

Preliminary process optimization

Optimum design and design strategy?

06-03-2025

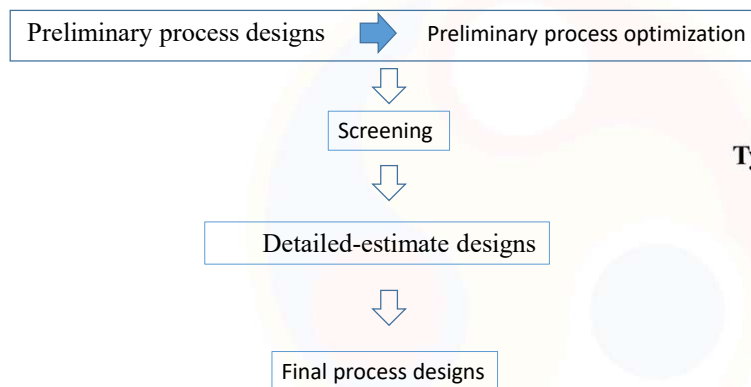
CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

197



197

Preliminary process optimization



Types of process design:

1. Order of magnitude of design
2. Study of factored design
3. Preliminary designs
4. Detailed-estimate designs
5. Final process designs

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

198



198

1

Optimum Design

- At the end of preliminary design synthesis, preliminary process optimization is performed with a **goal is to compare two or more process alternatives when each is close to its optimum design conditions.**
- A sufficient amount of accuracy is involved in the screening of alternatives at this stage.
- Selection of best alternatives → certain that we will proceed for Final design

Objective of an approximate optimization analysis:

- To determine the dominant economic trade-offs for each design variable.
- To rank/order the importance of design variable
- To estimate the incentive for optimizing a design (initial design is good enough or further try for improvement is needed)

Here, we want to get close to the optimum without necessarily determining the exact value of the optimum.

Shortcut design and cost models are used for the analysis



199

Optimum Design

Basic nature of design optimization is that a process design optimizations are always characterized by economic-trade-offs. i.e., criteria for optimality can ultimately be reduced to a consideration of costs or profits.

The factors affecting the economic performance of the design include:

- the type of processing technique used
- processing equipment used
- arrangement and sequencing of the processing equipment used in the design
- the actual physical parameters for the equipment

The operating conditions for the equipment are also of prime concern and importance.

Thus, the **optimum for a process design** is the most cost-effective selection, arrangement, sequencing of processing equipment and operating conditions for the design.



200

Optimum Design

Although cost considerations and economic balances are the basis of most optimum designs, at times factors other than cost can determine the most favorable conditions.

Ex: operation of catalytic reactor (optimum operation temp \leftrightarrow reactor size) \rightarrow equilibrium or reaction rate limitations.

The particular temperature could be based on based on the maximum percentage conversion or on the maximum amount of final product per unit time.

Design optimization problem: to determine the optimum thickness of insulation for a given steam pipe installation.

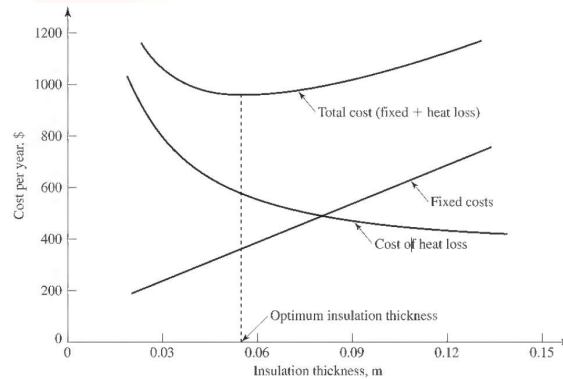


Figure: Illustration of the basic principle of an optimum economic design



Optimum Design

Optimum design analysis begins with the establishment of the optimization task. Which follows:

1. Selection of economic criteria

- done by objective function that is an economic performance measure

2. Definition of optimization problem

- It requires the establishment of *various mathematical relations and limitations* that describe the aspect of the design.
- The relations are used to explore the effects on the objective function, and then to determine the optimal values of the variables and constraints parameters that affect the process economic performance and objective function of the design



Selection of economic criteria

Economic criteria for rating investments → "best" investment strategy on the basis of the profitability analysis?

the best strategy is one that favors those **investments that meet or exceed an established minimum acceptable rate of return** for each investment, but that also ensures that no investment is made which does not meet that acceptable return standard

profitability methods—

- rate of return
- net return
- net present worth
- Etc.



203

Optimum Design

Definition of optimization problem:

1. **Basis for the optimization:** Objective function = $f(\text{structural and parametric variables and constraints})$ → maximization or minimization for a factor
 - Such factor could be total cost per unit production or per unit of time, profit, amount of final product per unit of time, and percent conversion.
 - an economic performance measure
2. **Determination of process variable** in the design that is to be optimized.
 - **Process variables** are the variables that affects the values of the objective functions.
 - Decision and dependent variables: Decision variables are variables that can be determined, or set, while dependent variables arise or are influenced by process constraints. Ex: such as temperature and pressure as well as equipment specification variables such as the number of trays in a distillation column
 - **Process constraints** are the constraints on the process. These are sometimes so obvious they are overlooked, but having these defined completely is critical. Common examples of process constraints include process operability limits, reaction chemical species dependence, or product purity and production rate.
 - large number of variables → reduced through screening analysis of a variable's relative impact on design performance and costs



204

Optimum Design

Optimization is often divided into two separate fields for convenience,

- **Structural optimization**
- Parametric optimization

Structural Optimization

- Topologic optimization concerns itself with equipment selection alternatives, arrangement, and inter- and intra-connectivity.
- This translates to such issues as potential arrangements of processing steps, considerations of alternative processing techniques, and considerations of alternative types of both individual and groupings of processing equipment.
- Structural optimization consists in finding one or more "best" flowsheets for a process.



Optimum Design

Optimization is often divided into two separate fields for convenience,

- Structural optimization
- **Parametric optimization**

Parametric Optimization

- Parametric optimization deals with process operating variables and equipment design variables other than those strictly related to structural concerns.
- Some of the more obvious examples of such decisions are operating conditions, recycle ratios, and stream properties such as flow rates and compositions.



Optimum Design

In the HDA process, optimization (i.e., economic trade-offs) at various scale can be perform:

- Conversion
- Purge composition
- Molar ration of reactor feeds
- Pressure of the flash drum and reactor pressure
- Approach temperature in heat exchanger
- Reflux ratio for distillation column
- Fractional recoveries in distillation columns



207

Design programming

Programming Optimization Problems

- The term programming as used in design optimization literally means optimization.
- Application programming is the *practice of assembling the mathematical relationships that describe a design process and its economic behavior and then using these relationships to explore and optimize the design.*
 - **continuous and discrete programing:** linear integer programming (LIP) and mixed-integer linear programming (MILP)
 - **Stochastic programming** methods:
 - optimization problems combining discrete or continuous and *constrained characteristics*.
 - particularly useful for dealing with uncertain processes that exhibit a certain degree of uncertainty or to evaluate process flexibility.
 - They are also in general less applicable to process design optimization.
 - bound constrained programming



208

Design programming



Figure: Programming approach methodology, divisions, and relations

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

209



209

Approaches to Optimization

The **overall optimization process** is summarized in the following steps:

1. Define an optimization problem
2. Quantify the optimization value assuming an ideal process
3. Identify the design conditions, assumptions and constraints
4. Strategize how to implement design changes
5. Evaluate the result of the optimization

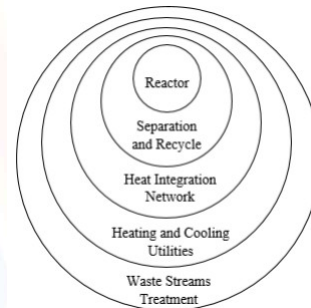


Figure: Hierarchy of Chemical Process Optimization

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

210



210

Chemical process Optimization: Example

University of Mississippi
eGrove

Honors Theses

Honors College (Sally McDonnell Barksdale
Honors College)

2016

A Practical Guide to Chemical Process Optimization: Analysis of a Styrene Plant

Fleur Phelps
University of Mississippi, Sally McDonnell Barksdale Honors College

Recommended Citation

Phelps, Fleur, "A Practical Guide to Chemical Process Optimization: Analysis of a Styrene Plant" (2016).
Honors Theses. 338.
https://egrove.olemiss.edu/hon_thesis/338

This Undergraduate Thesis is brought to you for free and open access by the Honors College (Sally McDonnell Barksdale Honors College) at eGrove. It has been accepted for inclusion in Honors Theses by an authorized administrator of eGrove. For more information, please contact egrove@olemiss.edu.

https://egrove.olemiss.edu/cgi/viewcontent.cgi?article=1337&context=hon_thesis

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

211



211

Approaches to Optimization

Optimization in Chemical Engineering by Prof. Debasis Sarkar

<https://www.youtube.com/playlist?list=PLbRMhDVUMngct1skDAxoR2xhblqOnAt0H>

Process Optimization in Chemical Engineering

https://www.youtube.com/watch?v=Jtrw_et-y4w&list=PLFK7DKgtfxu8IPROl2Oqlm4cgVibFg55

https://archive.siam.org/books/mo10/mo10_sample.pdf

<https://www.lsu.edu/mpri/files/process-optimization.pdf>

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

212



212

Process Retrofitting

Retrofitting also called **improvement of exiting chemical processes.**

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

213



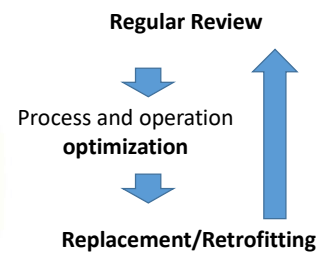
213

Process Retrofitting

Regular Review (performance of the existing process/plants and assess the possibilities for their improvement)

Following objectives:

- To reduce energy required and/or operating cost
- To improve conversion and/or selectivity of reactions
- To increase production/throughput of the process
- To use feed of different quality and/or alternative feed
- To meet new specifications of product(s)
- To produce new products
- To enhance the control of the process
- To improve the safety, reliability and flexibility of the process
- To reduce the adverse impact of the process on the environment.



06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

214



214

Process Retrofitting

Existing systems (old machine)
(with years of operating life, systems that required a substantial initial investment and are still in good working order)



Need to increase the **speed and efficiency of production** while significantly **improving the quality** of the final product and **reducing costs**.

Two option:

1. Replacement (cost-intensive)

Completely modernized (expensive with technical updates)

2. Retrofitting

Comparatively modernized (inexpensive with technical updates).
Cost-effective alternative to purchasing new equipment.
Extend its service life of old machine

- two words: “retro” (means **backward** in Latin) + “fit” (meaning **to adapt** in English)
- the word retrofit describes the process of “**turning old into new**”.
- In industry, it refers to the ***adaptation of existing equipment to current technical conditions***.

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

215



215

Process Retrofitting

Retrofitting means

- Making minor changes in the interconnections between process equipment } Structural change
- The replacement of one or more pieces of equipments by some other equipment or } PFD remain same
- Changes in the sizes of one or more pieces of equipments in an existing process. }
- Retrofitting is the addition of new technology or features to older systems.

To retrofit something imply the replacement of existing **parts** or the addition of new parts to improve the features of the machine or device, such as its performance or the safety of workers.

- Chemical Processes (continuous and batch) designs are retrofitted for the:
 - Product Quality and quantity (debottlenecking a process)
 - Operational efficiency: Improvement of Production Cost-Efficiency (economic performance)
 - Safety and Maintenance Performance
 - Energy efficiency

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

216



216

Process Retrofitting

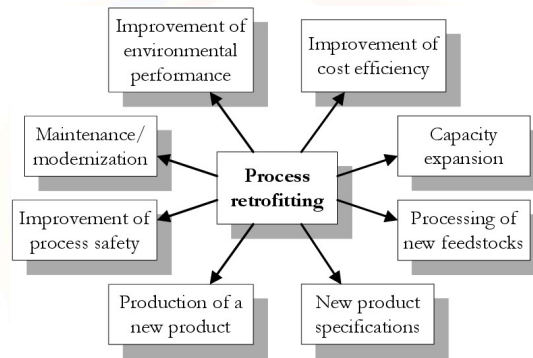


Figure: Typical retrofit incentives for chemical process design

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

217



217

Process Retrofitting

Two important perspective for Retrofitting:

1. Industry 4.0 Perspective

Retrofitting a Process Plant in an Industry 4.0 Perspective

- Transformation of an **old plant into a smart plant** capable of communicating quickly with operators to increase its safety and maintainability
- Costs and time to replace obsolete machines could be unsustainable

2. Emissions Reductions Perspective

Coal-Fired Power Plants

- Gas-fired power plant
- CO₂ capture etc

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

218



218

11

Process Retrofitting

Different Classes of Retrofit Problems:

Different kinds of retrofit problems → demands different levels of effort and expertise

Four broad classes of Retrofit Problems:

- I. Improvement studies on the efficiency of a particular unit operation.
- II. Integrating new technology (new unit operations) into an existing process.
- III. Studies to debottleneck the process.
- IV. Systematic studies that examine the entire process flow sheet and its interactions to either reduce costs or increase profits.

Concentrate on a particular unit operation and either make it operate more efficiently or replace it with something new and different.

Development of procedures to look at an entire process flow sheet and by considering the interactions between unit operations and process streams to find a way to increase profits

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

219



219

Process Retrofitting

Different Classes of Retrofit Problems:

- Optimization is an important issue in solving a retrofit problem.
- Basically two approaches to solving this structural optimization problem:
 - a. using sophisticated optimization theory to rigorously solve the underlying optimization problem
 - b. using heuristics derived from physics and economics and provided by experienced designers to try to “pick” a flow sheet structure or at least pick a small number of structures to evaluate. Useful especially in screening calculations where high accuracy is not expected.

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

220



220

Process Retrofitting

Systematic procedure for process retrofitting:

Proceeds through a **hierarchy of decisions**:

- i. Estimate an upper bound on the incentive for retrofitting.
- ii. Estimate the economic incentive for replacing the existing plant by using the using the same process flowsheet.
- iii. Estimate the economic incentive for replacing the existing plant with a better process alternative.
- iv. Estimate the incremental investment costs and savings in operating costs associated with changing the existing process.
- v. Refine the retrofit calculations.



221

Process Retrofitting

Procedure for **Screening Process Retrofit Opportunities** → simplified into a **systematic procedure for process retrofitting**, which proceeds through a **hierarchy of decisions**:

- i. **Estimate an upper bound on the incentive for retrofitting.**
 - Prepare operating cost diagram of an existing process (excluding capital cost)
 - Total cost of raw materials lost (as by-product or in waste streams)
 - All the energy cost
- ii. Estimate the economic incentive for replacing the existing plant by using the using the same process flowsheet.
- iii. Estimate the economic incentive for replacing the existing plant with a better process alternative.
- iv. Estimate the incremental investment costs and savings in operating costs associated with changing the existing process.
- v. Refine the retrofit calculations.



222

Process Retrofitting

Procedure for **Screening Process Retrofit Opportunities** → simplified into a **systematic procedure for process retrofitting**, which proceeds through a **hierarchy of decisions**:

- i. Estimate an upper bound on the incentive for retrofitting.
- ii. Estimate the economic incentive for replacing the existing plant by using the using the same process flowsheet.
 - Corresponds to the large capital investment
 - Estimate processing/operating costs (shortcut calculations of hierarchical decision procedures)
- iii. Estimate the economic incentive for replacing the existing plant with a better process alternative.
- iv. Estimate the incremental investment costs and savings in operating costs associated with changing the existing process.
- v. Refine the retrofit calculations.

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

223



223

Process Retrofitting

Procedure for **Screening Process Retrofit Opportunities** → simplified into a **systematic procedure for process retrofitting**, which proceeds through a **hierarchy of decisions**:

- i. Estimate an upper bound on the incentive for retrofitting.
- ii. Estimate the economic incentive for replacing the existing plant by using the using the same process flowsheet.
- iii. Estimate the economic incentive for replacing the existing plant with a better process alternative.
 - Profit potential for the **best possible alternative?** → gross-screening
 - Help in the identification of improved alternative or the changes in the existing flowsheet (go to ii. and then iv.)
- iv. Estimate the incremental investment costs and savings in operating costs associated with changing the existing process.
- v. Refine the retrofit calculations.

06-03-2025

CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG

224



224

Process Retrofitting

Procedure for **Screening Process Retrofit Opportunities** → simplified into a **systematic procedure for process retrofitting**, which proceeds through a **hierarchy of decisions**:

- i. Estimate an upper bound on the incentive for retrofitting.
- ii. Estimate the economic incentive for replacing the existing plant by using the using the same process flowsheet.
- iii. Estimate the economic incentive for replacing the existing plant with a better process alternative.
- iv. Estimate the incremental investment costs and savings in operating costs associated with changing the existing process.
 - Retrofit study should focus on incremental annualized costs and incremental savings in the operating costs.
- v. Refine the retrofit calculations.



Process Retrofitting

Procedure for Screening Process Retrofit Opportunities:


- i. Use an operating cost diagram to identify the incentive for raw materials and energy savings
- ii. Determine the incentive for completely replacing the entire plant
 - (a) estimate the optimum values of the design variables with current costs
 - (b) identify important process alternatives
- iii. Screen the process alternatives, and find the best flow sheet if we replace the plant
- iv. Modify the existing equipment sizes for the existing flowsheet or a structural alternative
 - (a) **eliminate the existing heat exchangers, but retain the heating and cooling utilities costs**
 - (b) **identify the dominant operating variables**
 - (c) **identify the equipment that constraints the dominant operating variables**
 - (d) **remove the equipment constraints by adding incremental equipment capacity until the incremental investment costs balance the incremental savings in operating costs**
 - (e) **develop a heat-exchanger network for the process**
 - (f) **modify the new heat-exchanger network in order to use as much existing heat-exchange equipment as possible**
 - (g) **Re-optimize the process flows and heat-exchanger network**
- v. Refine the retrofit calculations



Process Retrofitting

Read:

HDA process retrofitting example from the Douglas's *Conceptual design of chemical processes* book




Article

Retrofitting a Process Plant in an Industry 4.0 Perspective for Improving Safety and Maintenance Performance

Fabio Di Carlo ^a, Giovanni Mazzuto, Maurizio Bevilacqua  and Filippo Emanuele Ciarapica 

<https://doi.org/10.3390/su13020646>



Computers and Chemical Engineering 80 (2015) 177–188

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

ELSEVIER

Systematic retrofitting methodology for pharmaceutical drug purification processes

Gioele Casola ^{a,b}, Satoshi Yoshikawa ^a, Hayao Nakanishi ^d, Masahiko Hirao ^a, Hirokazu Sugiyama ^{b,c}

^a Department of Chemical System Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, 113-8656 Tokyo, Japan
^b Institute for Chemical and Bioengineering, ETH Zurich, Vladimir-Prelog-Weg 1, 8003 Zurich, Switzerland
^c Production Technology Department, Shionogi & Co., Ltd., 7 Moriya, Nohara, Kanagasaki-shi, Izuwa-gun, 028-4503 Iwate, Japan
^d Kanagasaki Plant, Shionogi & Co., Ltd., 7 Moriya, Nohara, Kanagasaki-shi, Izuwa-gun, 028-4503 Iwate, Japan

<http://dx.doi.org/10.1016/j.compchemeng.2015.05.024>

CrossMark

06-03-2025
CL 306 Process Engineering & Economics, Dr. Sumit kumar IITG
227 

227

Process Retrofitting

1. Retrofitting of Coal-Fired Power Plants for CO₂ Emissions Reductions, The MIT Energy Initiative's Symposium <https://energy.mit.edu/wp-content/uploads/2009/03/MITEI-Symposium-09-001-RP.pdf>
2. Retrofitting a Process Plant in an Industry 4.0 Perspective for Improving Safety and Maintenance Performance <https://doi.org/10.3390/su13020646>
3. Banimostafa, Alireza (2011). [Computer Aided Chemical Engineering] 21st European Symposium on Computer Aided Process Engineering Volume 29 || **Retrofit design of a pharmaceutical batch process considering green chemistry and engineering principles.**, (), 181–185. doi:10.1016/B978-0-444-53711-9.50037-7
4. David et. Al., 1990. A systematic procedure for retrofitting chemical plants to operate utilizing different reaction paths <https://doi.org/10.1021/ie00101a017>

228