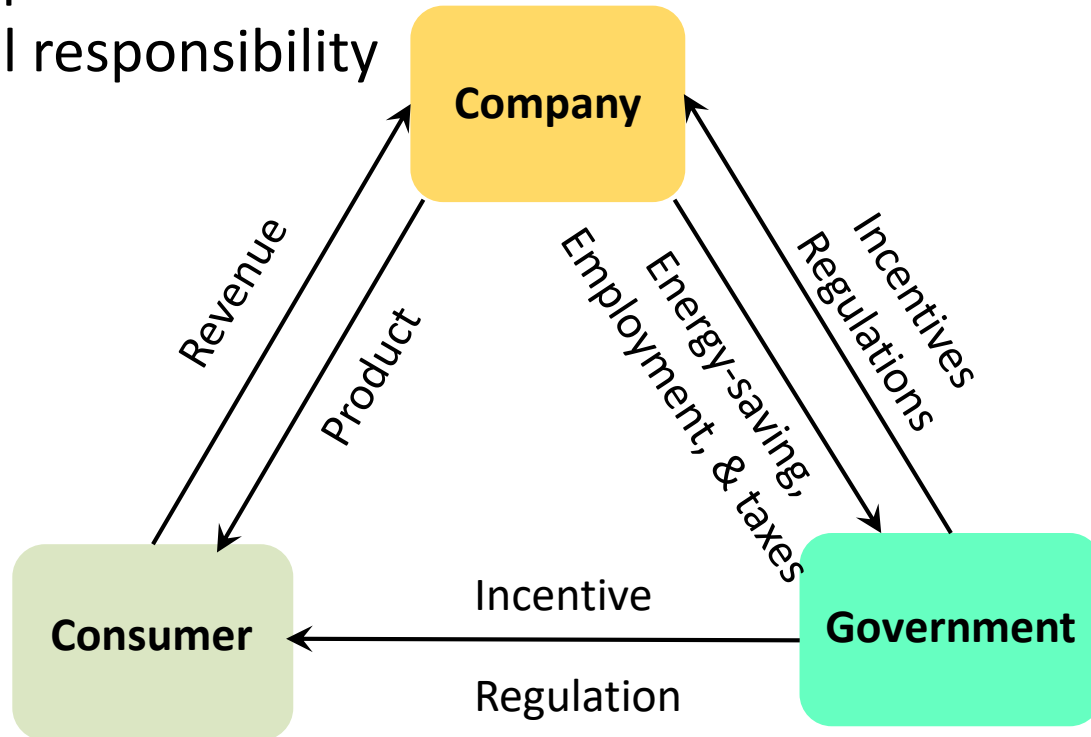
Make-Buy Analysis

- **A strategic choice is often made between producing an item internally (in-house) or buying it externally from an outside supplier (outsourcing)**
- **Items that are strategic in nature should be produced internally if at all possible**
 - **The item is critical to the success of the product, including customer perception of important product attributes;**
 - **The item requires specialized design and manufacturing skills or equipment, and the number of capable and reliable suppliers is extremely limited;**
 - **The item fits well within the firm's core competencies, or within those competencies the firm must develop to fulfill future plans**
- **Outsourcing of non-strategic items may be economically attractive**

Company-Consumer-Government Relationships (in 1 lecture); Graduate Level

Objectives

Net present value
Social responsibility



Objectives

Consumer satisfaction



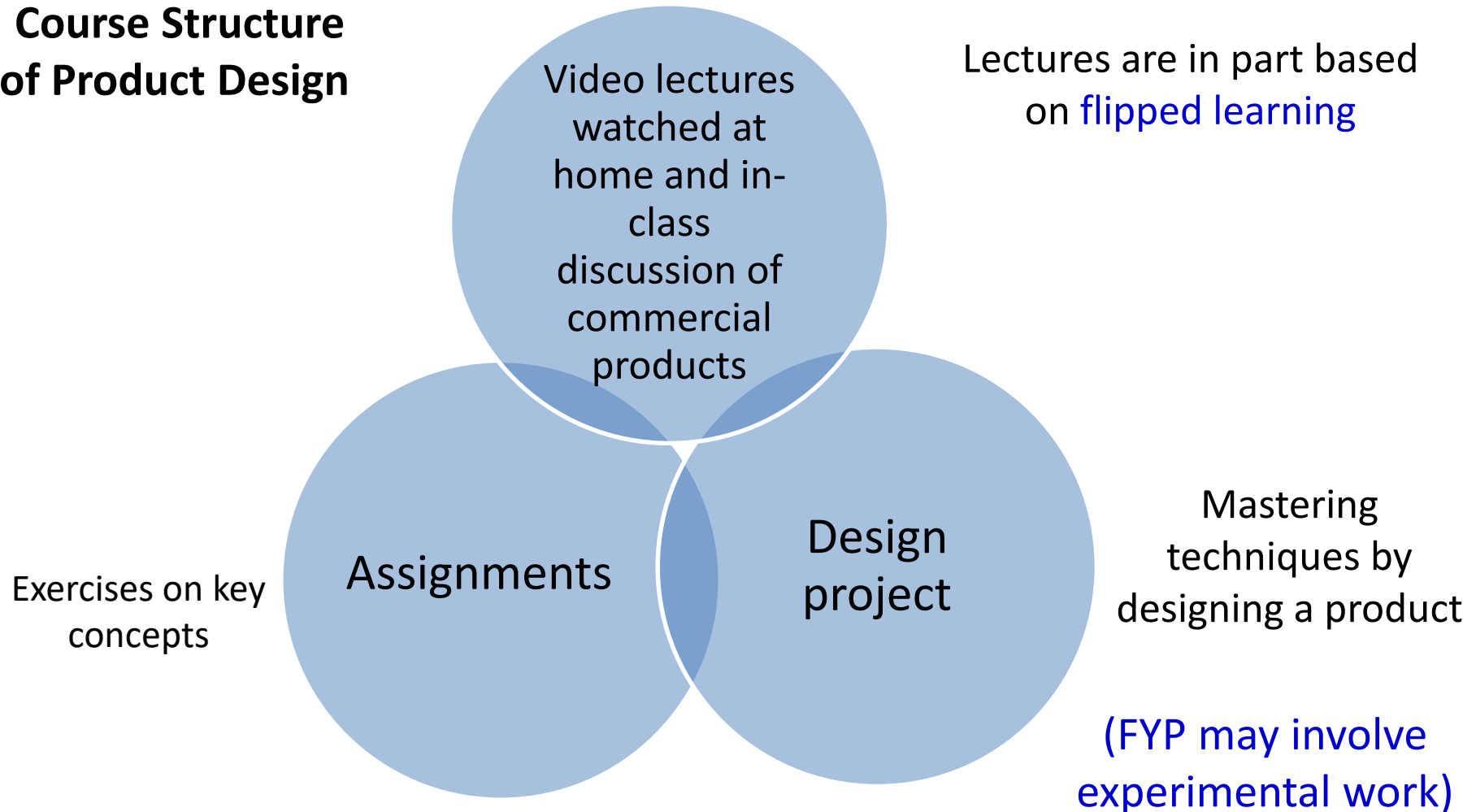
Objectives

Quality of life
Public safety
Competitiveness of society

Course Projects and Final Year Projects

These case studies are used in a product design course (UG / Graduate) or Final Year Project (FYP)

Course Structure of Product Design



Design Project Final Report Ch 23

- **Deliverables**
 - Describe the product and its **desired functions**.
 - Summarize the **market study** of the product; e.g., market size, major companies selling this and related products, competitive analysis, potential innovative products, and so on.
 - Identify the required **product attributes** to succeed in the marketplace.
 - **Conceptualize** the product; e.g., product microstructure, macrostructure, types of ingredients, and so on.
 - Determine the **product specifications**; e.g., the concentration of the ingredients, product performance, and so on.
 - Design the **product manufacturing process**; e.g., the flowsheet, equipment to be used, equipment operating conditions, material balances, and so on.
 - Provide a **financial analysis** accounting for the R&D cost, equipment cost, material cost, product life cycle, equipment salvage value, and so on.
- **The final report for course project (More is required for FYP)**
 - 20-min presentation (in the form of a **video**) + 5 min Q&A
 - A **power point file** that covers all the key deliverables listed above
 - An **executive summary** (3-4 pages) that summarizes the key ideas and results and an **appendix** (~ 5 pages) that provides further details to the executive summary.

A List of Selected Projects

- Wine Aerator
- Faucet Water Filter
- Conductive Ink
- Vitamin C Tablets
- Hand Lotion
- Laundry Detergent
- Shampoo
- Toothpaste
- Mosquito Repellent Vaporizer
- Mosquito Repellent Mat
- PM 2.5 Air Purifier
- Wound Dressing
- Magnetocaloric Fridge
- Desiccant Dehumidifier
- Refrigerator
- Air Conditioner with Green Refrigerants
- Building Air Conditioning System
- Phase Transition Type Heating Pad
- Energy Recovery Ventilator
- Conducting Paste for Printed Electronics
- Disposable Diaper

Further Developments

- These projects are also used by students interested in entrepreneurship.
- We have been developing / compiling case studies for teaching.
- Some of these projects can benefit from the participation of faculty outside of the chemical engineering department.



Second Prize in 2015 HKUST
One Million \$ Entrepreneurship
Competition



PRODUCT DESIGN PROJECTS

A Collection of Product Design Problem Statements and the Corresponding
Sample Solutions for Use as Final Year Projects in Chemical Engineering



JULY 12, 2017

Ka Yip Fung and Ka Ming Ng

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

A preliminary version of this compendium is in the workshop USB.

An NSF Project to Develop Innovative Chemical Products

- These product design projects need more depth and breadth.
- This can be achieved with the help of faculty members with expertise in a research area related to a specific class of chemical products.
- Warren Seider, Tom Edgar and I plan to submit a proposal through CACHE in the Fall of 2017 to the NSF Education Division for funding to develop these case studies.
- These projects should educate students to be leaders and innovators in product design, which is being carried out increasingly by chemical companies worldwide.

Project Plan

- We will invite collaborators with relevant domain knowledge to help develop around 25 new case studies. Some can be an extension of the initial case studies prepared by student design groups at HKUST and some can be proposed by the collaborators.
- Our aim is to produce a collection of case studies, a few of which will be aligned with the expertise profiles in each chemical engineering department.
- Tentatively, the project duration will be three years.
- During the first 6 months of the project, the PIs will help refine the objectives of the proposed case studies.
- After executing the project with one or two cohorts of students over ~ two years, the design project statement and solution alternatives will be documented by the collaborator.

Project Plan (Ctd)

- ~\$10,000 will be provided to each of the US faculty participants to cover costs.
- The case studies will be publicized in CACHE News and in AIChE Meeting sessions.
- They will be distributed at a small fee through CACHE, which has an extensive website (<http://cache.org/>) and has handled product orders in the past.
- Can you help us improve our project plans?

Contact Information



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PRODUCT DESIGN PROJECTS

A Collection of Product Design Problem Statements and the Corresponding
Sample Solutions for Use as Final Year Projects in Chemical Engineering



JULY 12, 2017

Ka Yip FUNG and Ka Ming NG

The Hong Kong University of Science and Technology

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Product 10: Mosquito Repellent Mat	
Product 11: IR Blocking Smart Window	
Product 12: PM 2.5 Air Purifier	
Product 13: Wound Dressing	
Product 14: Magnetocaloric Fridge	
Product 15: Refrigerator	
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Product 17: Building Air Conditioning System	
Product 18: Phase Transition Type Heating Pad	
Product 19: Energy Recovery Ventilator	
Product 20: Conductive Paste for Printed Electronics	
Product 21: Disposable Diaper	
Product 22: Desiccant Dehumidifier	
Product 23: Refrigerant Dehumidifier	
Product 24: Respirator	
Product 25: Portable Seawater Desalination System	
Product 26: Espresso Coffee Machine	
Product 27: Powdered Milk	
Product 28: Controlled Release Granule	
Product 29: Membrane Bioreactor	
Product 30: Aqueous Paint	

Introduction

Product and process design are integral tasks in the commercialization of any chemical product. Traditional chemical engineering focuses on process design because the product under consideration tends to be well defined and product design is not required. For these mature products, the company owning the product competes in the marketplace by reducing product cost. This is achieved by improving the production process or by switching to a cheaper feedstock, which often necessitates the development of a new process. With the recent rapid changes in the global environment, companies can no longer prosper by merely producing mature products. Consumers demand innovative chemical products that meet their needs in their daily lives. For these consumer products, product design is crucial. Thus, the designer has to select the proper product ingredients and design the process to configure these ingredients in such a way that the final product provides the desired product attributes.

Since product design has not received much attention in the chemical engineering community until the late 90s, there are significantly fewer case studies for teaching product design than for process design. And not surprisingly most final year projects in a typical chemical engineering curriculum are related to process design, simulation and optimization.

The purpose of this compendium is to facilitate the expansion of chemical engineering design to product design by providing case studies that can be used as final year product design projects. Each case study includes a problem statement as well as references and web links guiding the students to complete the project. Because of the open-ended nature, these design problems do not have unique and complete solutions. Nonetheless, sample solutions are provided for some of the design problems. Part of these solutions are the course work solutions submitted by the students at the Hong Kong University of Science and Technology. They should be viewed with a degree of scepticism because the solutions depend on the assumptions used in a particular design report. Indeed, different students often come up with totally different products for the same problem statement. For example, the design of disposable diapers was one of the design projects. One group of students considered a product that focused on reusing part of the disposable diaper, while another group designed a product that comes with an RFID wetness sensor.

Despite the diversity of products, the approach to product design and the issues to be considered are the same. The students are given a list of issues to consider and have a great deal of freedom on how the relevant issues should be addressed. Often, a group of students work as a team on a final year design project. Advice and comments are provided to these students throughout the project. At the end of the project, the team submits a written report and presents a power point presentation summarizing all the main points. To guide the students to complete the design tasks and to think about their own performance, an assessment rubric is provided to the students at the outset.

The Design Project

Scope

In each project, product and process design concepts and methods are used to design a specific product. The first step is to carry out a market study to determine the market size, the desired product attributes, and the attributes of competing products. A lot of information on various products can be found in market analyses, company reports, and trade sites on the internet. The second step is to conceptualize the desired product and make a decision on the desired market share. Methods such as house of quality and business model canvas are used to keep track of the information in this phase of the product development project. The product technical specifications such as the active and supporting ingredients as well as the product structure should be determined. Then, product performance is determined by model-based methods or experiments. Throughout the entire product development process, the economic potential of the proposed product is periodically evaluated by means of financial analysis, quantified by metrics such as NPV and IRR.

Consultation

Meetings are scheduled with each team on a regular basis to provide comments, advice, and resources to complete the project. Subject to necessity and availability of equipment, experiments are performed as part of the product design project.

Report and Presentation

The project report is limited to 20 pages. It includes an executive summary (2 pages) that summarizes the main points, the body of the report (maximum 10 pages) and an appendix (maximum 8 pages) that provides further details to the report. The following items are addressed in the written report:

1. Describe the product and its desired functions.
2. Summarize the market study of the product; e.g., market size, major companies selling this and related products, competitive analysis, potential innovative products, etc.
3. Identify the required product attributes to succeed in the marketplace.
4. Conceptualize the product; e.g., product microstructure, macrostructure, types of ingredients, and so on.
5. Determine the product specifications; e.g., the concentration of the ingredients, product performance, etc.
6. Design the product manufacturing process; e.g., the flowsheet, equipment to be used, equipment operating conditions, material balances, and so on.
7. Provide a financial analysis accounting for the R&D cost, equipment cost, material cost, product life cycle, equipment salvage value, etc.

All materials and ideas borrowed from various sources such as the internet, books, and scientific papers should be cited.

The product design team gives a 20 min powerpoint presentation in front of the entire class at the end of the project. The presentation is followed by a Q&A session of about 10 minutes.

Assessment of Student Performance

This is broken down as shown in the project assessment rubric. The instructor after consulting with all members of the project team assigns a multiplying factor ranging from 0-100% to each team member which reflects the contribution from the individual team member. The actual grade is obtained by the project grade times the multiplying factor.

Assessment Rubric for Product Design Project

	Exemplary	Competent	Developing	Beginning
Technical skills				
Product introduction (5%)	Give a clear introduction of the product and define the design scenario clearly.	Give a clear introduction of the product, but the design scenario is not sufficiently clear.	Give an acceptable introduction of the product, but the design scenario is not defined clearly.	Fail to introduce the product and the design scenario clearly.
Market study and identification of product attributes (10%)	Provide a comprehensive competitors' analysis and a reasonable estimate on market size with sound justification. Identify the most important product attributes to be designed.	Provide a comprehensive competitors' analysis and a reasonable estimate on market size, but with weak reasoning. Identify the most important product attributes to be designed.	Provide an acceptable competitors' analysis and a reasonable estimate on market size, but with weak reasoning. Fail to identify the major product attributes to be designed.	Fail to provide an acceptable competitors' analysis and a reasonable estimate on market size. Fail to identify major product attributes to be designed.
Product conceptualization (ingredients and product structure) (30%)	Explain clearly and quantitatively on why the product is designed as is. Major product attributes are designed and supported with sound scientific and engineering principles.	Explain clearly why the product is designed as is. Major product attributes are designed with scientific and engineering principles, but with minor mistakes in the analysis.	Explain why the product is designed as is, but not with sufficient details to allow clear understanding. Major product attributes are designed with scientific and engineering principles, but with major mistakes in the analysis.	Fail to explain why the product is designed as is. Major product attributes are not supported with scientific and engineering principles.
Product manufacture (20%)	Describe clearly and quantitatively the process required to manufacture the product, with clear explanations on the logic behind it	Describe clearly the process required to manufacture the product, but the reasoning is not sufficiently clear	Describe the process required to manufacture the product, but without enough quantitative results and the reasoning behind is not clear	Fail to describe a reasonable process to manufacture the product
Financial analysis (10%)	Provide a sound and justifiable financial	Provide a financial analysis with justification	Provide a financial analysis without	Provide a financial analysis with quite a

	analysis	for most of the numbers, but fail to justify all parameters	justification for most of the numbers, and occasionally incorrect for some calculations	number of errors and mistakes
Presentation skills				
Organization (10%)	Good organization at the level of each point and sentence. Good transitions from one point to another. Audience can follow the train of thought of the speaker and form a clear mental picture.	Good organization at the level of main messages. Mostly sensible sequence of topics. Occasional unclear transitions from point to point	Basic organization at the overview level only. Only occasional logical transition between each slide or each sentence. Use terms or concepts before they are introduced or defined.	No logical sequencing or organization of topics. Impossible to follow.
Questions & Answers (10%)	Provide to-the-point and thoughtful answers. Good command of the discussion, with meaningful back-and-forth with audience. Graceful response to difficult questions.	Respond to all questions with mostly to-the-point answers. Q&A is largely unilateral. Do not know how to handle difficult questions.	Provide incomplete, dead-ended, and sometimes irrelevant answers. Appear defensive or diffident.	Fail to comprehend or respond to most questions.
Visual aids (5%)	Slides are clear, appealing and error-free. Innovative and appropriate use of figures or animations to explain concepts. Slides complement the speech well.	Slides are adequate to deliver message most of the time. Occasionally effective use of figures or animations. Slides somewhat complement the speech.	Some slides are poorly designed, unclear or error-prone. Little or ineffective use of figures. Slides and speech do not complement each other very much.	Most slides are poorly designed, unclear, error-prone. Slides appear to be hastily put together without much care.

Design Projects

Product 1: Wine Aerator

A device that mixes air with red wine to soften the tannins in the red wine

Project Statement

The term tannin refers to a class of molecules that bind relatively non-specifically to protein molecules [Payne *et al.*, 2009]. Tannin found in red wines binds with salivary protein, forming protein-tannin complexes that reduce lubricity of saliva in the oral cavity, thereby creating dry and puckering taste within the mouth, called astringent sensation. The astringency can be softened by tannin oxidation or conventionally known as wine aging process by using wine aerator or decanter [McRae and Kennedy, 2011].

Wine aerator is able to soften the astringent sensation of red wines, making the bouquet of lower grade red wines comparable to that of higher grade red wines. The chemistry behind softening wine astringency, involving the interaction of astringent agents, alcohol, sugar content in wine, and the salivary protein in oral cavity, is complex [Smith *et al.*, 1996; Payne *et al.*, 2009].

Astringent agents in a wine are classified into two categories, hydrolysable and condensed tannin. Hydrolysable tannin is incorporated during storage in wood or oak vessel and treatment with wood or oak chip. This type of tannin readily degrades at the pH of wine, hence not giving any astringency sensation to the wine. Condensed tannin consists of extracts from grape seeds and skins, is stable at the pH of wine, binds with salivary protein, and is responsible for the astringency of a red wine [Payne *et al.*, 2009].

Wine aging is a series of oxidation process of tannins and other agents. This series of oxidation can be catalysed by introducing a trace amount of transition metal ions [Waterhouse and Laurie, 2006] or increasing the amount of oxygen in the wine, hence increasing the rate the oxidation. The aims of wine aerator device can be better understood after some basic understanding in red wine making [<http://www.wineanorak.com/howwineismade.htm>]. Chemistry involved in tannin oxidation may be also useful in designing a wine aerator [Fulcrand *et al.*, 2006; Waterhouse and Laurie, 2006].

In addition to designing a functional wine aerator, the economic viability of the product has to be considered as well. Students are advised to perform a competitive analysis based on information available at online trade sites such as Amazon and Alibaba as well as competitors' company websites. Based on the competitive analysis, students will be able to evaluate and identify key product attributes of the wine aerator sold in the market.

Generally, wine aerator devices available in the market can be divided into two types: electrical and non-electrical. Electrical type involves moving parts such as stirrer and bubbler whereas a non-electrical aerator design usually involves pressure difference between wine and ambient air. Sometimes, transition metal ions are introduced into the wine as a catalyst. Consider using basic fluid mechanics such as the Bernoulli equation in designing a wine aerator.

References

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- <http://www.wineanorak.com/howwineismade.htm> (Accessed on 9 Sep, 2016)

Sample Solutions to Design of Wine Aerator

1.1 The product and its functions

Tannins found in red wine are plant polyphenols that originate from grapes seeds and skins. These plant polyphenols bind and precipitate salivary protein, forming protein-tannin complexes. Aggregation and precipitation of protein-tannin complexes reduces the lubricity of saliva through increasing the feel of “friction” in the oral cavity [Payne *et al.*, 2009], hence producing a drying sensation, so called astringency. Astringency is a complex process with multiple interactions between the astringent agents [Smith *et al.*, 1996]. The astringency could also be produced by the polymerization of tannins in the wine.

Red wine aging reduces the astringency by reducing the amount of protein-tannin complexes through a series of oxidation reactions. The oxidation process is initiated by the singlet oxygen free radical ($O_2^{\bullet}$), whose generation is relatively slow in an acidic wine medium, especially in the absence of light. Its generation can be catalyzed by metal ions such as Fe(III) so that the oxidation reaction is faster [Fulcrand *et al.*, 2006; Waterhouse and Laurie, 2006]. However, iron concentration in red wine is usually not sufficient for effective wine aging. This can be helped by introducing iron into the wine during the aging process, which is usually carried out in conventional wine decanter, wine aerator or directly bubbled air into the wine after bottle opening.

The aim of this project is to design a wine aerator which also adds trace amount of metal ions into the red wine before it mixes with the air.

1.2 Market study

The red wine market is large and complex, fragmented into different grades, and sources of origin. Low- and mid-grade red wines account for the majority of the market, while high-grade red wines contribute only a small portion of it. Usually, low- and mid- grade red wines need to be aerated as they contain a significant amount of tannins.

In 2009-2013, red wine accounts for the largest portion (54.78%) in the world wine consumption, equivalent to 17.78 billion bottles. The world wine consumption is somewhat steady, and is estimated to be further increased by 1% in 2014–2018, equivalent to 17.96 billion bottles in 2014-2018. [<http://www.wineindustryadvisor.com/2015/02/02/us-wine-market-drives-growth/>].

Assume a consumer purchases 6 bottles of wine a year (i.e. 30 bottles in 2014-2018) and 10% of the consumers would like to buy a wine aerator which has to be replaced every 5 years, 59.9 million pieces of wine aerators is needed for the next 5 years, equivalent to an annual sales of 12 million pieces of wine aerators in 2014-2018. We aim at capturing 5% market share, equivalent to an annual sales of 599,000 wine aerators.

Wine aging devices, with different working principles and product specifications, are available in the market. A preliminary analysis of few competitor’s product has been summarized in Table

1.1. Vinturi and Oster utilize Venturi effect for aeration, have an excellent level of aeration and require a short aeration time. Vinturi has a stand to contain dripping wine after use and is cheaper than Oster. Decanter is also available in the market, with a wide range of price. But, the required aeration time is much longer, and is too large to be portable.

Table 1.1 Summary of competitors' products.

Type (Brand Name)*	Working Principle	Level of aeration	Aeration time	Size	Price	Others
Hand-held injection type (Vinturi)	Venturi effect	Excellent	< 10s	Portable	US\$ 18.95	Stand available to contain dripping wine after use
Funnel type (Oster)	Venturi effect	Excellent	< 10s	Portable	US\$ 25.44	Without stand
Decanter	Exposing wine in air	Good	10-15min	Large	US\$ 20- 299 or above	Complex shaped container and hard to clean

*Company websites are listed in the reference.

1.3 Product attributes and technical parameters

The consumer preferences of a wine aerator are listed below.

- Aerates wine quickly
- Convenient to hold the aerator
- Easy to clean
- Portable
- Cheap

These consumer preferences are converted into product/technical parameters in the House of Quality (Table 1.2). The first column lists the consumer preferences on the wine aerator, while the first row lists the product/technical parameters. The relationships between consumer preferences and product/technical parameters are summarized in the table, with 0 indicating no relationship, 1 indicating a weak relationship and 9 indicating a strong relationship. For example, how fast the wine is aerated is highly related to the aeration principle and the air flowrate, but is not related to the material, size, etc. With the weighting factors of all consumer preferences, as listed in the table, the importance weighting of each product/technical parameter can be calculated. For example, the ease of cleaning and price are related to the use of material. The importance weighting for the use of material can be calculated as: $(5 \times 1) + (9 \times 3) = 32$. Among all product/technical parameters, aeration principle and airflow rate are the most important factors, which will be discussed in more detail in product conceptualization. The same table also summarizes the comparison between our product and the competitors' product.

Table 1.2 House of Quality.

Consumer Preference / Technical Parameter (rated from 1 to 9, with a larger number indicating a stronger relationship)	Use of material	Aeration principle	Aerator Size	Parts Removable	Air flow rate	Aerator stand	Weighting factor	Competition (5 is the best)			
								Our Product	Vinturi	Oster	Decanter
Aerates wine quickly	0	9	0	0	8	0	4	4	4	4	2
Convenient to hold the aerator	0	0	0	0	0	9	2	4	4	1	4
Easy to clean	5	0	6	9	0	0	1	2	2	3	1
Portable	0	0	9	7	0	0	1	4	4	3	1
Cheap	9	5	6	0	5	3	3	4	2	2	5
Importance weighting	32	51	33	16	47	27					

1.4 Governing physicochemical phenomena

Air can be introduced into the wine by direct bubbling (electrical type) or entrainment (non-electrical type). To make a low-cost wine aerator, direct bubbling is not selected. Pressure drop can be created along a channel to entrain air into the wine for oxidation. Venturi, nozzle, and orifice designs can be used to induce pressure drop in the channels (Figure 1.1). Among the three designs, venturi has the smallest pressure drop (Figure 1.2) and is selected for use in the wine aerator.

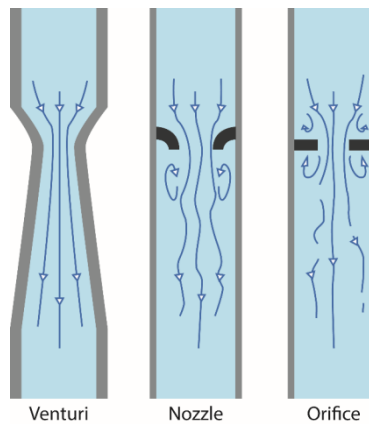


Figure 1.1 Venturi, nozzle and orifice designs.

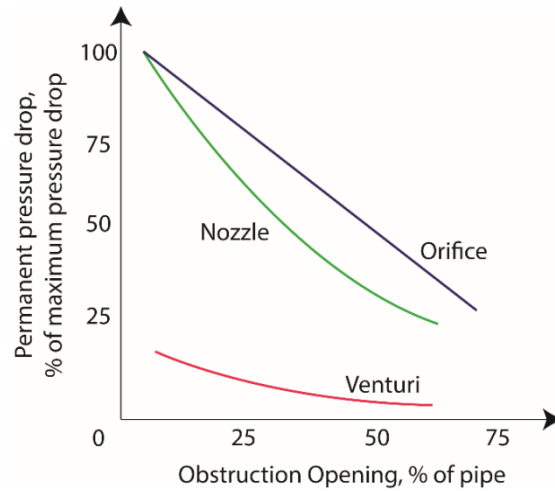


Figure 1.2 Pressure drop for different designs [Munson *et al.*, 2006].

1.5 Product conceptualization

The configuration of the wine aerator is depicted in Figure 1.3. The wine aerator has an aluminum coated Fe_2O_3 filter to filter any wine sediments and to introduce trace amount of Fe^{3+} ion into the passing wine for catalytic oxidation. The reducer in the wine aerator aims at creating an accelerated wine flow, which also slightly reduces the pressure in the wine. This small pressure difference between the wine and the ambient air sucks air into the wine through the entrainer tube for wine oxidation and aging.

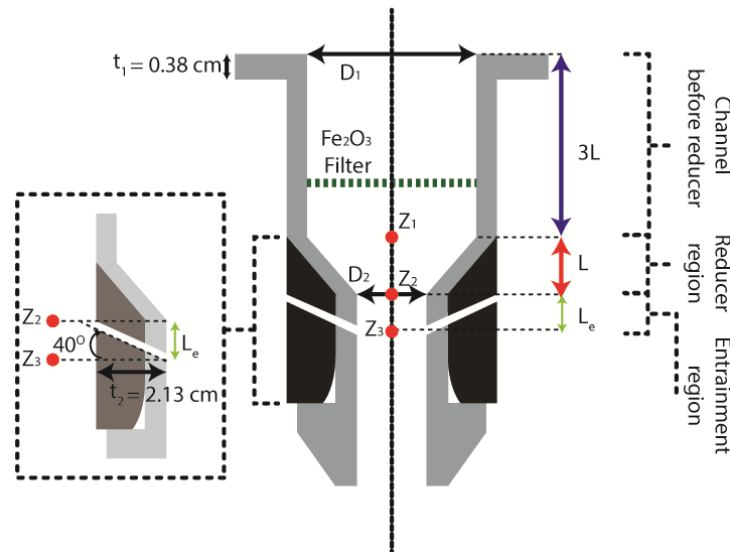


Figure 1.3 Schematic diagram of the wine aerator.

Polystyrene is selected as the raw material in this project as it is chemically inert with alcohol, possesses good mechanical strength, transparent, and requires a low processing temperature. Its price is also lower and more stable in comparison with other polymer materials such as polycarbonate (PC) and polyethylene terephthalate (PET).

1.6 Determination of the product specifications

The dimensions of the proposed wine aerator are first determined. The channel before reducer and the reducer region are designed to hold a volume of $\sim 50 \text{ cm}^3$ of red wine (V). It is further assumed that the ratio of the length of channel before reducer and the length of the reducer region is 3:1. The diameter of the channel before reducer (D_1) and after reducer (D_2) are specified to be 4 cm and 0.5 cm, respectively.

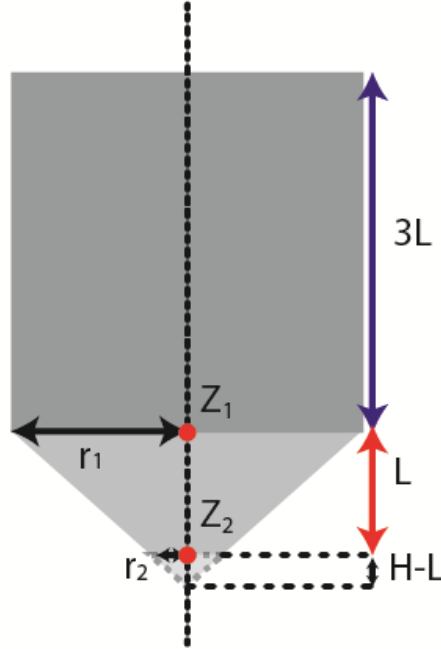


Figure 1.4 Dimensions of the wine aerator.

The volume V can be expressed as follows

$V = \text{Volume of the channel before reducer} + \text{Volume of the reducer region}$

Volume of the channel before reducer $= 3\pi r_1^2 L$

Volume of the reducer region $= \frac{1}{3}\pi r_1^2 H - \frac{1}{3}\pi r_2^2 (H - L)$

So, we have

$$V = 3\pi r_1^2 L + \frac{1}{3}\pi r_1^2 H - \frac{1}{3}\pi r_2^2 (H - L) = 50 \text{ cm}^3 \quad (1)$$

By similarity of triangles,

$$\frac{r_2}{H-L} = \frac{r_1}{H} \quad (2)$$

Solving the above equations, we get $L = 1.18 \text{ cm}$. Therefore, the length of the channel before reducer is 3.53 cm and the length of the reducer region is 1.18 cm.

The entrainment tube is designed to be inclined at an angle of 40° , so the height of the entrainment section (L_e) can be calculated.

$$L_e = \tan 40^\circ \times 2.13 \text{ cm} = 1.79 \text{ cm} \quad (3)$$

With the aerator dimensions, Bernoulli equation can be used to calculate the amount of air being entrained into the wine. The following assumptions are made in the calculation:

- Viscous effect is negligible
- Steady state flow
- Incompressible flow
- Applicable along streamline
- Constant volumetric flowrate throughout the wine aerator

In pouring the wine through the wine aerator, the wine continues to flow down the channel and we assume here that the wine usually fills up the reducer region only. So, by applying the Bernoulli equation across the reducer and the entrainment section,

$$P_1 - P_3 = \frac{\rho_w}{2} (v_{w,3}^2 - v_{w,1}^2) + \rho_w g (Z_3 - Z_1) \quad (4)$$

Here, g is the gravity acceleration and equals 9.8 m/s^2 , ρ_w is the wine density. Note that the subscripts 1 and 3 refer to the location before the reducer and after the entrainment section, respectively. We assume that the wine contains an alcoholic percentage of 12.9%, so the wine density is 1095 kg/m^3 [<http://winemaking.jackkeller.net/hydrom.asp>].

The aerator is designed to aerate a glass of red wine ($\sim 150 \text{ cm}^3$) in 10 s, so the volumetric flowrate Q can be calculated as:

$$Q = 150 \text{ cm}^3 / 10 \text{ s} = 15 \text{ cm}^3/\text{s} \quad (5)$$

Assume constant volumetric flowrate, the wine velocity before and after the reducer region can be calculated.

$$Q = A_1 v_{w,1} = A_2 v_{w,2} \quad (6)$$

The wine velocity before the reducer ($v_{w,1}$) is

$$v_{w,1} = Q / \pi r_1^2 = 1.2 \text{ cm/s} \quad (7)$$

Similarly, the wine velocity after the reducer ($v_{w,2}$) is 76.4 cm/s . As the cross-sectional area is the same in the entrainment section, we have $v_{w,3} = v_{w,2}$.

With $Z_3 - Z_1 = -(L + L_e)$, and after substituting all parameters,

$$P_1 - P_3 = 0.853 \frac{\text{kg}}{\text{m s}^2} = 8.42 \times 10^{-6} \text{ atm} \quad (8)$$

The entrainment tube is designed to suck air into the passing wine for oxidation. Bernoulli equation can be applied to the entrained air.

$$P_2 - P_3 = \frac{\rho_a}{2} (v_{a,3}^2 - v_{a,2}^2) + \rho_a g (Z_3 - Z_2) \quad (9)$$

The pressure drop of air in the entrainment tube is same as the pressure drop in wine. So, we have

$$\frac{\rho_a}{2} (v_{a,3}^2 - v_{a,2}^2) + \rho_a g (Z_3 - Z_2) = 8.42 \times 10^{-6} \text{ atm} \quad (10)$$

Here, ρ_a is the air density at STP which equals 1.184 kg/m^3 [Munson *et al.*, 2006] and $Z_3 - Z_2 = -L_e$.

By assuming the inlet air velocity ($v_{a,2}$) equals 0 m/s , the velocity of air sucking into the flowing wine ($v_{a,3}$) is 1.34 m/s . The diameter of the entrainment tube is designed to be 0.5 cm , leading to an air flowrate of $26.3 \text{ cm}^3/\text{s}$, equivalent to $0.031 \text{ g of air /s}$ or $0.0065 \text{ g of O}_2/\text{s}$.

The oxygen in air is used to oxidize tannins in wine. The reaction rate can be expressed by the following equation.

$$\frac{d[T]}{dt} = -k[T][O_2] \quad (11)$$

Here, k is the reaction rate constant and equals $2 \times 10^2 \text{ m}^3 / \text{mol s}$, $[T]$ and $[O_2]$ are the concentration of tannins and oxygen in wine. By assuming $[O_2]$ is in excess and remains constant, the rate equation can be integrated with the boundary conditions ($t = 0, [T] = [T]_0$; $t = t, [T] = [T]$) to give

$$[T] = [T]_0 e^{-k[O_2]t} \quad (12)$$

The initial tannins concentration $[T]_0$ in red wine is reported to be around 200 ppm (Harbertson et al., 2008). We assume that 1% of the inflow O_2 can be dissolved into the wine for oxidation, so that $[O_2]$ in the wine medium is:

$$[O_2] = \frac{0.0065 \times 1\%}{15} = 4.36 \frac{g \text{ } O_2}{m^3} = 0.136 \frac{mol \text{ } O_2}{m^3} \quad (13)$$

Assume the reaction time is around 5 s, the fast oxidation of tannins provides almost no tannins in the red wine ($[T] = 1.48 \times 10^{-57} \text{ ppm}$).

1.7 Design of product manufacturing process

With an annual sales of 599,000 wine aerators, plastic injection moulding, with relatively low processing cost, is considered to be the most suitable processing technique to handle a relatively large throughput.

Food grade impact-modified polystyrene is used as the raw material to produce transparent wine aerators with moderate impact strength and glossy outer surface. No additives are added to the process; and fillers such as glass fibres are strictly prohibited by regulations for manufacturing components that are in contact with foods or drinks. Similarly, no regrind or reuse of defected plastic parts is allowed for these goods.

Polystyrene resins are preheated in a hopper at 80°C for few hours to remove any moisture. Dry resins are then melted in the barrel of an injection machine, and the melted plastic is injected into a mould with highly polished surface, which is important to produce wine aerator with highly glossy surface. The hot melt is cooled by the cooling water channels running around the mould. When the melt is solidified, the products are ejected from the mould by an ejector pin.

To design the injection moulding machine, issues such as mould size and design, ejection force, etc. have to be considered. Detailed information can be found in polymer engineering textbooks (Jones, 2008). The cost estimation for injection moulding machine is readily available in the internet [<http://www.custompartnet.com/estimate/injection-molding/>] and is used below for financial analysis.

1.8 Financial analysis

The financial analysis of a 5-year wine aerator product is summarized in Table 1.3. With a sales volume of 599,000 pieces at \$12.99 per piece, we have an annual sales of \$7,781,010. The sales volume is expected to be the same for the subsequent years.

During product development (Year -1 and 0), fixed cost includes \$180,000 for office rent and \$480,000 for staff wages (per annum). After product launch, an annual advertising cost of \$200,000 is added to the fixed cost. This increases the fixed cost from \$660,000 in Year -1 and 0 to \$860,000 in Year 1 to 3. A development cost of \$1,000,000 is spent in the first year (year -1) for R&D and product design, which includes tooling design, prototype functional test and regulatory test. The capital investment in Year 0 is assumed to be \$50,000, and the net working capital is assumed to be \$250,000.

For Year 1 to 3, the variable cost includes manufacturing cost and packaging cost, which can be estimated by an online feature-based estimator [<http://www.custompartnet.com/estimate/injection-molding/>] with input parameters summarized in Appendix A. The results show that the manufacturing cost, which includes material cost, production cost, and tooling cost, is US\$ 0.699 per unit. With an unit cost of US\$ 0.09 for a Fe₂O₃ filter, the manufacturing cost of a wine aerator is US\$ 0.708. Similarly, the packaging cost is also estimated to be US\$ 0.098 per unit. This leads to a variable cost of US\$ 0.806 per unit, equivalent to US\$ 482,794 per annum.

With all the cost information, income from operations (*IFO*), earnings before income tax (*EBIT*), after tax operating income (*ATOI*), operating cash flow (*OCF*), and project cash flow (*PCF*) are calculated by the following equations.

$$IFO = S - C_{ED} \quad (14)$$

$$EBIT = IFO - D = S - C_{ED} - D \quad (15)$$

$$ATOI = (1 - t) EBIT = (1 - t) (S - C_{ED} - D) \quad (16)$$

$$OCF = ATOI + D = (1 - t) (S - C_{ED} - D) + D = (1 - t) (S - C_{ED}) + t D \quad (17)$$

$$PCF = OCF - \text{Development cost} - \text{Increase in NWC} - \text{Project capital spending} \quad (18)$$

Here, *S* is the sales, *C_{ED}* is the fixed and variable costs, *D* is depreciation which is assumed to be linear depreciation over 5 years, *t* is tax rate which is assumed to be 40%, *NWC* is the net working capital.

Table 1.3 Financial analysis of a wine aerator product for a 5 year product cycle. (All the money is shown in USD and in thousands.)

Year	-1	0	1	2	3
Sales	0	0	7,781.01	7,781.01	7,781.01
Fixed Cost	660.0	660.0	860.0	860.0	860.0
Variable Cost	-	-	482.8	482.8	482.8
IFO	-	-	6,438.2	6,438.2	6,438.2
Depreciation	-	-	10.0	10.0	10.0
EBIT	-	-	6,428.2	6,428.2	6,428.2
Taxes (40%)	-	-	2,571.3	2,571.3	2,571.3
ATOI	-	-	3,856.9	3,856.9	3,856.9
OCF	-660.0	-660.0	3,866.9	3,866.9	3,866.9
NWC	-	250.0	-	-	-250.0

Development cost	1,000.0	-	-	-	-
Capital Spending	-	50.0	-	-	
PCF	-1,660.0	-960.0	3,866.9	3,866.9	4,116.9

Net present value (NPV) is used to calculate the profitability of the wine aerator project. A discount rate (R) of 20% and a bank interest rate of 5% are assumed in this evaluation.

$$NPV = \sum_{j=-n}^m \frac{PCF_j}{(1+R)^j} \quad (19)$$

Here, n is the number of periods for product development, and m is the number of periods for product life cycle. Note that the unit of NPV is in thousand USD.

$$NPV = -1660(1+R) - 960.0 + \frac{3866.9}{1+R} + \frac{3866.9}{(1+R)^2} + \frac{4116.9}{(1+R)^3} \quad (20)$$

With $R = 0.2$, NPV equals US\$ 5,338,291, which meets the management's expectation.

To determine IRR, NPV is set to 0. It becomes

$$0 = -1660(1+R) - 960.0 + \frac{3866.9}{1+R} + \frac{3866.9}{(1+R)^2} + \frac{4116.9}{(1+R)^3} \quad (21)$$

Using Microsoft Excel to solve the above equation, IRR equals 81.9%, which is larger than the bank interest rate of 5%. Therefore, the wine aerator project can be presented to the management for approval.

1.9 References

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- Waterhouse AL, Laurie VF. Oxidation of wine phenolics: A critical evaluation and hypotheses. *American Journal of Enology and Viticulture*. 2006;57:306-313.

Webpage information

Market information:

- <http://www.wineindustryadvisor.com/2015/02/02/us-wine-market-drives-growth> (Accessed on 9 Sep, 2016)

- Oster website - <http://www.oster.com> (Accessed on 9 Sep, 2016)
- Vinturi website - <https://www.vinturi.com/> (Accessed on 9 Sep, 2016)

Technical information:

- <http://winemaking.jackkeller.net/hydrom.asp> (Accessed on 9 Sep, 2016)
- <http://www.custompartnet.com/estimate/injection-molding/> (Accessed on 9 Sep, 2016)

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Appendix A. Parameters for CustomPartNet for the cost estimation of injection molding.

	Wine aerator
Part information	
Rapid tooling	No
Quantity	599000
Material	Polystyrene, Impact Modified
Envelope X-Y-Z (mm)	47 × 47 × 130
Max. wall thickness (mm)	3.8
Projected area	48.3% of the envelope
Projected Holes	No
Volume	49.9% of the envelope
Tolerance (mm)	Moderate precision (≤ 0.25)
Surface roughness (μm)	High gloss polish ($R_a \leq 0.2$)
Complexity	Simple
Injection Molding Process parameters	
Material	
Defect rate (%)	10
Material price (US\$/kg)	2.2
Regrind Ratio (%)	0
Additives ratio (%)	0
Material markup (%)	25
Production	
Hourly rate (US\$/h)	35
Machine setup time (h)	8
Machine uptime (%)	95
Post-processing time (h)	0
Production markup (%)	10
Tooling	
Mold-making rate (US\$/h)	65
Packaging process parameters	
Material	
Box price (US\$/box)	3.32
Filler	Yes
Filler price (US\$/m ³)	44.14
Production	
Part spacing (mm)	25.4
Pack time per part (s)	5
Packing rate (US\$/h)	35

Product 2: Faucet Water Filter

A device that removes pollutants from tap water

Project Statement

A faucet water filter is a device that removes pollutants such as bacteria, organics, and heavy metals from the tap water. Various technologies such as ultrafiltration, reverse osmosis, and adsorption can be used for such purpose. Students are required to design a faucet water filter for pollutants removal. They can refer to the Environmental Protection Agency (2013) for more information on the pollutants contained in tap water and Crittenden et al. (2012) for the basic information on water purification techniques.

Students are advised to perform a market study and a competitive analysis on the faucet water filters. Online trade sites such as Amazon and Alibaba as well as competitor's company website provide such information. Examples of companies providing faucet water filters include Brita [<https://www.brita.com/intl/>] and Culligan [<http://www.culligan.com/>]. Students should remember that market information is always fragmented and students should not rely on a single source of information. After the market study, the market size and the market price of the faucet water filter can be estimated. The competitive analysis also helps the students identify the key product attributes of the water filters. Students can also conduct a market survey to understand which of these attributes are more important to their target customers.

With the key product attributes, students should relate them to the technical requirements of a water filter by tools such as quality function deployment. Product form and the operating mechanism of the water filter are decided next. Adsorption or membrane filtration theories and models (McCabe et al. 2005) can be used to design the water filters. With the design of the water filter, the manufacturing process is proposed next, followed by a financial analysis to determine if the proposed product is profitable.

References

- Brita's website. <https://www.brita.com/intl/> (Accessed on 9 Sep, 2016)
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Sample solutions to design of faucet water filter

2.1 The product and its functions

Organics and heavy metals are the major contaminants found in water collected from a faucet (EPA, 2013). For example, lead was found in the tap water of few public housing estates in Hong Kong in 2015 due to the use of lead containing solder in pipe welding (Chan and Lai, 2015). Water filters have to install under the faucets for removing lead from drinking water. Various pollutant removal mechanisms can be used in these faucet water filters. This project is to design a cheap water filter that removes contaminants from tap water.

2.2 Market study

Household product companies such as Brita, Panasonic and Culligan provide faucet water filters of various technologies such as ultrafiltration, reverse osmosis, adsorption and ion exchange (Table 2.1). All of these filters remove more than 99% of lead from the tap water. The price varies from US\$ 23-127 which depends on the mechanism of pollutants removal and its handling capacity. All these products produce a flowrate from 1.6 to 2.2 L/min. Note that the typical water flowrate from a faucet is around 7.5 L/min.

Table 2.1 Commercial faucet water filters

Brand*	Model	Mechanism	Price (USD)	Flowrate (L/min)	Handling capacity (L)
Panasonic	TKCJ21	Ultrafiltration	\$127	1.8	4000
Culligan	FM-15A	Carbon Adsorption	\$23	1.9	757
Culligan	FM 25	Carbon Adsorption	\$25	1.9	757
Brita	Advanced Faucet Filtration System FF-100	Carbon and ion-exchange resin adsorption	\$29.99	2.2	378
Philips	Micro X-Pure WP 3812	GAC and ion-exchange resin adsorption; membrane filtration	\$90	1.6	1500

* Brand's websites are listed in the reference

Based on market research, the desired product attributes of a water faucet purifier are

1. Contaminants removal (pathogens, metals e.g. lead, organics)
2. Low price
3. Long working life
4. Small in size
5. With a replaceable cartridge
6. With an indicator for replacing the filter cartridge

In order to understand which product attributes are more important to the customers, a survey is conducted with the questionnaire in Appendix A. The customers are asked to give a rank for each product attribute (1 being the least important and 5 being the most important), and the average score $\bar{x}$ is calculated as follows

$$\bar{x} = \sum x_i n_i / n \quad (1)$$

Here, x_i is the score (1 to 5), n_i is the number of respondent for score i , and n is the total number of respondents (i.e. 100 in this study). Table 2.2 summarizes the results of the survey which shows that contaminants removal and low price are the product attributes that the consumers mainly concern. A long working life and a replaceable cartridge are also considered to be relatively important, while size and a cartridge replacement indicator are the least important.

Table 2.2 Results of the consumer survey

Desired product attributes	1	2	3	4	5	Average	Rank
Contaminants removal	0	0	15	55	30	4.15	1
Low price	0	10	10	45	35	4.05	2
Long working life	5	15	25	35	20	3.50	4
Small in size	30	40	25	5	0	2.05	6
With a replaceable cartridge	10	5	25	30	30	3.65	3
With an indicator for replacement	5	15	50	30	0	3.05	5

After the market survey, the specifications of the water filter are summarized as

1. Low concentration of lead in the filtered water (0ppm) [Note that lead is used as the reference contaminant in this study]
2. A selling price of around US\$ 10
3. The filter can lasts for 6 months before replacement
4. Compact in size
5. A removable and replaceable filter cartridge.
6. With a reasonable operational flow rate of 1.9L/min

The company aims at selling the faucet water filter to local families in Hong Kong. With an estimate of 2,400,000 families in Hong Kong and a target of capturing 20% market share in the first five years, an annual sales of 96,000 water filters is expected .

2.3 Governing physicochemical phenomena

Ultrafiltration, reverse osmosis, and adsorption are the most common techniques used in faucet water filters. Ultrafiltration and reverse osmosis use a membrane to filter the pollutants, in which pressure is applied to force water across the membrane such that pollutants such as particulates and ions are retained in the concentrate and remove from the filtered water. Adsorption is a process in which pollutants are adsorbed onto the adsorbent by physical forces. A highly porous material is beneficial as it provides a larger surface area for adsorption to take place. Adsorption is selected to be the technique of pollutants removal in this study, as it is widely used in faucet water filters and its price is lower when compared to membrane filtration techniques.

2.4 Product attributes and technical parameters

The product attributes are converted to technical requirements in the house of quality (Figure 2.1). A higher score (5) indicates a stronger relation between the product attribute and the technical requirement, whereas a lower score (1) indicates a weaker relation. For example,

contaminants removal is strongly related to the lead concentration in the filtered water and moderately related to the flowrate of the filtered water. The importance of each product attribute is obtained with reference to the average score in the consumer survey. The importance of each technical requirement is also calculated. For example, the importance of lead concentration in filtered water is calculated as: $5 \times 5 + 5 \times 4 = 45$. Among all the technical requirements, lead concentration in the filtered water and the handling capacity before filter replacement are the most important.

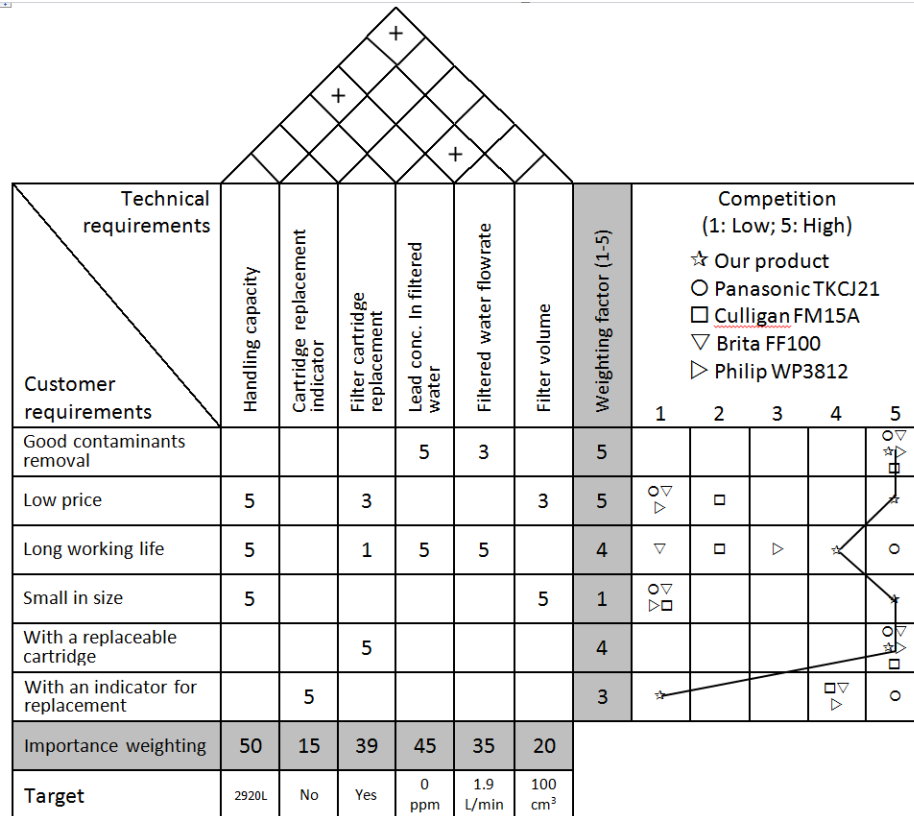


Figure 2.1 A house of quality for faucet water filter

In order to achieve the required product specifications, the technical requirements of the water filter are specified below. Note that the bold items are the two important technical requirements identified above.

- 1. A handling capacity of 2920L before filter replacement (assume a consumption of 16L/day for a 4-member family and replace the cartridge once every 6 months)**
- A removable and replaceable filter cartridge, but no replacement indicator to reduce the product cost
- 3. Low concentration of lead in the filtered water (0 ppm)**
- A filtered water flow rate of 1.9L/min
- A filter volume of ~100 cm³

2.5 Product conceptualization and determination of product specifications

The configuration of the faucet water filter is illustrated in Figure 2.2. It consists of three components: outer case, connection port, and filter cartridge. The filter cartridge contains adsorbent which removes pollutants and connects to the faucet by a connection port.

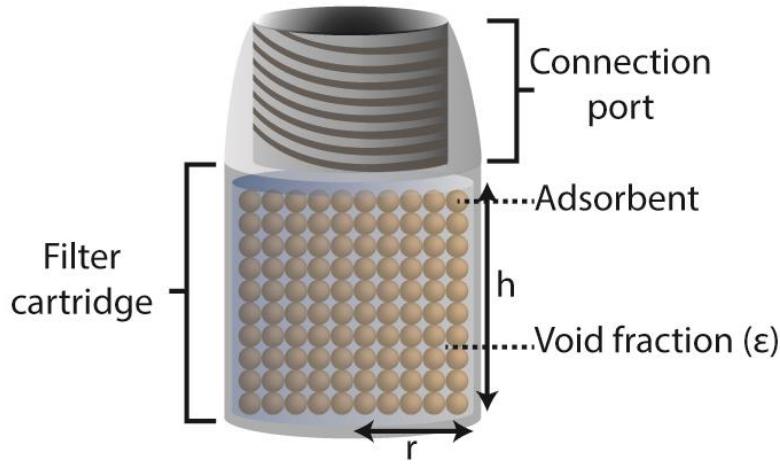


Figure 2.2 Configuration of the faucet water filter

In order to determine the filter volume and its dimensions, the velocity of contaminant (lead) movement (u in cm/min) in the filter bed is determined by Eqn. 2.

$$u = \frac{v_i}{1 + \frac{1-\varepsilon}{\varepsilon} \rho \left(\frac{q_2 - q_1}{c_2 - c_1} \right)} \quad (2)$$

Here, v_i is the interstitial fluid velocity (cm/min), ε is the external void fraction in the water filter and is assumed to be 0.4, ρ is the particle density of the adsorbent, and q_1 (c_1) and q_2 (c_2) are the lead concentration in the adsorbent (fluid) before and after solute feeding, respectively.

The interstitial fluid velocity v_i is related to the volumetric flowrate of filtered water (V) and the filter dimensions by Eqn. 3

$$v_i = \frac{V}{\pi r^2 \varepsilon} \quad (3)$$

Here, r is the filter radius and is designed to be 3 cm by considering the filter is connected to a faucet. With a target water flowrate of 1.9 L/min (1900 cm³/min), v_i can be calculated as

$$v_i = \frac{1900}{\pi \times 3^2 \times 0.4} = 168 \frac{\text{cm}}{\text{min}} \quad (4)$$

The adsorbent bed is assumed to be clean before solute feeding. Therefore, $q_1 = 0$ mg/g. Similarly, $c_1 = 0$ mg/L. After solute feeding, the concentration of lead in the adsorbent (q_2) can be related to that in the water (c_2) by the Langmuir isotherm (Eqn. 5), assuming local equilibrium, and negligible dispersion and diffusion effects.

$$q_2 = \frac{q_{\max} K_A c_2}{1 + K_A c_2} \quad (5)$$

Here, $q_{\max}$ and K_A are the maximum adsorption capacity and the adsorption constant, respectively. Ion exchange resin and activated carbon are the two most common adsorbent used for lead removal, and their data for Langmuir isotherm are summarized in Table 2.3.

Table 2.3 Data of adsorption isotherm for ion exchange resin and activated carbon

Absorbent*	$q_{\max}$ (mg/g)	K_A (L/mg)	Reference
Ion exchange resin (Lewatit CNP 80)	65.4	1.22	Vergili et al., 2013
Activated Carbon (Calgon Carbon Corporation)	54.9	0.938	Payne and Abdel-Fattah, 2004

* $\rho_{\text{resin}} = 1190 \text{ g/L}$, $\rho_{\text{AC}} = 800 \text{ g/L}$; cost of resin = US\$ 975 / ton, cost of AC = US\$ 840 / ton

With the isotherm data, q_2 can be calculated by assuming the lead concentration in the inlet water (c_2) to be 0.11 mg/L. Lewatit CNP 80 ion exchange resin is used as an example to illustrate the calculations below.

$$q_2 = \frac{q_{\max} K_A c_2}{1 + K_A c_2} = \frac{65.4 \times 1.22 \times 0.11}{1 + 1.22 \times 0.11} = 7.74 \frac{\text{mg}}{\text{g}} \quad (6)$$

Thus, the velocity of lead movement in the resin bed is

$$u = \frac{v_i}{1 + \frac{1-\varepsilon}{\varepsilon} \rho \left(\frac{q_2 - q_1}{c_2 - c_1} \right)} = \frac{168}{1 + \frac{1-0.4}{0.4} \times 1190 \times \frac{7.74}{0.11}} = 1.34 \times 10^{-3} \text{ cm/min} \quad (7)$$

The bed height (h_{bed}) is determined next to ensure that the lead solute front is still within the filter bed before the handling capacity of 2920 L is reached.

$$h_{\text{bed}} = 1.34 \times 10^{-3} \times \frac{2920}{1.9} = 2.06 \text{ cm} \quad (8)$$

With the height of the filter bed, the total mass of the ion exchange resin (m_{resin}) is

$$m_{\text{resin}} = \rho \pi r^2 h_{\text{bed}} (1 - \varepsilon) = 1.19 \times \pi \times 3^2 \times (2.06) \times (1 - 0.4) = 41.5 \text{ g} \quad (9)$$

With a cost of US\$ 975 per ton of resin, the cost of the resin bed is US\$ 0.041 per unit. Similarly, the cost of the adsorbent is US\$ 0.052 per unit if activated carbon is used. As using Lewatit CNP 80 ion exchange resin is cheaper, it is selected for the faucet water filter.

A plastic case is needed to hold the filter cartridge. Acrylonitrile butadiene styrene (ABS) is selected as the raw material as it is light in weight and widely used in making drinking bottles. The filter cartridge is connected to the faucet by a connection port made of ABS, with a height of 2 cm and a diameter same as that of the plastic case housing the filter cartridge. The material cost of the ABS plastic will be estimated by an online estimator in the financial analysis.

2.6 Design of product manufacturing process

The faucet water filter consists of a filter cartridge, a connection port, and a plastic case. Figure 2.3 depicts the process flow diagram to manufacture the faucet water filter. The filter cartridge containing Lewatit CNP 80 ion exchange resin is provided by the supplier, while the connection port and the plastic case are manufactured by injection molding. The three components are then assembled and packed for shipping.

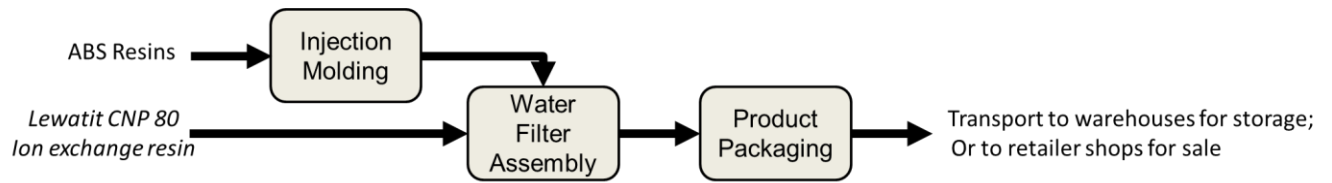


Figure 2.3 Process flow diagram of manufacturing faucet water filter.

2.7 Financial analysis

The financial analysis of the faucet water filter is summarized in Table 2.4. With an expected sales of 96,000 filters at US\$ 10 per unit for the first five years, the annual sales is US\$ 960,000 in year 1 to 5. During product development (year -1 and 0), fixed cost includes US\$ 20,000 for office rent and daily operations. A development cost of US\$ 200,000 is spent in year -1 for R&D and product design such as tooling design and prototype test. A capital spending of US\$ 100,000 is required in year 0 to start the production line.

Table 2.4 Financial analysis of faucet water filter (All the money is shown in USD and in thousands.)

Year	-1	0	1	2	3	4	5
Sales	-	-	960.00	960.00	960.00	960.00	960.00
Fixed Cost	20.00	20.00	77.60	77.60	77.60	77.60	77.60
Variable Cost	-	-	97.76	97.76	97.76	97.76	97.76
IFO	-	-	784.64	784.64	784.64	784.64	784.64
Depreciation	-	-	20.00	20.00	20.00	20.00	20.00
EBIT	-	-	764.64	764.64	764.64	764.64	764.64
Taxes (40%)	-	-	305.86	305.86	305.86	305.86	305.86
ATOI	-	-	458.78	458.78	458.78	458.78	458.78
OCF	-20.00	-20.00	478.78	478.78	478.78	478.78	478.78
NWC	-	260.00	-	-	-	-	-260.00
Development Cost	200.00	-	-	-	-	-	-
Capital Spending	-	100.00	-	-	-	-	-
PCF	-220.00	-380.00	478.78	478.78	478.78	478.78	738.78

After product launch, an annual advertising cost of US\$ 57,600 (6% of target sales) is added to the fixed cost. For the variable cost, it includes the manufacturing cost of the cartridge, connection port and the plastic case, as well as the cost for assembly and packaging. The manufacturing cost of the connection port and the plastic case by injection molding is estimated by an online feature-based estimator [<http://www.custompartnet.com/estimate/injection-molding/>] with the input parameters summarized in Appendix B. The results show that the manufacturing cost of the connection port and the plastic case are US\$ 0.485 and US\$ 0.309 per unit, respectively. Note that the estimated manufacturing cost includes material cost, production cost, and tooling cost. With the cost of the ion exchange resin to be US\$ 0.041 per unit, the total cost

of manufacturing the three components in the water filter is US\$ 0.835 per unit, equivalent to US\$ 80,160 per year. For assembly the three parts in the production line, it is assumed that a worker can assemble 4 filters in one min and the hourly wage of the worker is US\$ 10. Therefore, the cost of assembly is US\$ 4,000 per year. Similarly for packaging, the same assumption on labor requirement is used. With a unit cost of US\$ 0.1 for the packaging material, the cost of packaging is US\$ 13,600 per year. Therefore, the total variable cost equals US\$ 97,760 per year, equivalent to US\$ 1.02 per unit.

With all the cost information, income from operations (*IFO*), earnings before income tax (*EBIT*), after tax operating income (*ATOI*), operating cash flow (*OCF*), and project cash flow (*PCF*) are calculated by the following equations.

$$IFO = S - C_{ED} \quad (10)$$

$$EBIT = IFO - D = S - C_{ED} - D \quad (11)$$

$$ATOI = (1 - t) EBIT = (1 - t) (S - C_{ED} - D) \quad (12)$$

$$OCF = ATOI + D = (1 - t) (S - C_{ED} - D) + D = (1 - t) (S - C_{ED}) + t D \quad (13)$$

$$PCF = OCF - \text{Development cost Increase in NWC} - \text{Project capital spending} \quad (14)$$

Here, *S* is the sales, *C_{ED}* is the fixed and variable costs, *D* is depreciation which is assumed to be linear depreciation over the project period, *t* is tax rate which is assumed to be 40%, *NWC* is the net working capital.

Net present value (NPV) is used to calculate the profitability of the water filter project, as expressed in Eqn. 15.

$$NPV = \sum_{j=-n}^m \frac{PCF_j}{(1+R)^j} \quad (15)$$

Here, *R* is the discount rate set by the management, *n* is the number of years for product development, and *m* is the number of years of the product life. With a discount rate of 20%, NPV equals US\$ 892,345.

Similarly, internal rate of return (IRR) can be determined by setting NPV to be 0 and solve for the discount rate *R*. Using Solver in Microsoft excel, IRR equals 61.2% which exceeds the 5% bank interest rate. Therefore, the project can be presented to the management team for approval.

2.8 References

- Chan G, Lai YK. Lead 80 times the safe limit found in water at Hong Kong public housing estate where scandal broke. *South China Morning Post*. 12 Sep 2015.
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- Vergili I, Soltobaeva G, Kaya Y, Gonder ZB, Cavus S, Gurdag G. Study of the removal of Pb(II) using a weak acidic cation resin: kinetics, thermodynamics, equilibrium, and breakthrough curves. *Industrial & Engineering Chemistry Research*. 2013;52:9227-9238.

Webpage information

Market information:

- Panasonic: <http://www.panasonic.hk/> (Accessed on 9 Sep , 2016)
- Culligan: <http://www.culligan.com/> (Accessed on 9 Sep , 2016)
- Brita: <https://www.brita.com/intl/> (Accessed on 9 Sep , 2016)
- Philips: <http://www.philips.com.hk> (Accessed on 9 Sep , 2016)

Technical information:

- <http://www.custompartnet.com/estimate/injection-molding/> (Accessed on 9 Sep , 2016)

Appendix A. Sample questionnaire for consumer survey

We are a group of students from the Hong Kong University of Science and Technology (HKUST). We are now conducting a survey about the faucet water filter in Hong Kong. The survey will be anonymous and can be completed in around 3 minutes.

1. Background information:

- a. Gender: ☐ Male ☐ Female
- b. Age: ☐ 14 or under ☐ 15 - 18 ☐ 19 - 24 ☐ 25 - 29
☐ 30 - 39 ☐ 40 - 59 ☐ 60 or over
- c. Family monthly salary: ☐ < \$10,000 ☐ \$10,000 - \$ 19,000 ☐ \$19,000 - \$31,000
☐ \$31,000 - \$50,000 ☐ >\$50,000
- d. Number of people living with: _____

2. Brand Recognition:

- a. Have you ever heard of the following brands for faucet water filters?

	☐ Yes	☐ No		☐ Yes	☐ No
	☐ Yes	☐ No		☐ Yes	☐ No

- b. Please rank the following product features that is important to your decision in selecting a faucet water purifier (1 = the least important; 5 = the most important):

	1	2	3	4	5
Contaminants removal (e.g. bacteria, metals, inorganics)	☐	☐	☐	☐	☐
Low price	☐	☐	☐	☐	☐
Long working life	☐	☐	☐	☐	☐
Small in size	☐	☐	☐	☐	☐
With a replaceable cartridge	☐	☐	☐	☐	☐
With an indicator for replacement	☐	☐	☐	☐	☐
Others (Please specify)					

-End-

Appendix B. Parameters for CustomPartNet for the cost estimation of injection molding

	Connection Port	Filter Case
Part information		
Rapid tooling	No	No
Quantity	96000	96000
Material	ABS, Molded	ABS, Mold
Envelope X-Y-Z (mm)	70.00 x 70.00 x 30.00	70.00 x 70.00 x 30.00
Max. wall thickness (mm)	5	2.5
Projected area	67.7% of the envelope	67.7% of the envelope
Projected Holes	Yes	Yes
Total Area of the hole	25.6 % of the envelope	25.6 % of the envelope
Volume	42.04% of the envelope	11.2% of the envelope
Tolerance (mm)	Not critical (>0.5)	Not critical (>0.5)
Surface roughness (μm)	Not critical ($R_a > 0.8$)	Not critical ($R_a > 0.8$)
Complexity	Very Simple	Very Simple
Injection Molding Process parameters		
Material		
Defect rate (%)	5	5
Material price (US\$/kg)	0.63	0.63
Regrind Ratio (%)	0	0
Additives ratio (%)	0	0
Material markup (%)	25	25
Production		
Hourly rate (US\$/h)	35	30.00
Machine setup time (h)	8	8
Machine uptime (%)	95	95
Post-processing time (h)	0	0
Production markup (%)	10	10
Tooling		
Mold-making rate (US\$/h)	65	65

Product 3: Conductive Inkjet Ink

A conductive ink that prints conductive tracks for printed electronics

Project Statement

Conductive ink is increasingly used in various applications in recent years, as inkjet printing is more environmental friendly and produces less waste in fabricating printed circuit boards, as compared to conventional vacuum deposition and lithography techniques. It can be used in drop-on-demand inkjet printing to print conductive tracks for printed electronics, photovoltaics, biosensors, etc.

As conductive ink and inkjet printing are not covered in a typical chemical engineering curriculum, students are advised to first understand how inkjet printing prints conductive tracks and the basic requirements of the conductive ink such as the required ink conductivity for different applications. After that, a market study has to be conducted to summarize the market size and the competing products in the market. Examples of companies producing conductive ink include DuPont and Novacentrix. The product attributes of the conductive ink are identified from market analysis and printing technology handbooks (Kipphan, 2001).

The identified product attributes are converted to technical parameters by methods such as House of Quality. For example, whether droplets can be formed in the printing process depends on the nozzle size, the ink viscosity and surface tension. The base case formula is then determined by rule-based methods, model-based methods, database, and experiments. Students can refer to Tam et al. (2016) and Magdassi (2010) for a database of the common ingredients in a conductive ink, heuristics to shortlist candidates for a specific ink component, and models to select the ingredients and determine its concentration such that the product specifications are met. After formulating the base-case, experiments are conducted to verify the major physicochemical properties and to print on a substrate to verify its printing performance. The formulation is then iterated, guided by a causal tablet, to meet the product specifications. The product manufacturing process of the conductive ink is then synthesized and a financial analysis is performed to evaluate the profitability.

References

- Kipphan H. *Handbook of Print Media: Technologies and Production Methods*. Berlin; Hong Kong: Springer-Verlag, 2001.
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- Tam SK, Fung KY, Poon GSH, Ng KM. Product design: Metal nanoparticle-based conductive inkjet inks. *AIChE Journal* 2016;62(8):2740-2753.

Sample solutions to design of conductive inkjet ink (Tam et al., 2016)

3.1 The product and its functions

Conductive ink is used in drop-on-demand (DoD) inkjet printing to print conductive traces for different applications, including printed electronics, photovoltaics, and biosensors. A metal nanoparticle-based conductive ink, which is a suspension of conductive nanoparticle fillers in a dispersing medium, is the most common one in the printed electronics industry. Conductive ink receives a growing demand as inkjet printing produces less waste in fabricating printed circuit boards, when compared to conventional vacuum deposition and lithography techniques. A typical inkjet printing process includes several steps. First, the conductive ink is transported from a liquid reservoir to an inkjet printhead. Then, a specific volume of the conductive ink is ejected from the printhead nozzle to form an ink droplet that deposits on the desired position of a substrate. After reaching the solid surface, the droplet spreads and coalesces with the previously deposited droplets to form a line. The printed line is then dried and sintered to form a conductive solid track.

3.2 Market study

The market size of conductive inks and pastes keeps increasing in recent years. Grand View Research (2016) reported that the global market exceeded USD 3 billion in 2015, in which the Asia Pacific market accounted for >70% of the total market revenue (i.e. USD 2.1 billion). Conductive inks and pastes have been applied in various market sectors, including photovoltaics, automotive, printed electronics, and sensors. Among them, photovoltaics is the largest (Savastano 2015).

Among all the products in the market, silver and copper paste used for screen printing still dominate the market, as conductive inks used for inkjet printing cannot yet produce a film with sufficient thickness and conductivity for various applications. Only limited products have been developed for inkjet printing, which has a resolution higher than that of screen printing. Although the conductivity of the ink-jet printed film is lower, it is sufficient for certain applications such as touch panel. This conductive ink for inkjet printing will be designed in this project. Examples of conductive ink in the market are summarized in Table 3.1, together with their product specifications.

Table 3.1. Summary of conductive inks in the market

Company	Product	Filler	Volume resistivity ($\mu\Omega$ cm)	Viscosity (cP)	Reference
Novacentrix	Metalon® JS-A102	Ag (40 wt%)	47	8-12	Novacentrix (2016)
NanoDimension	Ag Cite ink	Ag (20-70 wt%)	2.8	5-35	NanoDimension (2016)
DuPont	DUPONT™ PE410	Ag	12.5	20-40	DuPont (2016)

Most conductive inks use silver as filler, as silver is less prone to oxidation. However, silver ink is more expensive and the market price from trade website is around USD 800-1600 per kg of ink. The above inks are mainly used for applications such as printed circuit boards and antennas, and hence requiring a lower volume resistivity. In our discussion with printed electronics experts, the required volume resistivity can be higher (300-400 $\mu\Omega$ cm) if the inks are used for touch panels.

3.3 Product attributes and technical parameters

Based on a study of the market products, the required product attributes of a conductive ink are summarized in the left column of the House of Quality in Figure 3.1. The product attributes can be grouped into two states: metal nanoparticle suspension and printed solid track. For the nanoparticle suspension, it has to be stable against sedimentation and agglomeration. During printing, stable droplets have to be formed. The deposited droplets should wet the substrate and coalesce with previously deposited droplets to form a uniform line. For the printed track, it should be conductive with minimum pores and cracks, and also free of coffee ring stains.

These product attributes are related to technical product specifications in the House of Quality. Note that the product use conditions such as substrate and printer specifications also affect certain product attributes. For example, the stability of the ink against sedimentation is related to the product shelf life and is mainly determined by the size of the nanoparticle filler, whereas the formation of stable droplets during printing depends on the viscosity and specific surface energy of the ink, the nozzle diameter, and the droplet diameter and velocity. Readers can refer to Tam et al. (2016) for a more detailed discussion of Figure 3.1.

			Product use conditions					Product specifications						Related ingredients
								Suspension			Printed track			
			Substrate	Droplet diameter and nozzle diameter	Droplet velocity	Transverse printing speed and droplet spacing	Curing conditions, e.g. drying or sintering	Shelf life	Ink viscosity	Ink specific surface energy	Track width	Track thickness	Track volume resistivity	
Suspension	Stability	Stable against sedimentation											Filler	
		Stable against aggregation											Dispersant	
	Printability	Stable droplet formation		○	○			○	○				Dispersing medium	
		Good wettability on substrate	○						○				Dispersing medium	
		Droplets coalescence to form uniform lines				○		○	○	○			Dispersing medium	
Printed track	Conductivity	Free of coffee ring stains							○				Cosolvent	
		Fully sintered with minimum pores and cracks				○		○			○	○	Binder	

Figure 3.1. House of Quality for metal nanoparticle based conductive ink. (Tam et al., 2016)

In this design project, the conductive ink is designed for a shelf life of 4 months at room temperature. Dimatix Materials Printer DMP-2800 with printhead DMC-11619 and settings summarized in Table 3.2 is used to print the conductive tracks (Fujifilm-Dimatix, 2013). A piezoelectric printhead is used and the required ink viscosity is 8-15 mPa·s (Kipphan, 2001). The printed track has a width of 250 μm, a thickness of 1 μm, and a volumetric resistivity of <400 μΩ cm. As the track is rather wide, the printing is repeated 4 times, with the newly printed line next to the just printed line. Thus, the desired track width (w) is 62.5 μm, which is related to the droplet diameter (d₀), the contact angle of the ink on the substrate (θ), and the center-to-center drop spacing (p) by Eqn. 1 derived based on the conservation of volume (Stringer and Derby, 2010).

$$w = \sqrt{\frac{2\pi d_0^3}{3p\left(\frac{\theta}{\sin^2 \theta} - \frac{\cos \theta}{\sin \theta}\right)}} \quad (1)$$

Therefore, the required contact angle of the conductive ink is determined to be 45°.

Table 3.2. Printing conditions and printer settings

Substrate	PET
Temperature, T	298 K
Droplet diameter, d ₀	30 μm
Droplet velocity, v	5 m/s
Nozzle diameter, d _{nozzle}	21.5 μm
Printing speed, U _T	2.4 m/s
Drop spacing, p	25 μm
Curing conditions	Thermal sintering under N ₂ environment

3.4 Generation of a base case formula

Common ingredients in a conductive ink include electrical conductive filler, dispersing medium, dispersant, and binder, and their examples are listed in Table 3.3 with the selection heuristics summarized in Tam et al. (2016). Only heuristics that are applied in this design project are explained below, alongside with the ingredient selection in formulating the base case. Students can consult a chemist or formulation scientist who is familiar with inkjet or screen printing for more detailed information.

Table 3.3. Common ingredients in conductive ink (Tam et al., 2016)

Ingredient	Desired function	Examples	Typical amount (wt%)
Electrical conductive filler	Provides the conductive material for the ink	Metal: silver, nickel, copper, nanoparticles Metal precursor: copper oxide, nickel oxide nanoparticles	10-60
Dispersing medium	Provides the continuous phase	Non-polar solvent: tetradecane, cyclohexane Polar solvent: water, ethanol, propanol, ethylene glycol, diethylene glycol, glycerol, formamide	30-70
Dispersant	Prevents fillers from aggregation	Polymeric dispersant: Polyvinylpyrrolidone (PVP), sodium polyacrylate, anionic phosphated alkoxyated polymer (Solsperse 40), Small-molecule dispersant: fatty acid, alkylamine, alkythiol	2-10
Binder	Increases the cohesiveness of filler or provides adhesion to the substrate	Organic binder: PVP, acrylic resin Inorganic binder glass frits, borate nanoparticle	3-10

Selection of filler material. As silver ink is of high price, a cheaper conductive ink is designed in this project. Copper nanoparticles are selected to be the conductive filler as copper has an electrical conductivity similar to that of silver, but at a much lower cost. As copper nanoparticles are easily oxidized, a dispersant which also acts as a passivating agent is also needed.

Selection of dispersing medium (the continuous phase of the ink). The wettability of the ink on the substrate and the suppression of coffee ring stain formation during drying are the two major considerations in selecting the dispersing medium. Among all the dispersing medium in Table 3, ketone, aromatic and halogenated solvent are excluded as they are not compatible with the polyethylene terephthalate (PET) substrate, and ketone readily oxidizes copper nanoparticles. Next, the wettability of the dispersing medium on the PET substrate is considered using the Owens-Wendt-Rabel-Kaelble (OWRK) method (Owens and Wendt, 1969; Janssen et al., 2006). The first step in the OWRK method is to measure the equilibrium contact angle (θ_{eq}) of at least three solvents (i.e. water, ethylene glycol, glycerol) with known polar (γ_L^P) and dispersive (γ_L^D) contribution to the specific surface energy of the substrate used for printing (i.e. PET). The contact angles measured for the three solvents, together with their γ_L^P and γ_L^D , are summarized in Table 4. Using these data points, the polar (γ_S^P) and dispersive (γ_S^D) contribution of the substrate, which highly depend on its preparation method, are determined through regression:

$$\frac{(\gamma_L^P + \gamma_L^D)(\cos\theta_{eq} + 1)}{2\sqrt{\gamma_L^D}} = \sqrt{\gamma_S^P} \frac{\sqrt{\gamma_L^P}}{\sqrt{\gamma_L^D}} + \sqrt{\gamma_S^D} \quad (2)$$

By plotting $\frac{(\gamma_L^P + \gamma_L^D)(\cos\theta_{eq} + 1)}{2\sqrt{\gamma_L^D}}$ vs. $\frac{\sqrt{\gamma_L^P}}{\sqrt{\gamma_L^D}}$, γ_S^P and γ_S^D are obtained from the slope and the intercept of the regression line and equal 20.8 mJ/m² and 17.6 mJ/m², respectively. The contact angles of other solvents with known γ_L^P and γ_L^D on the same substrate are then estimated by Eqn. 2, and the results are also summarized in Table 3.4. Solvents that spread on the PET substrate are excluded, leaving water, ethylene glycol, glycerol, diethylene glycol, and formamide as potential candidates for the dispersing medium.

Table 3.4. Specific surface energy and contact angle on PET of various solvents. (Tam et al., 2016)

Solvent	Boiling point (°C)	Specific surface energy (mJ/m ²)			Contact angle*	
		Polar γ_L^P	Dispersive γ_L^D	Total		
Water	100	51.0	21.8	72.8	Measure	66.0°
Ethylene glycol	197	29.3	18.9	48.2		39.9°
Glycerol	290	43.1	20.2	63.3		55.1°
Tetradecane	254	26.4	0.0	26.4	Estimated	spreading
Cyclohexane	81	25.5	0.0	25.5		spreading
Ethanol	79	5	17	22.0		spreading
Propanol	97	3.6	19	22.6		spreading
Diethylene glycol	245	13.2	31.6	44.8		34.3°
Formamide	210	19.0	39.0	58.4		52.2°

*The contact angles of water, ethylene glycol and glycerol were measured by the sessile drop technique. The contact angles of other solvents were estimated by the OWRK method.

After considering the wettability of the dispersing medium on the substrate, the prevention of coffee ring stain formation during drying is considered next. Coffee ring is formed at the contact line as the liquid near the contact line evaporates faster than that at the center, which creates a flux that moves the copper nanoparticles towards and concentrates near the contact line. This can be suppressed by providing a Marangoni flow directing inwards along the liquid-air interface that moves the nanoparticles back to the droplet center. Marangoni flow is generated when there is a difference in specific surface energy at the liquid-air interface, which can be induced by concentration gradient. Park and Moon (2006) reported that an effective Marangoni flow can be induced in a binary solvent mixture, one solvent with low boiling point and high specific surface energy and one solvent with high boiling point and low specific surface energy. At the contact line region, the solvent with a low boiling point first evaporates during drying, leading to the specific surface energy at the contact line region lower than that at the center, thus inducing an inward Marangoni flow. Therefore, it is desirable to select two solvents with large specific surface energy difference and low viscosity, so that the Marangoni flow can be enhanced. Among the five solvents shortlisted above, water and diethylene glycol are selected to form a

binary solvent system, as they have the largest different in specific surface energy. Finally, their composition are determined to provide the ink with the desired contact angle (45°). Experimental data (Figure 3.2) show that a mixture of 40wt% water and 60wt% diethylene glycol (DEG) meets this requirement. Based on the data reported in the literature (MEGglobal, 2013), this dispersing medium has a viscosity of 5.8 mPa·s, a specific surface energy of 53 mJ/m², and a density of 1,082 kg/m³ at room temperature.

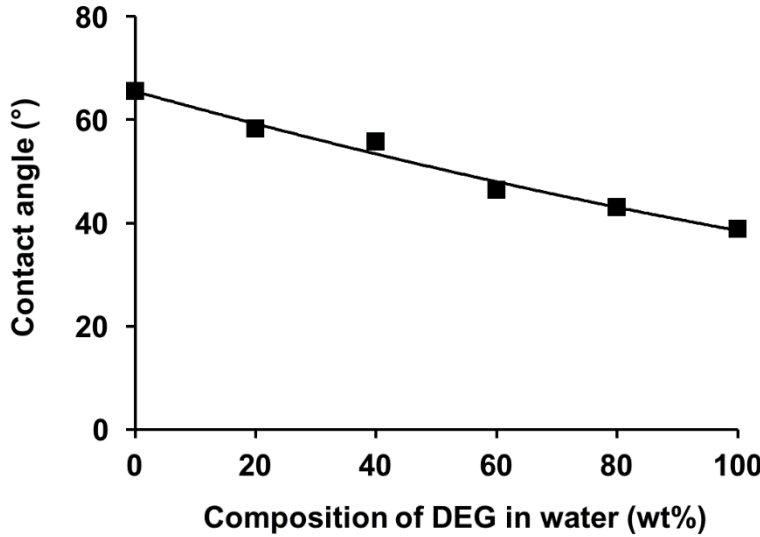


Figure 3.2. Contact angle at different weight fractions of DEG in water. (Tam et al., 2016)

Determination of Filler Particle Diameter. The size of the nanoparticle fillers is considered next. In order not to clog the nozzle, the maximum diameter of the filler should be less than one-hundredth of the nozzle diameter (Fujifilm-Dimatix, 2013). As the particle fillers should not settle before printing, the Brownian motion of the nanoparticles should counteract the sedimentation flux, which can be achieved by setting the distance travelled by a nanoparticle due to Brownian motion longer than its sedimentation distance over the same period of time. Therefore, the maximum nanoparticle filler diameter (d_p) can be expressed as (Rhodes, 2013):

$$d_p = \left(\frac{216k_B T \mu_m}{\pi g^2 (\rho_p - \rho_m)^2 t} \right)^{1/5} \quad (3)$$

Here, k_B is the Boltzmann constant which equals $1.38 \times 10^{-23} \text{ m}^2 \text{kg/s}^2 \cdot \text{K}$, T is temperature, ρ_p is the density of the filler particles (8960 kg/m^3), t is the required shelf life, μ_m is the viscosity of the dispersing medium, and ρ_m is the density of the dispersing medium. With a required 4-month shelf life and the selected dispersing medium, the maximum particle diameter is 30 nm, which is smaller than one-hundredth of the nozzle diameter (i.e. 215 nm).

Selection of dispersant. To keep the filler nanoparticles dispersed, dispersant is needed in the conductive ink. Some parts of the dispersant are adsorbed onto filler surface while the rest is freely suspended in the dispersing medium to provide steric repulsion and minimize particles aggregation. Polymeric dispersant is often preferred because it is more effective than small-molecule dispersant. Polyacrylic acid (PAA) is selected here as it is compatible with the dispersing medium and can be decomposed into carbon dioxide and water during sintering.

The molecular weight of the dispersant is determined next to ensure that the surface adsorption layer (adlayer) is sufficiently thick to resist particle aggregation. The interaction force among the particles determines the required thickness of the adlayer (l). The overall interaction potential includes the van der Waals potential and the steric repulsion potential, and varies with the distance between two particles. When two particles are separated by $2l$, the steric repulsion is zero and the overall interaction potential reaches a minimum ($\Phi_{T,min}$) and equals the van der Waals potential (Φ_{vdW}). To prevent particles aggregation, $\Phi_{T,min}$ has to be greater than the Boltzmann threshold stabilization energy ($-3/2k_B T$) (Saunders et al., 2010):

$$\Phi_{T,min} = \Phi_{vdW} \geq -3/2k_B T \quad (4)$$

The van der Waals potential of two particles with the same size d_p in a medium can be expressed as:

$$\Phi_{vdW} = -\frac{A_{p,m}}{6} \left[\frac{d_p^2}{2D(2d_p+D)} + \frac{d_p^2}{2(d_p+D)^2} + \ln \frac{D(2d_p+D)}{(d_p+D)^2} \right] \quad (5)$$

Here, $A_{p,m}$ is the Hamaker constant of particles in the dispersing medium (water and DEG), and can be estimated from the Hamaker constant of the particle in vacuum ($A_{p,v}$) (Anand et al., 2008):

$$A_{p,m} \approx \left[\sqrt{A_{p,v}} - (\phi_w \sqrt{A_{w,v}} + \phi_{DEG} \sqrt{A_{DEG,v}}) \right]^2 \quad (6)$$

Here, ϕ_w (ϕ_{DEG}) and $A_{w,v}$ ($A_{DEG,v}$) are the volume fraction and the Hamaker constant of water (DEG) in vacuum, respectively. $A_{p,v}$ and $A_{w,v}$ can be obtained from the literature and equal 40×10^{-20} J (Royer et al., 2010) and 3.7×10^{-20} J (Stokes and Evans, 1997), respectively. No experimental data can be found for $A_{DEG,v}$, which can be estimated by the Lifshitz theory and equals 6.1×10^{-20} J (MEGlobal, 2013). With a density of 1170 kg/m^3 for DEG, the volume fraction of water (ϕ_w) and DEG (ϕ_{DEG}) equal 0.438 and 0.562, respectively. In Eqn. 5, D is the surface-to-surface separation between the two particles. The minimum adlayer thickness to keep the particles dispersed can be obtained by substituting Eqn. 5 into Eqn. 4 and specifying $D = 2l$. With the Hamaker constants and the particle size determined in the last step (i.e. 30 nm), the minimum adlayer thickness is 3.48 nm. For polymeric dispersant with high molecular weight, the adlayer thickness in nm can be related to the molecular weight of the dispersant (M_w) by an empirical correlation (Kirby et al., 2004):

$$l \approx 0.06(M_w)^{0.5} \quad (7)$$

Therefore, an adlayer thickness of 3.48 nm corresponds to a molecular weight of 3,364 for polyacrylic acid.

The dispersant polyacrylic acid can also function as a passivating agent to prevent copper from oxidation. However, sodium polyacrylate, instead of polyacrylic acid, is usually used as the passivating agent in synthesizing copper nanoparticles. By accounting for the molecular weight difference between polyacrylic acid and sodium polyacrylate repeating unit, the desired molecular weight of sodium polyacrylate is 4,420. As only sodium polyacrylate of certain molecular weight are available in the market, sodium polyacrylate with a molecular weight of 5,100, closet to the desired value, is selected. This is equivalent to a molecular weight of 3,880 for polyacrylic acid, corresponding to an adlayer thickness of 3.74 nm.

Determination of the amount of filler and dispersant. Assume the solid track after drying and sintering has no pores and all the other ingredients are removed during sintering so that the track contains only nanoparticle fillers, the volume fraction of nanoparticle fillers in the ink (ϕ_p) equals the volume of the solids track with the desired thickness ($\delta_{thickness}$) divided by the total volume of droplets deposited onto the substrate.

$$\phi_p = \frac{w(Np)\delta_{thickness}}{N\left(\frac{\pi d_0^3}{6}\right)} = \frac{6wp\delta_{thickness}}{\pi d_0^3} \quad (8)$$

Here, N is the number of droplets printed. Note that w and p are defined in Eqn. 1. With a desired thickness of 1 μm and a track width (w) of 62.5 μm , the amount of fillers in the conductive ink is estimated to be 11 vol%.

The amount of dispersant required to fully cover the nanoparticle surface is determined next. For a particle coated with dispersant, the volume of the adlayer (V_d) equals:

$$V_d = \frac{\pi}{6} [(d_p + 2l)^3 - d_p^3] \quad (9)$$

Assume all dispersant are adsorbed onto the filler surface, the volume fraction of dispersant (ϕ_d) and filler particles in the ink are related to the adlayer volume and particle volume (V_p):

$$\frac{\phi_d}{\phi_p} = \frac{V_d}{V_p} \quad (10)$$

With an adlayer thickness of 3.74 nm, ϕ_d equals 5.4 vol%.

Selection of binder and determination of its amount. Binder is needed in a conductive ink to provide adherence among nanoparticle fillers and between filler and substrate. To increase the conductivity of the printed solid track, it has to be decomposed and removed during sintering. Organic polymer that is easily decomposed by heating is commonly used. Polyvinylpyrrolidone (PVP) with a molecular weight of 10,000 is selected here. As pores remained in the solid track after binder decomposition would lower the track conductivity, the amount of binder should be minimized, yet providing the required ink viscosity (i.e. 8-15 mPa·s for piezoelectric nozzle). In this case study, the desired viscosity μ_{ink} is set to be 12 mPa·s. The amount of binder needed can be determined by Eqn. 11 (Krieger and Dougherty, 1959) and Eqn. 12:

$$\mu_{ink} = \mu_m \mu_{r,binder} \left[1 - \frac{\phi_d + \phi_p}{\phi_{max}} \right]^{-[\mu] \phi_{max}} \quad (11)$$

Here, μ_m is the viscosity of the dispersing medium, $\mu_{r,binder}$ is the relative binder viscosity, $[\mu]$ is the intrinsic viscosity, and ϕ_{max} is the volume fraction of filler particles at the maximum packing condition. For monodispersed particles, $[\mu] = 2.5$ and $\phi_{max} = 0.63$ (Stuart et al., 2006). With the desired ink viscosity (12 mPa·s), $\mu_{r,binder}$ equals 1.29, which can be related to the binder concentration in the dispersing medium (C in wt%) by the Fikentscher's K-value (Wu, 2004).

$$\log \mu_{r,binder} = \left(\frac{75(K/1000)^2}{1 + 1.5(K/1000)C} + (K/1000) \right) C \quad (12)$$

For the selected binder, K equals 15, and the binder concentration in the dispersing medium (C) is 3.6 wt%.

Summary of the base case formulation. As a summary, the conductive ink contains 11 vol% of copper nanoparticles (conductive filler), 5.4 vol% of polyacrylic acid (dispersant), and the remaining (83.6 vol%) is dispersing medium and binder. Binder (polyvinylpyrrolidone) accounts for 3.6 wt% in the dispersing medium which contains water and diethylene glycol in a mass ratio of 4:6. All compositions are converted to weight fractions in the conductive ink, as summarized in Table 3.5.

Table 3.5. Formulation of the conductive ink

Ingredients	Components	Base case composition (wt%)	Modified ink composition (wt%)
Dispersed phase			
Conductive filler	30 nm Cu nanoparticles	50.5	50.5
Dispersant	Polyacrylic acid	3.2	3.2
Continuous phase			
Dispersing medium	Water	17.9	17.2
	Diethylene glycol	26.8	25.9
Binder	Polyvinylpyrrolidone	1.7	3.2

3.5 Measurement of physicochemical properties that cannot be predicted by experiments

As binder viscosity affects whether the ink can be successfully ejected from the nozzle and the specific surface energy determines whether the ink provides sufficient wetting to the substrate, they are verified by measurements. The conductive ink with the base case formulation was prepared. The viscosity of the ink was measured by a viscometer and equaled 13 mPa·s, whereas the specific surface energy was measured by the Wilhelmy plate method and equaled 51.6 mJ/m². These closely match with the values used in generating the base case (i.e. viscosity = 12 mPa·s; specific surface energy = 53 mJ/m²).

The prepared conductive ink was stored for four months. No particles sedimentation was observed and the conductive ink remained stable, thus satisfying the required shelf life. The ink was printed on a PET substrate and the quality of the printed track was evaluated. However, the printed track was non-conductive as micro-cracks were formed (Figure 3.3).

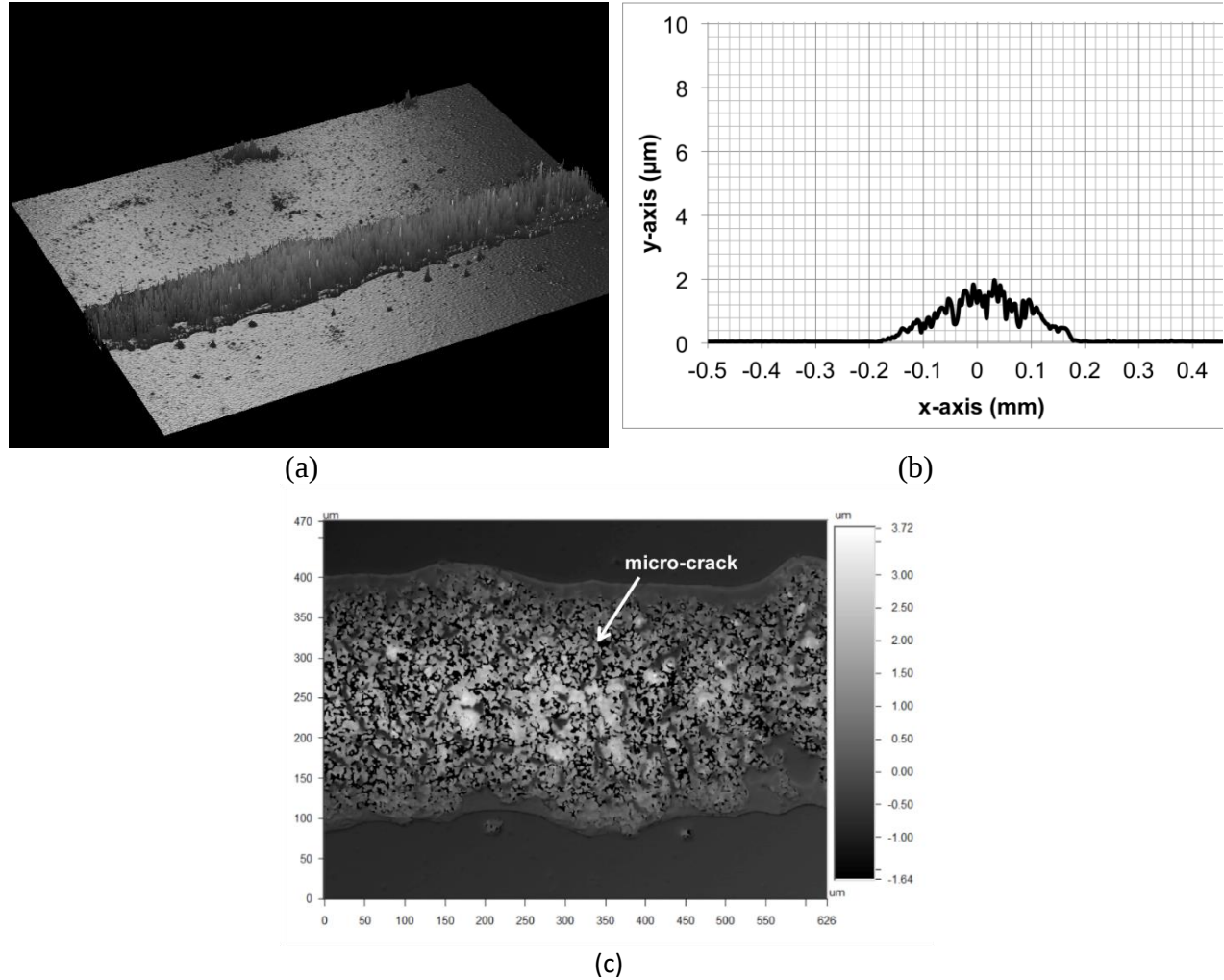


Figure 3.3. Copper track printed by the base-case formulation under optical profiler a) perspective view; b) cross-sectional view; and c) top view of printed track. (Tam et al., 2016)

3.6 Iterate guided by a causal table

As the base case formulation cannot provide a printed track with the desired conductivity, the formulation has to be modified according to the causal table summarized in Tam et al. (2016). The causal table points out that the cracks in the solid track can be reduced by increasing the amount of binder in the conductive ink. Therefore, the binder concentration in the conductive ink is increased to 3.2 wt%, giving an ink with an estimated viscosity of 15 mPa·s. The formulation of the modified ink is also summarized in Table 3.5. The modified ink was tested for its performance. The printed track was evaluated and no cracks or coffee rings were observed (Figure 3.4). The film thickness was measured to be 1 μm, meeting the product specification. The average sheet resistivity was measured by the 4-point probe method to give 3.55 Ω/sq. Therefore, the average volume resistivity calculated by multiplying the average sheet resistivity with the film thickness was 355 μΩ cm, again meeting the product specification (<400 μΩ cm).

The measured ink viscosity was 18 mPa·s. Although this is higher than the suggested range for the piezoelectric nozzle, experiments showed that the ink can still be ejected from the nozzle.

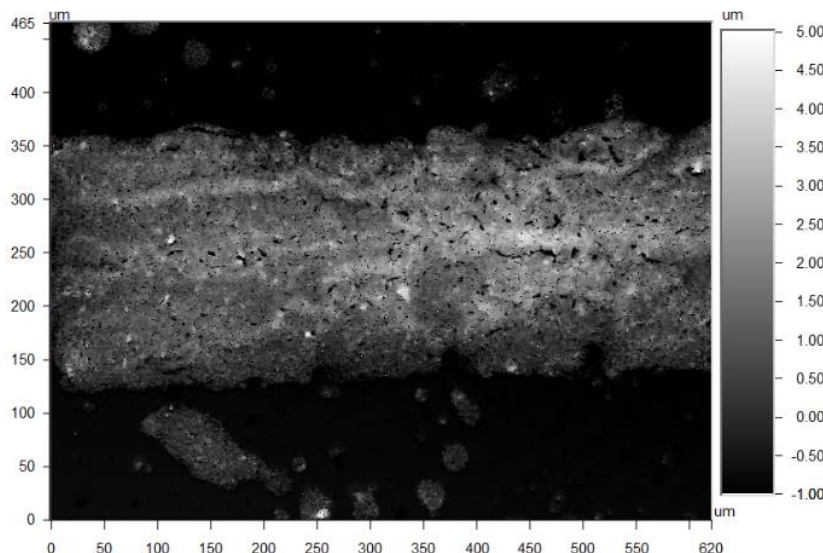


Figure 3.4. Copper track printed with the modified ink formulation under optical profiler. (Tam et al., 2016)

3.7 Design of product manufacturing process

The manufacturing process of the conductive inkjet ink is very simple. Copper nanoparticles coated by dispersant or passivating agent are added to a binder-containing dispersing medium in a mixing vessel. Mixing is provided by an overhead stirrer to mix the dispersed phase and the continuous phase under vacuum, so that no air bubbles are trapped inside the conductive ink.

The copper nanoparticles can either be synthesized in-house or purchased from a supplier. Cheng et al. (2016) provided guidelines for this make-buy decision. As copper nanoparticles synthesized by the chemical reduction method (Tam and Ng, 2015) can be of better quality than those available in the market, the manufacturing technology is better to be kept in-house and the nanoparticles are synthesized by the company. Copper acetate monohydrate was added to an aqueous solution containing ammonia to form a blue solution. Potassium hydroxide was then added to form a pale blue slurry. Then, aqueous hydrazine solution was added as a reducing agent with vigorous stirring at room temperature and under nitrogen for 15 min to form copper nanoparticles. Sodium polyacrylate was then added and coated onto the copper nanoparticles as a passivating agent under gentle mixing. As polyacrylic acid is not soluble in methanol, methanol was added under nitrogen with vigorous stirring for 1 h to settle the copper nanoparticles, which were then collected by centrifugation and washed with water to remove any impurities.

3.8 Financial analysis

There are limited copper inks available in the market so that a reference selling price is hard to obtain. Silver ink is sold at a price of around US\$ 800-1600 per kg. As copper is much cheaper than silver, the price of copper ink can be lower and is set to be US\$ 600 per kg. As copper ink

has not yet been well accepted by the industry, we provide copper ink samples for consumer testing. As we have close collaborations with several big companies, we aim at an average production capacity of 30 kg/month in Year 1 and 2 and increase to 50 kg/month in Year 3 and 4. Therefore the sales revenue are calculated to be US\$ 216,000 in Year 1 and 2 and US\$ 360,000 in Year 3 and 4, giving a total of US\$ 1,152,000 for a project period of 4 years.

After consulting with personnel who are more familiar with nanoparticles and ink production, the capital investment and operating cost are estimated and summarized in Table 3.6. A capital investment of US\$ 50,000 is required to set up a reaction system for copper nanoparticles production and a mixing system for copper ink production. The material and consumables cost and utility cost for producing 1 kg of copper ink are estimated to be US\$ 200/kg and US\$ 75/kg, respectively. As marketing personnel have to visit our collaborators and promote copper ink in trade shows (e.g. IDTechEx), a marketing budget of US\$ 20,000 for Year 1 and 2, and US\$ 30,000 for Year 3 and 4 are estimated.

Table 3.6. Financial summary of conductive copper ink (All the money is shown in USD)

Year	1	2	3	4
Production capacity (kg/month)	30	30	50	50
Sales revenue (600/kg)	216,000	216,000	360,000	360,000
Expenses				
Capital investment	50,000			
Material and consumables cost (200/kg)	72,000	72,000	120,000	120,000
Utility cost (75/kg)	27,000	27,000	45,000	45,000
Rental and office expenses (5000/month)	60,000	60,000	60,000	60,000
Marketing cost	20,000	20,000	30,000	30,000
Total expenses	229,000	179,000	255,000	255,000

Return on investment (ROI) is used to calculate the financial return in this project:

$$ROI = \frac{\text{Total revenue} - \text{Total expenses}}{\text{Total expenses}} \quad (13)$$

With all the revenue and expenses estimated in Table 3.6, ROI is calculated to be 25.5%.

3.9 References

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Product 4: Vitamin C Tablet

Project Statement

Dietary supplements provide nutrients to our body to make up for the insufficient intake of essential nutrients such as vitamins, minerals, fatty acids and amino acids from our daily meals. The products can be of various forms, with tablets and capsules being the most common one. Vitamin C tablets are designed in this case study. Vitamin C is taken daily by many people with the belief that they are less likely to catch a cold with a strengthened immune system.

Students should first start with a market analysis to investigate the market size of vitamin products and to perform a competitive analysis to compare various products on the market. In addition to visiting online websites, students can also visit departmental stores to collect information such as ingredients, price, number of tablets per bottle, etc. for different brands of vitamin C products. After the competitive analysis, students can identify the key product attributes of vitamin C tablets. Note that market analysis may not provide all important product specifications (e.g. mechanical strength and dissolution time of tablets), students are advised to refer to textbooks on pharmaceutical dosage forms (Lieberman et al., 1989) or product standards (United States Pharmacopeia, 1990).

With the key product attributes, students should relate them to the technical requirements of vitamin C tablets. The base case formulation is then determined by rule-based methods, model-based methods, and database. Students can refer to Fung and Ng (2003) or Kibbe (2000) for a database of common ingredients used in vitamin C tablets, its selection heuristics, and some models to ensure that the formulation and product structure meet the required product specifications. After formulating the base-case, the physicochemical properties of the vitamin C tablets are evaluated and the formulation is iterated, guided by a causal tablet, to meet the product specifications. Finally, the product manufacturing process is synthesized and a financial analysis is conducted to evaluate the profitability.

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Sample solutions to design of vitamin C tablet (Fung and Ng, 2003)

4.1 The product and its functions

Vitamin C (ascorbic acid) is a water soluble and essential nutrient for humans. It can be obtained in our everyday intake of fruits and vegetables. Vitamin C is required for the biosynthesis of collagen, L-carnitine, and certain neurotransmitters. It is also involved in protein metabolism, is an important physiological antioxidant and plays an important role in our immune system. The recommended amount for adults is 90 mg for male and 75 mg for female (Institute of Medicine, 2000). For people who do not obtain sufficient Vitamin C through meals, they can take Vitamin C dietary supplements which can be in the form of tablets, capsules and liquid with Vitamin C tablets as the most common product form.

4.2 Market study

The global vitamin supplements market was valued at USD 37.4 billion in 2013, with Asia-Pacific being the largest market. With increasing life expectancy, vitamin consumption is on an upward trend and its global sales is expected to reach USD 59.6 billion in 2020 (Persistence Market Research, 2015). Within the vitamin supplements market, Vitamin C supplements account for a sales of 221.3 million in the U.S. in 2011 (Watson, 2011). There are various brands of Vitamin C tablets on the market, as summarized in Table 4.1. All of them provide either 500 mg or 1000 mg dosage of ascorbic acid, with varying number of tablets per bottle. The price could vary from USD 15 per bottle to USD 35 per bottle, depending on whether the product is a time-released one, whether rosehips or bioflavonoids is added, tablet dosage, and number of tablets per bottle.

Table 4.1. Vitamin C tablets in the market.

Brand name	No. of tablets per bottle	Amount of Vitamin C per tablet (mg)	Price (USD)*	Remark
GNC	90	1000	35	
GNC	100	1000	27	Rosehips added
Doctor's Choice	60	500	19	Bioflavonoids added
Doctor's Choice	40	1000	21	Rosehips added; Time-released tablet
Blackmores	90	500	24	Rosehips and Bioflavonoids added; slow release
Blackmores	60	1000	21	Bioflavonoids added
Jamieson	100	1000	28	
Jamieson	100	500	15	
Jamieson	100	500	17.5	Time release
AG natural health	120	500	28	Rosehips and Bioflavonoids added; time release

* Note that the price of vitamin supplements can be very different in different countries.

4.3 Product attributes and technical parameters

The required product attributes of a Vitamin C tablet is summarized in Table 4.2. The tablet should disintegrate in the stomach within 30 min (United States Pharmacopeia, 1990) and the ascorbic acid be absorbed by the gastrointestinal tract quickly. The tablet has to stay intact during processing, packaging, transportation, and dispensing, stable under anticipated environmental conditions, and also easy and pleasant to swallow by consumers. The customers also expect the tablets to be of consistent quality (i.e. similar weight and composition among tablets of different batches).

With the required product attributes, the corresponding technical parameters are also identified, as summarized in Table 4.2. For tablets to disintegrate in our stomach, the solubility of the active ingredient and the tablet porosity are important. As ascorbic acid is water soluble, the dissolution time can be expected to be short. For tablets to remain intact during handling, binder selection to provide sufficient tablet tensile strength is critical. In order to keep the tablets stable under storage and are pleasant to swallow, a film coating is applied to the Vitamin C tablets. To ensure consistent quality among tablets, the mixing process and whether granulation is needed in the manufacturing process is critical.

Table 4.2. Required product attributes of a Vitamin C tablet and the corresponding technical parameters

Product attribute	Corresponding technical parameter
Disintegrate in stomach within 30 min	Solubility of the active ingredient, tablet porosity
Dissolve and absorb into gastrointestinal tract quickly	Solubility of ascorbic acid in water
Remain intact during processing, packaging, transportation, and dispensing	Binder selection, tablet tensile strength
Keep stable under anticipated environmental conditions	Apply coating to the tablets
Easy and pleasant to swallow	
Consistent quality - minimum batch-to-batch variation in weight and composition	Good mixing and includes a granulation step in the manufacturing process

4.4 Generation of a base case formula

With reference to the products on the market, most Vitamin C tablets provide a dosage of 500 or 1000 mg Vitamin C, which is much higher than the recommended amount. Although excess ascorbic acid can be excreted, it is of no use to the body. Therefore, tablets with a lower dosage of Vitamin C (350 mg) are designed in this case study. Similar to many products on the market, bioflavonoids (50 mg) are added to the product to increase the market acceptance.

Excipients such as diluent, binder, disintegrant and lubricant are commonly added to a tablet. Therefore, the weight of a Vitamin C tablet is designed to be 500 mg and its diameter is set at 10 mm. Common excipients and their typical amounts are summarized in Fung and Ng (2003). Readers can also refer to Kibbe (2000) for a more comprehensive database. Note that some

ingredients can serve various functions and it is desirable to have an excipient that serves multiple purpose in a tablet. Common ingredients are selected for the base case formulation: microcrystalline cellulose as the diluent, Povidone as the disintegrant, and magnesium stearate as the lubricant. Binder selection and product structure parameters such as tablet height and porosity are determined next to make sure the product specifications are met.

With the tablet mass m_t and the particle density ρ_p , tablet height H can be determined.

$$\frac{\pi D^2}{4} H (1 - \varepsilon) = \frac{m_t}{\rho_p} \quad (1)$$

where D is the tablet diameter (10 mm) and ε is the tablet porosity which is assumed to be 7.5% in this case study. As the tablet mainly contains ascorbic acid, the particle density of ascorbic acid (1650 kg/m³) is used. Therefore, the tablet height is 4.17 mm. Tablet density can be calculated by dividing the tablet mass with the table volume and equals 1526 kg/m³.

The selection of the above parameters has to provide a tablet that meets the required disintegration time. As ascorbic acid is soluble in water, tablet disintegration depends on the rate of dissolution of the soluble component. The disintegration time t_d can be estimated as (de Jong, 1991):

$$t_d = \frac{2m_t^2}{\rho_t^2 \pi^2 D^4 D_i \varepsilon (1 - \varepsilon)^2} \quad (2)$$

where ρ_t is the tablet density and D_i is the diffusivity of the soluble component in liquid and is assumed to be 2×10^{-8} m²/s. This provides a disintegration time of 28.2 min which meets the product specifications. Note that Darcy law and Blake-Kozeny equation have to be used if the major component in the tablet is not water soluble (Fung and Ng, 2003).

Next, we determine if binder has to be added to provide cohesion among powders to withstand any compaction stress σ_c under normal handling situations, which can be expressed as (Stuart-Dick and Royal, 1992):

$$\sigma_c = \rho_t v_t^2 \sin^2 \theta \quad (3)$$

where v_t is the impact velocity and θ is the angle of impact of the tablet onto a surface. Here, v_t and θ are assumed to be 15 m/s and 90°, respectively. A relatively high impact velocity is assumed here to account for some extreme conditions (e.g. accidentally throwing the tablets onto floor). For tablets to remain intact, the table tensile strength has to be larger than the compaction stress. In this case study, the required tensile strength is defined to be 1.5 σ_c (i.e. a safety factor of 50%). Tensile strength σ_T can be related to the adhesion force (van der Waals force) among powders F_{adh} which in turn relates to the binder Hamaker constant A as (Pietsch, 1997; Visser, 1989):

$$\sigma_T = \frac{9}{8} \frac{1 - \varepsilon}{\varepsilon} \frac{F_{adh}}{d_p^2} \quad (4)$$

$$F_{adh} = \frac{A d_p}{12 z^2} \quad (5)$$

where d_p is the constituent particle size (5 μ m), and z is the separation distance between particles and can be taken as 4 Å when particles are in close contact (Dahneke, 1971). Therefore, the required Hamaker constant is 3.6×10^{-19} J. As the Hamaker constant of ascorbic acid is 4.5×10^{-20} J, binder has to be added to provide sufficient cohesion. In many cases, diluent can also serve as a binder and the required Hamaker constant of the diluent for providing sufficient cohesion can be estimated by

$$A \approx (\sqrt{A_{API}} - \sqrt{A_{diluent}})^2 \quad (6)$$

In this case study, if the diluent also serves as a binder, the required Hamaker constant of the diluent is 1.5×10^{-19} J, which is close to that of microcrystalline cellulose (1.85×10^{-19} J). Therefore, microcrystalline cellulose also serves as binder in this case study.

In the base case formulation, the amount of excipients takes the lowest amount suggested in Fung and Ng (2003). Therefore, 2.5 mg of Povidone is added as disintegrant and 1.25 mg of magnesium stearate is added as lubricant. With 350 mg of ascorbic acid and 50 mg of bioflavonoids, the balance is the microcrystalline cellulose (96.25 mg), as diluent and binder.

4.5 Measurement of physicochemical properties that cannot be predicted by experiments/ Iterate guided by a causal table

As the disintegration time is one of the major product attributes for Vitamin C tablets, it is measured for tablets prepared with the base case formulation. The powders are mixed and compressed in a tablet compaction machine. The pressure P required to produce tablets with the desired porosity can be determined from the following equation (Heckel, 1961):

$$\ln \frac{1}{\varepsilon} = \frac{1}{3}YP + \ln \frac{1}{1-D_A} \quad (7)$$

where Y is the yield strength and D_A is the relative density corresponding to die filling and particle rearrangement. After that, they are put into an apparatus for disintegration testing. Readers can refer to the United States Pharmacopeia (2008) for the detailed specifications of the apparatus and the operating procedure. Experimental results show that the disintegration time is 40 min, which is longer than the product specification. Causal table summarized in Fung and Ng (2003) suggests that more disintegrant can be added to the tablet formulation. For example, the amount of disintegrant can be increased to 5 mg and the amount of diluent reduces to 93.75 mg to keep the same tablet mass.

4.6 Design of product manufacturing process

The manufacturing process of the Vitamin C tablets is illustrated in Figure 4.1. As the particle size of ascorbic acid and microcrystalline cellulose (diluent and binder) are larger than the desired constituent particle size in the tablet (5-10 μm), they are crushed before mixing. To minimize batch-to-batch variations in the tablets, granulation is recommended before compression and wet granulation is selected in this case study. As the diluent also serves as the binder, only water (solvent) is added to the granulator. After granulation, a crusher is usually used to fine-tune the particle size distribution and a dryer is used to dry the granules. After drying, the particles are screened to collect particles with the desired particle size. Oversized particles are recycled back to the crusher whereas undersized particles are recycled back to the granulator. Particles with the desired particle size are mixed with Povidone (disintegrant) and magnesium stearate (lubricant), and compressed in a tablet compression machine. As ascorbic acid is water soluble, a film coating is applied to ensure that the tablet is stable under anticipated environmental conditions and also to mask the acidic taste of ascorbic acid.

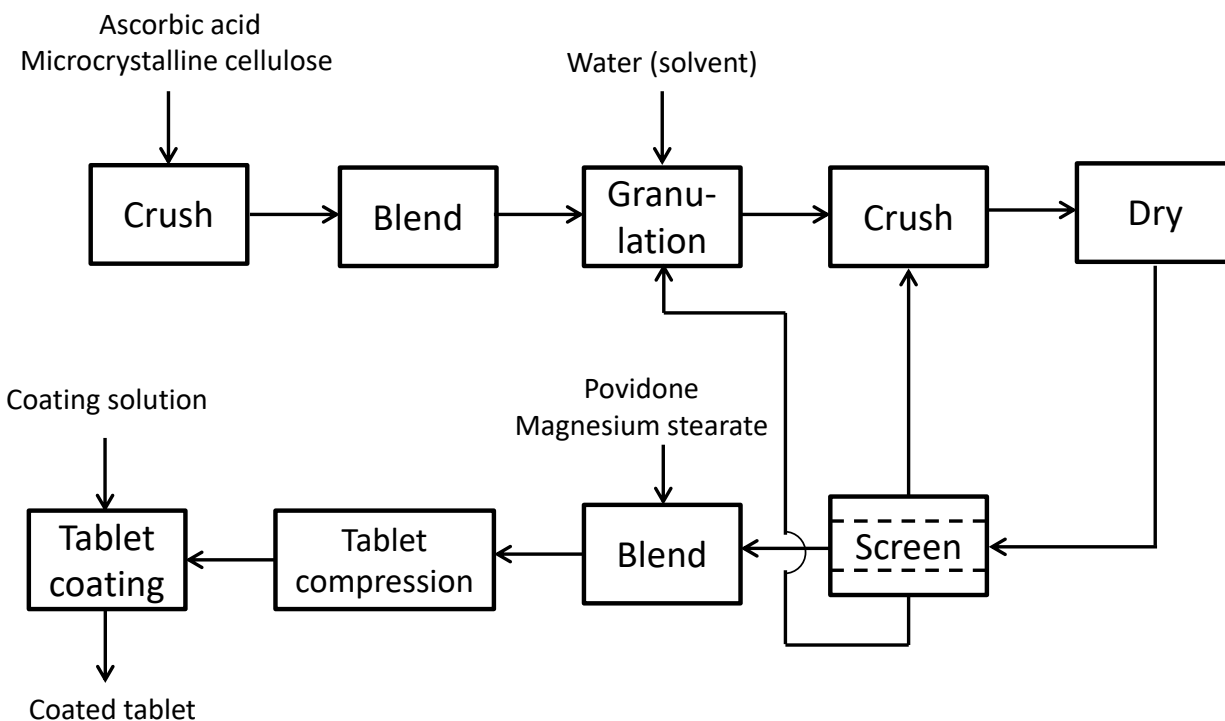


Figure 4.1. Process flowsheet for coated Vitamin C tablet manufacture.

4.7 Financial analysis

The financial analysis of a 7-year Vitamin C tablet product is summarized in Table 4.3. As the market is very competitive, it takes a relatively long time to gain a substantial market share. The development cost of the project is estimated to be USD 700,000 which includes identifying the best formulation for the product and determining the specifications of the process units. The capital spending is assumed to be USD 800,000 and the fixed cost in the first two years is estimated to be USD 1.5 million.

As the market is very competitive, penetration pricing strategy is adopted in this case study. With reference to similar products in the market, the product is set at a lower price (USD 23 per bottle of 100 tablets) in the first two years and increases to USD 26 per bottle in Year 3 to 5. As the price is lower than similar products in the market, we expect a fast growth in Year 1 and 2 (i.e. 300,000 and 500,000 bottles sold in Year 1 and 2, respectively). The growth becomes slower in Year 3 to 5 as the product returns to its standard price. However, we still expect a small growth because of the returning customers and a positive brand image being developed. The fixed cost (excluding the marketing cost) is increased to 3 million in Year 1 and 2 to account for more production and supporting staff. As there are many competitors, a substantial marketing cost has to be invested. When the product returns to its standard price in Year 3, the marketing expenses is increased from USD 1.5-2 million in Year 1 to 2 to USD 4 million in Year 3 to 5. Similarly, the fixed cost is increased to USD 4 million to account for more sales and marketing staff in Year 3 to 5. The variable cost of the product is assumed to be USD 5 per bottle.

With all the cost information, income from operations (IFO), earnings before income tax (EBIT), after tax operating income (ATOI), operating cash flow (OCF), and project cash flow (PCF) are calculated by the following equations.

$$IFO = S - C_{ED} \quad (8)$$

$$EBIT = IFO - D = S - C_{ED} - D \quad (9)$$

$$ATOI = (1 - t) EBIT = (1 - t) (S - C_{ED} - D) \quad (10)$$

$$OCF = ATOI + D = (1 - t) (S - C_{ED} - D) + D = (1 - t) (S - C_{ED}) + t D \quad (11)$$

$$PCF = OCF - \text{Development cost} - \text{Increase in NWC} - \text{Project capital spending} \quad (12)$$

Here, S is the sales, C_{ED} is the sum of fixed cost, marketing cost and variable cost, D is depreciation which is assumed to be linear depreciation over 5 years, t is tax rate which is assumed to be 40%, NWC is the net working capital.

Table 4.3. Financial analysis of a Vitamin C tablet product for a 7 year product cycle (All numbers are shown in USD and in thousands).

Year	-1	0	1	2	3	4	5
No. of bottles sold			300	500	600	650	700
Sales			6,900	11,500	15,600	16,900	18,200
Fixed Cost	1,500	1,500	3,000	3,000	4,000	4,000	4,000
Marketing cost			1,500	2,000	4,000	4,000	4,000
Variable Cost			1,500	2,500	3,000	3,250	3,500
IFO			900	4,000	4,600	5,650	6,700
Depreciation			160	160	160	160	160
EBIT			740	3,840	4,440	5,490	6,540
Taxes (40%)			296	1,536	1,776	2,196	2,616
ATOI			444	2,304	2,664	3,294	3,924
OCF	-1,500	-1,500	604	2,464	2,824	3,454	4,084
NWC		250					-250
Development cost	700						
Capital Spending		800					
PCF	-2,200	-2,550	604	2,464	2,824	3,454	4,334

Net present value (NPV) is used to calculate the profitability of the project. A discount rate (R) of 20% and a bank interest rate of 5% are assumed in this evaluation.

$$NPV = \sum_{j=-n}^m \frac{PCF_j}{(1+R)^j} \quad (13)$$

Here, n is the number of periods for product development, and m is the number of periods for product life cycle. Note that the unit of NPV is in thousand USD.

$$NPV = -2200 (1 + R) - 2550 + \frac{604}{1+R} + \frac{2464}{(1+R)^2} + \frac{2824}{(1+R)^3} + \frac{3454}{(1+R)^4} + \frac{4334}{(1+R)^5} \quad (14)$$

With $R = 0.2$, NPV equals US\$ 2,066,143, which meets the management's expectation.

To determine IRR, NPV is set to 0. It becomes

$$0 = -2200(1 + R) - 2550 + \frac{604}{1+R} + \frac{2464}{(1+R)^2} + \frac{2824}{(1+R)^3} + \frac{3454}{(1+R)^4} + \frac{4334}{(1+R)^5} \quad (15)$$

Using Microsoft Excel to solve the above equation, IRR equals 31.1%, which is larger than the bank interest rate of 5%. Therefore, the Vitamin C tablet project can be presented to the management for approval.

4.8 References

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