Process Simulation

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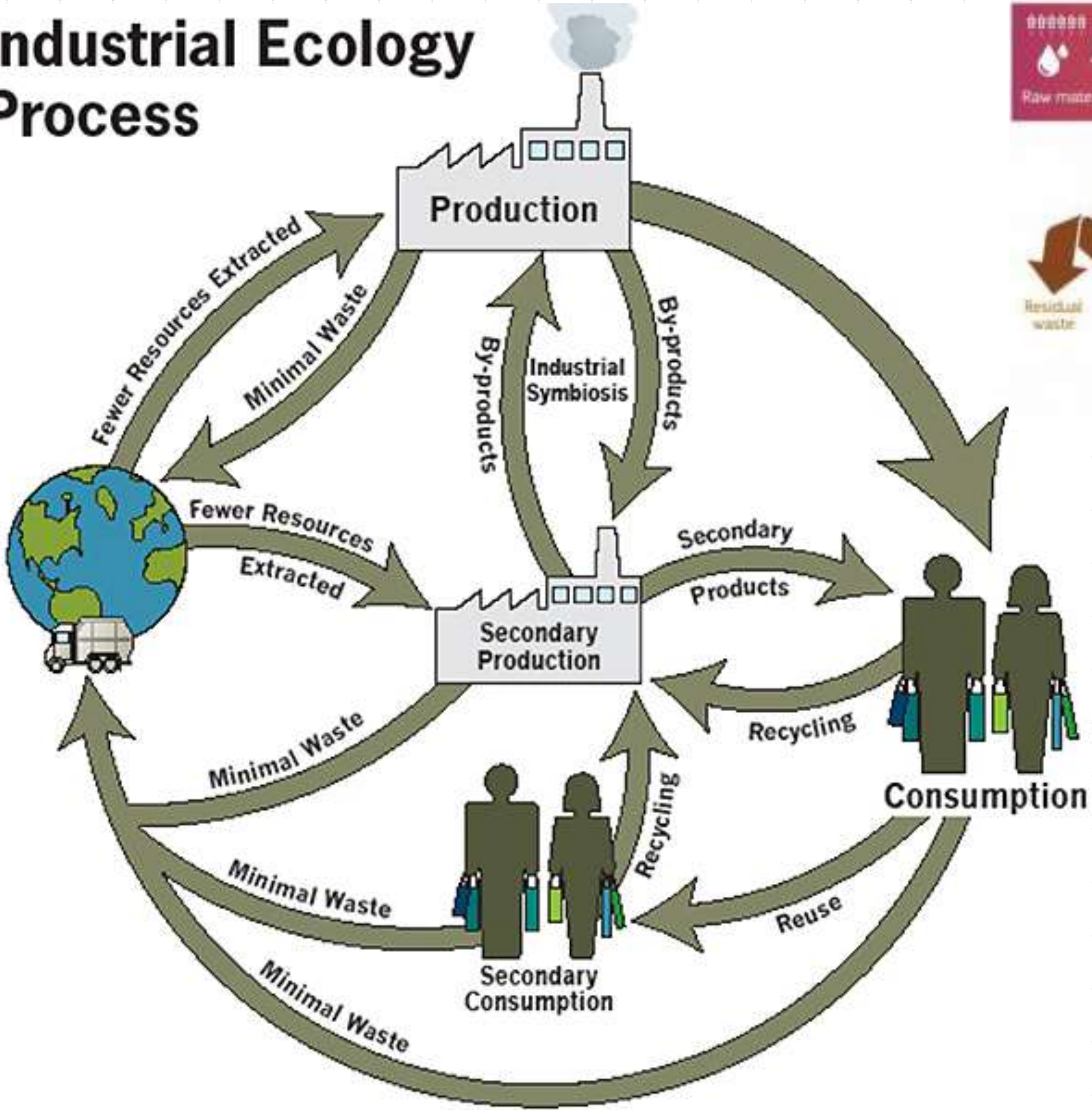
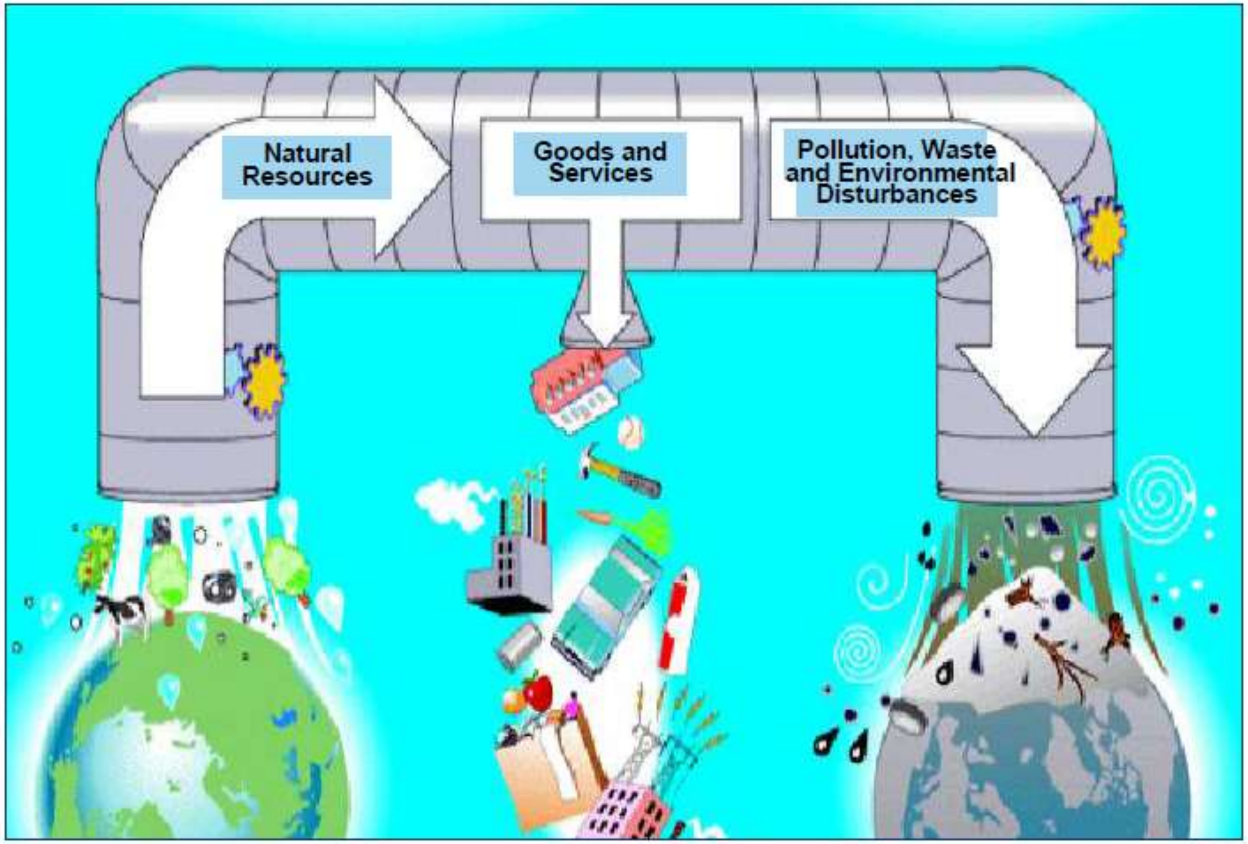
Industrial Ecology Process



Motivation: are our products and processes sustainable?

Only 25 wt% of what goes into the pipe comes out as goods and services – scope for significant improvements



Adapted from Drioli, 2005

Without significant improvements, our products-processes are not sustainable

Failure to adopt new ideas & techniques

G. Agricola, *De Re Metallica*, 1556

Is it possible to achieve more improvements in design for these equipments?

Chemical Process Industry, 2006

How to find new & innovative solutions?

A vision… how a future plant may look vs. a conventional plant.

(Rendering courtesy of DSM)

OPERATING with NON POLLUTING PROCESSES involving

PROCESS INTENSIFICATION

SAVINGS ABOUT 30 % (RAW MATERIALS + ENERGY + OPERATING COSTS)

How many **Earths** do we need?

1.7 Earths

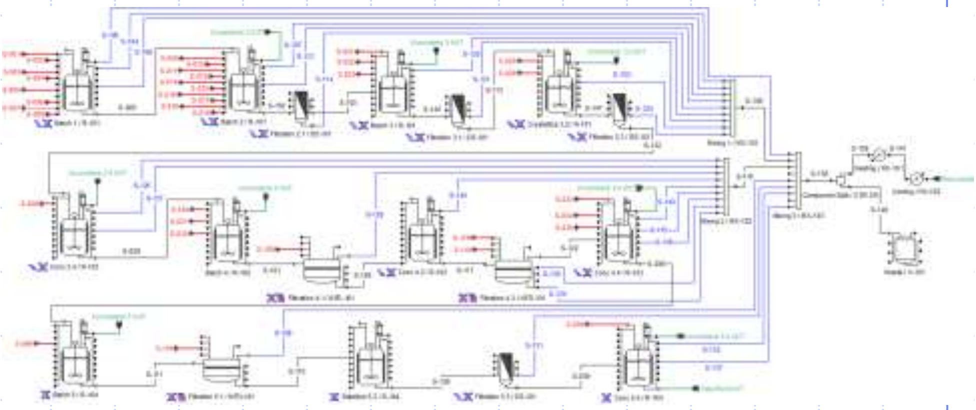
Global Footprint Network®

(Biocapacity/human ecological footprint) x365 = earth overshoot day

Source: Global Footprint Network National Footprint and Biocapacity Accounts 2019

Global Footprint Network
Advancing the Science of Sustainability

Global Vision

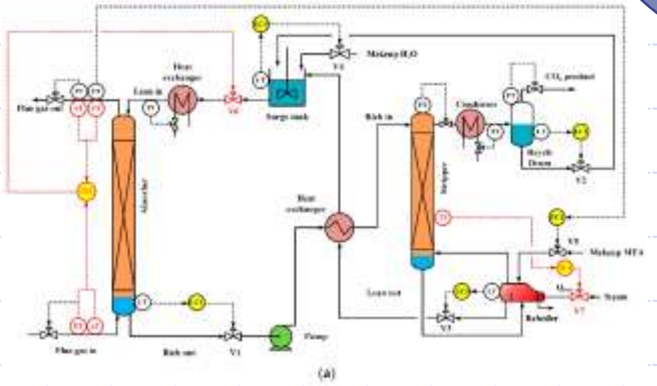


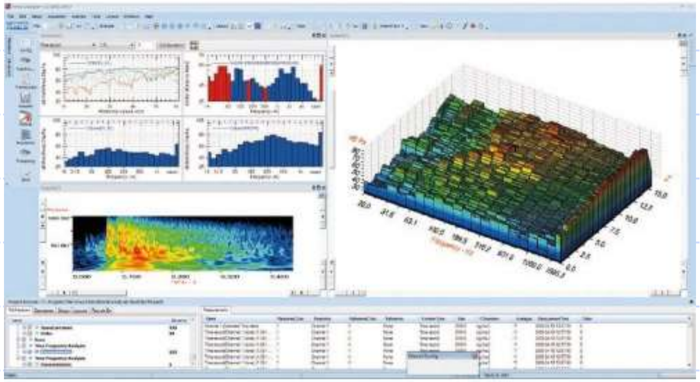
Process Simulation

Process Control

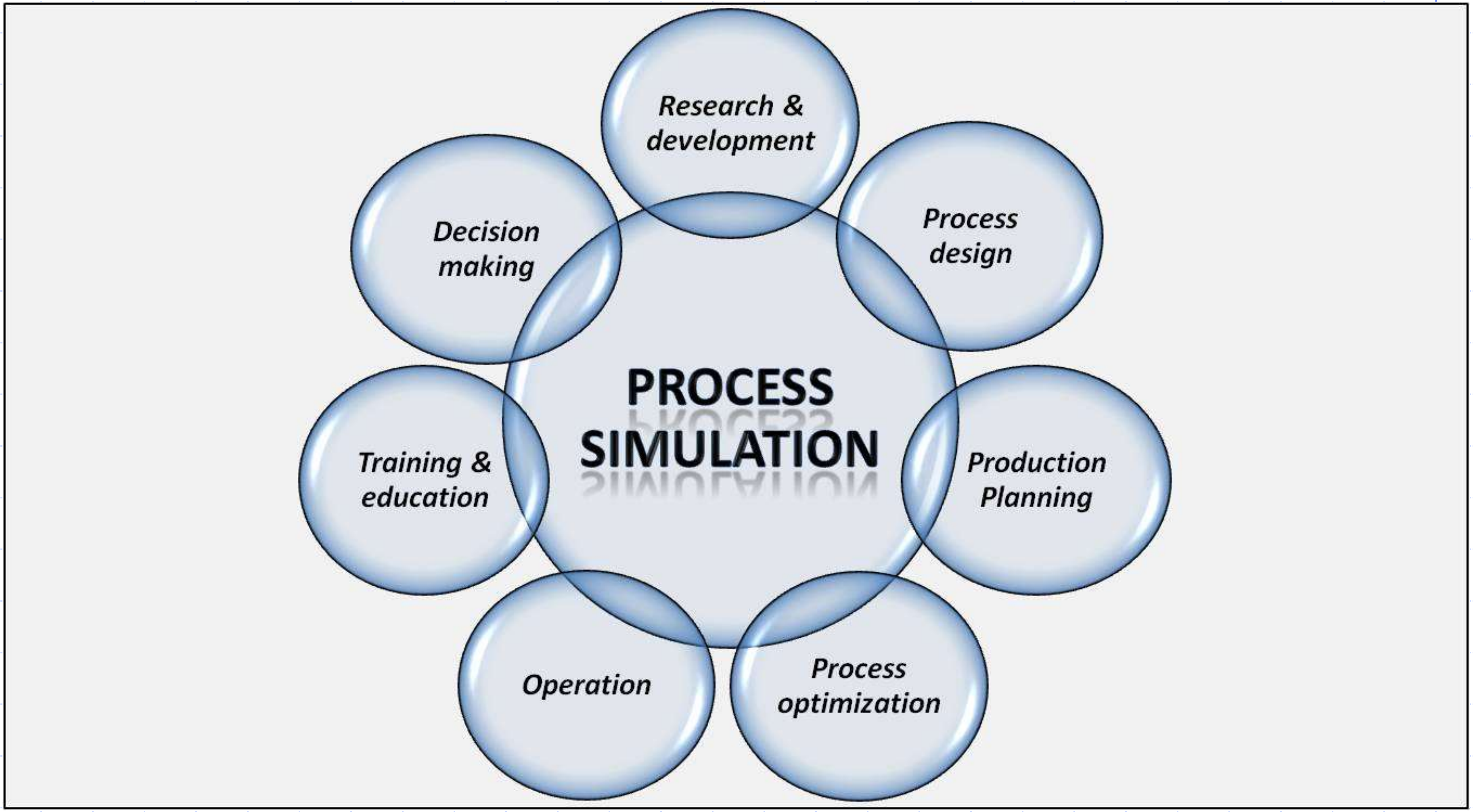
Sustainable Development

Environmental Simulation

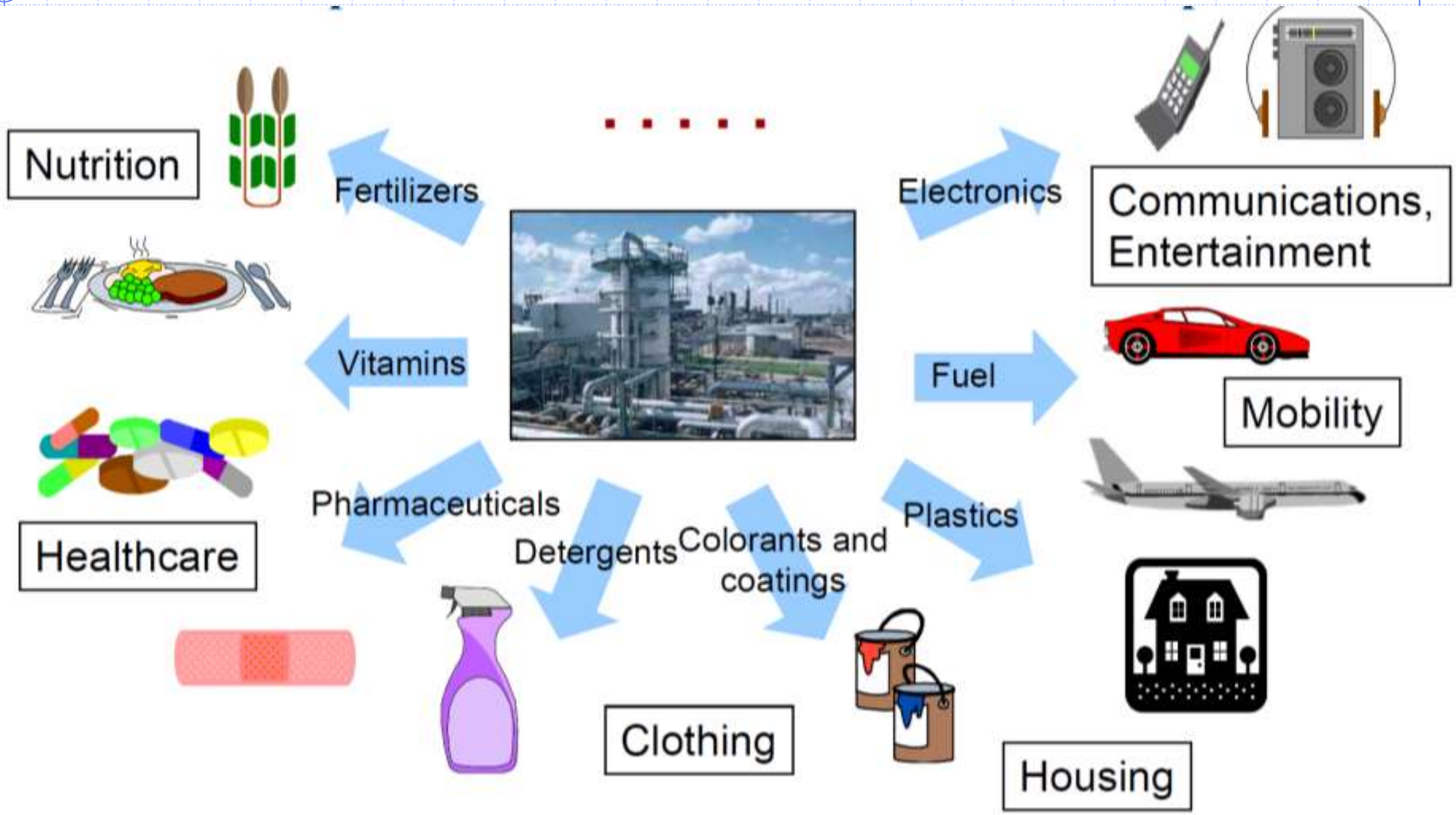




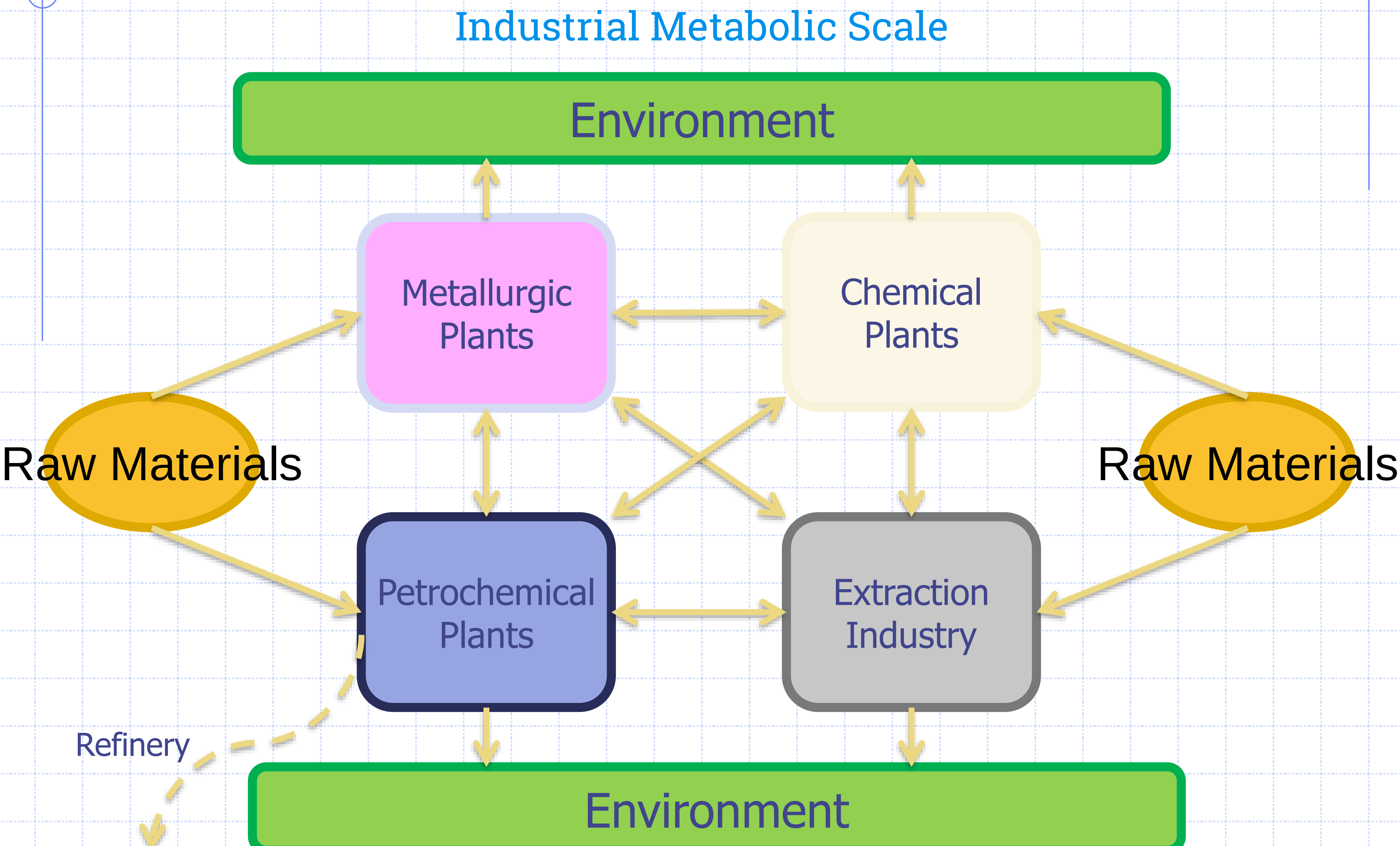
Process simulation as the key discipline of chemical engineering



Can Process simulation be used for all these products?

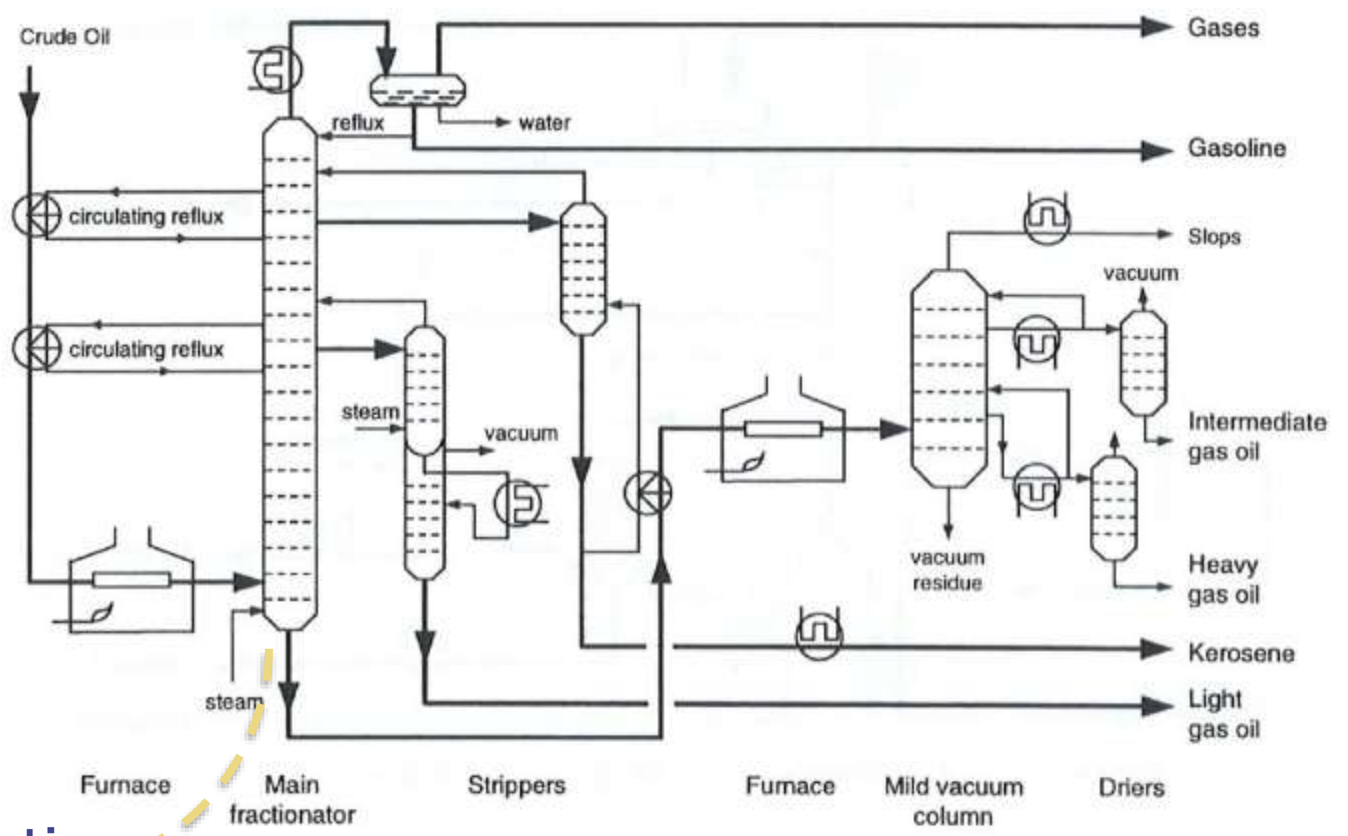


Macroscale Analysis: Industrial Ecology



Mesoscale Analysis: Refinery

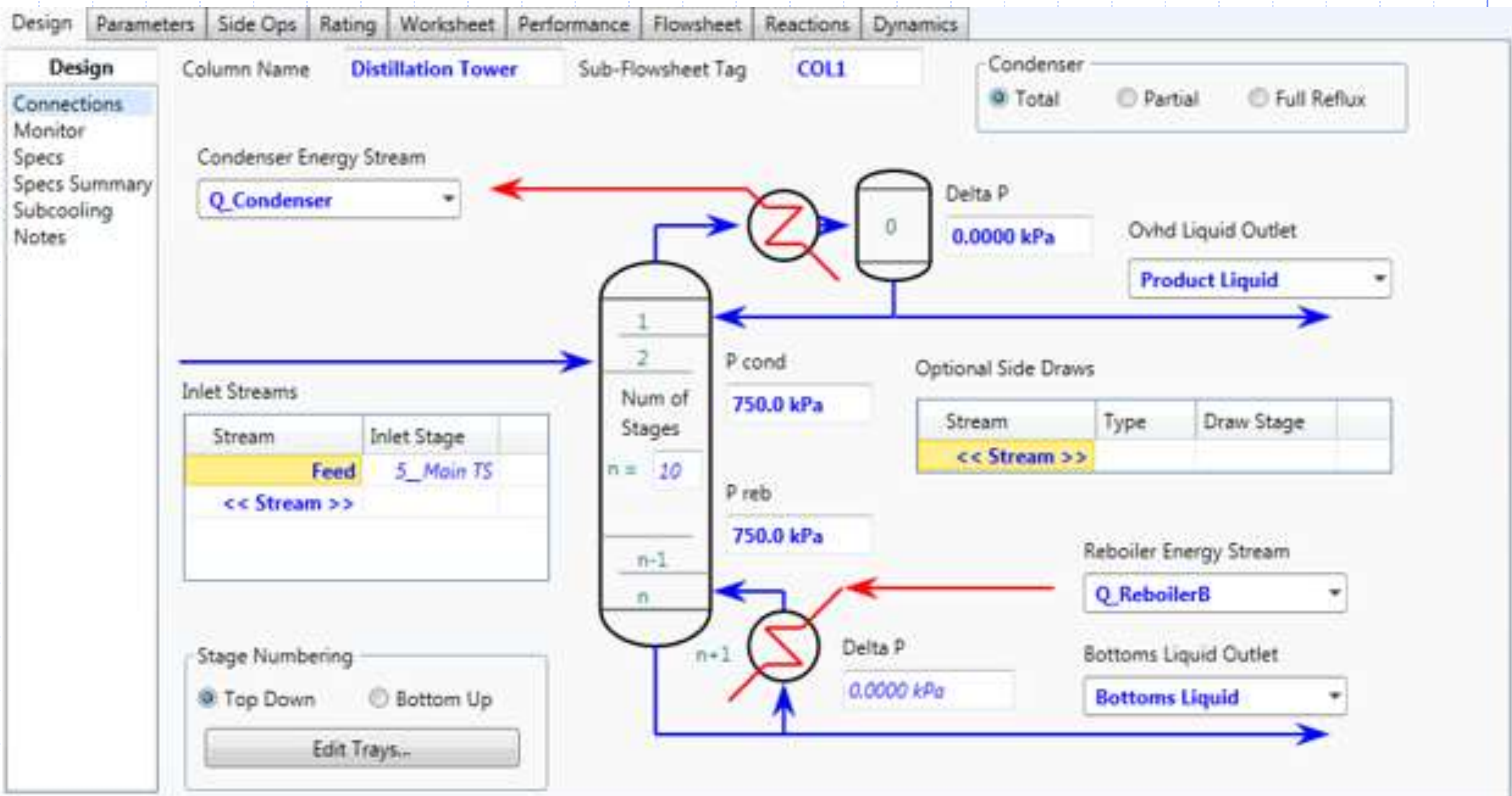
Process Engineering Scale



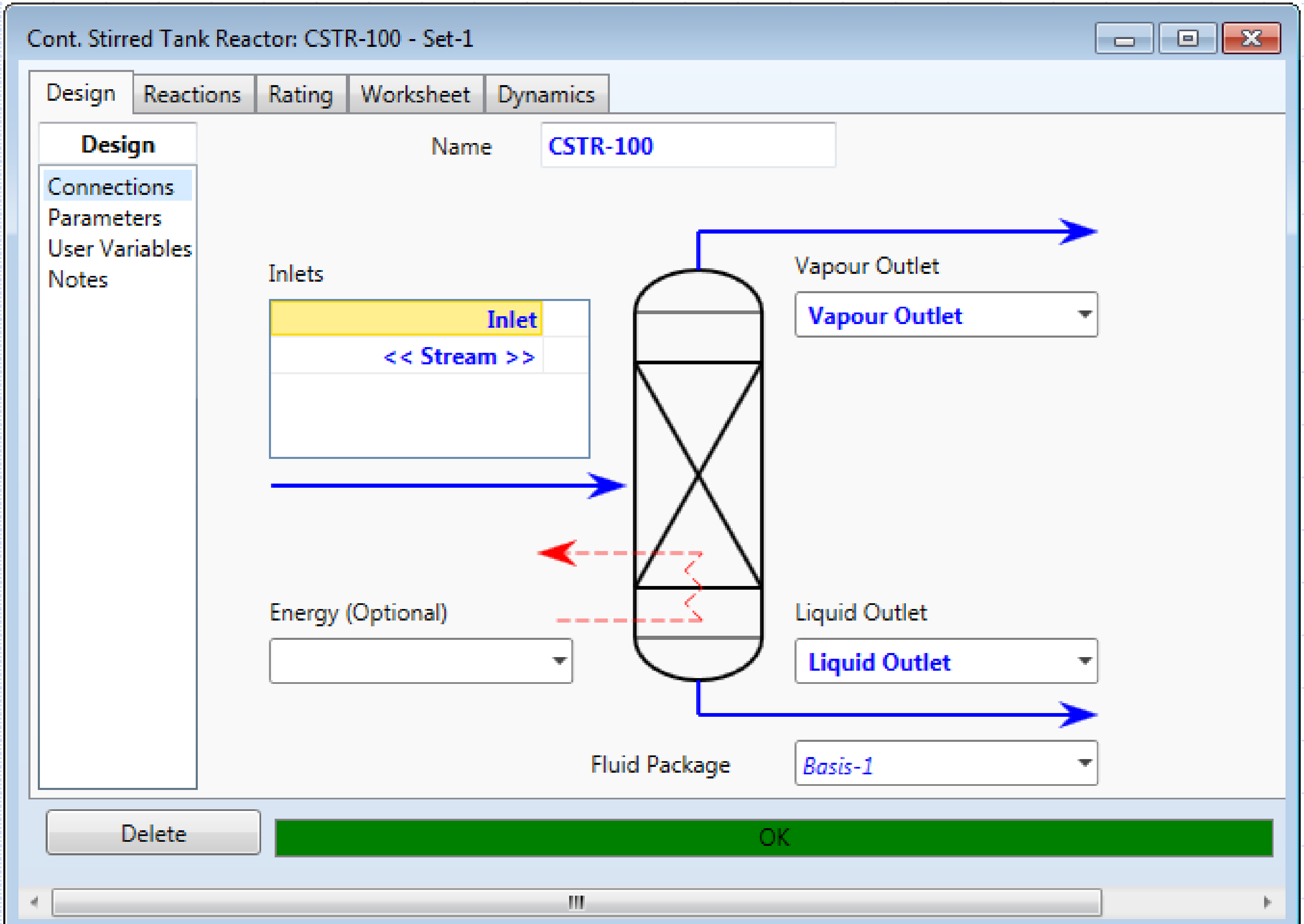
Separation Tower

Microscale Analysis: Separation Tower

Process Engineering Scale

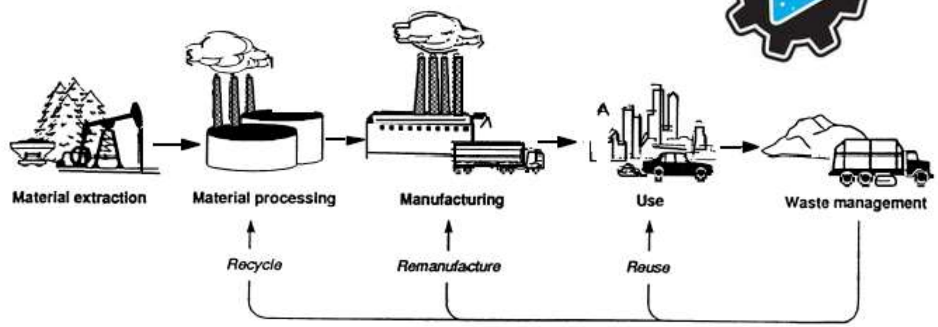


Microscale Analysis: CST reactor

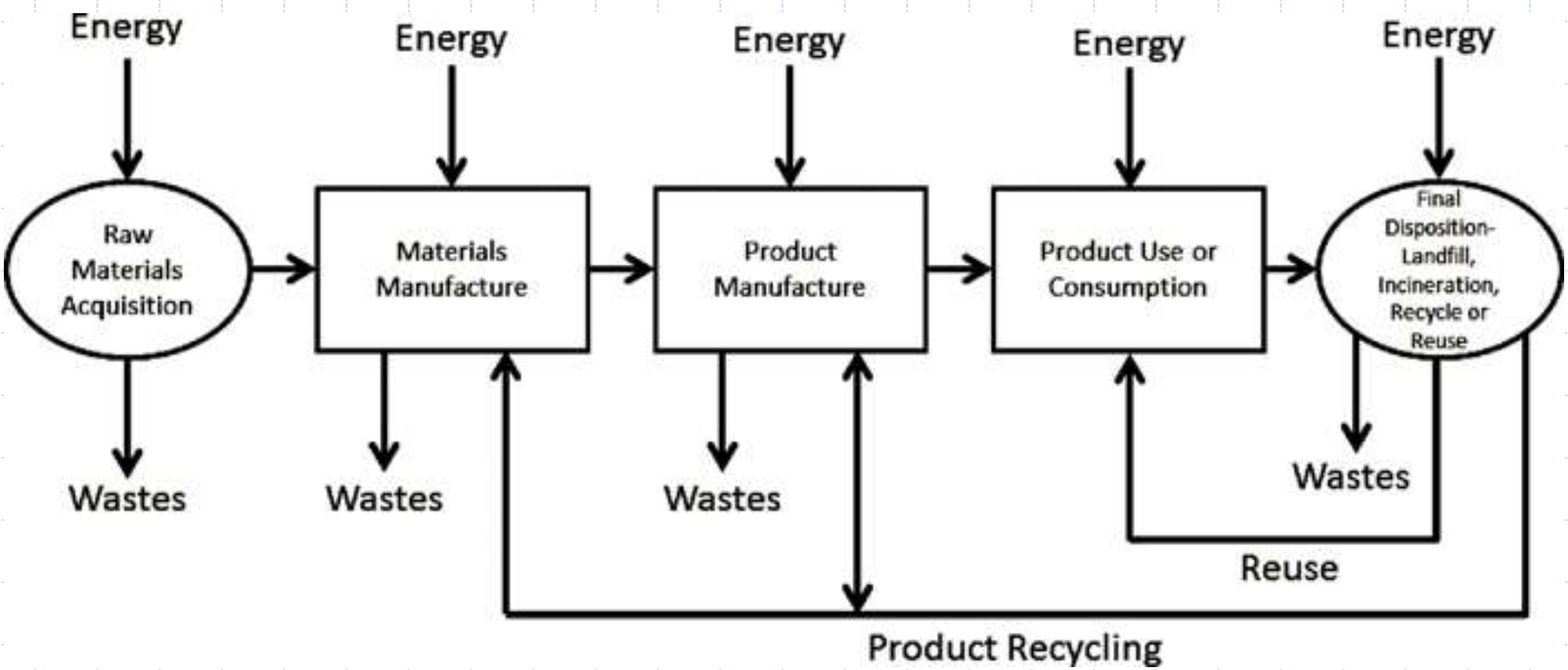


LCA

- Reconsider '**common linear path**'
- Introduce '**disposition pathways**'
  - Reuse
  - Remanufacturing
  - recycling



Stages of life cycle (OTA, 1992)



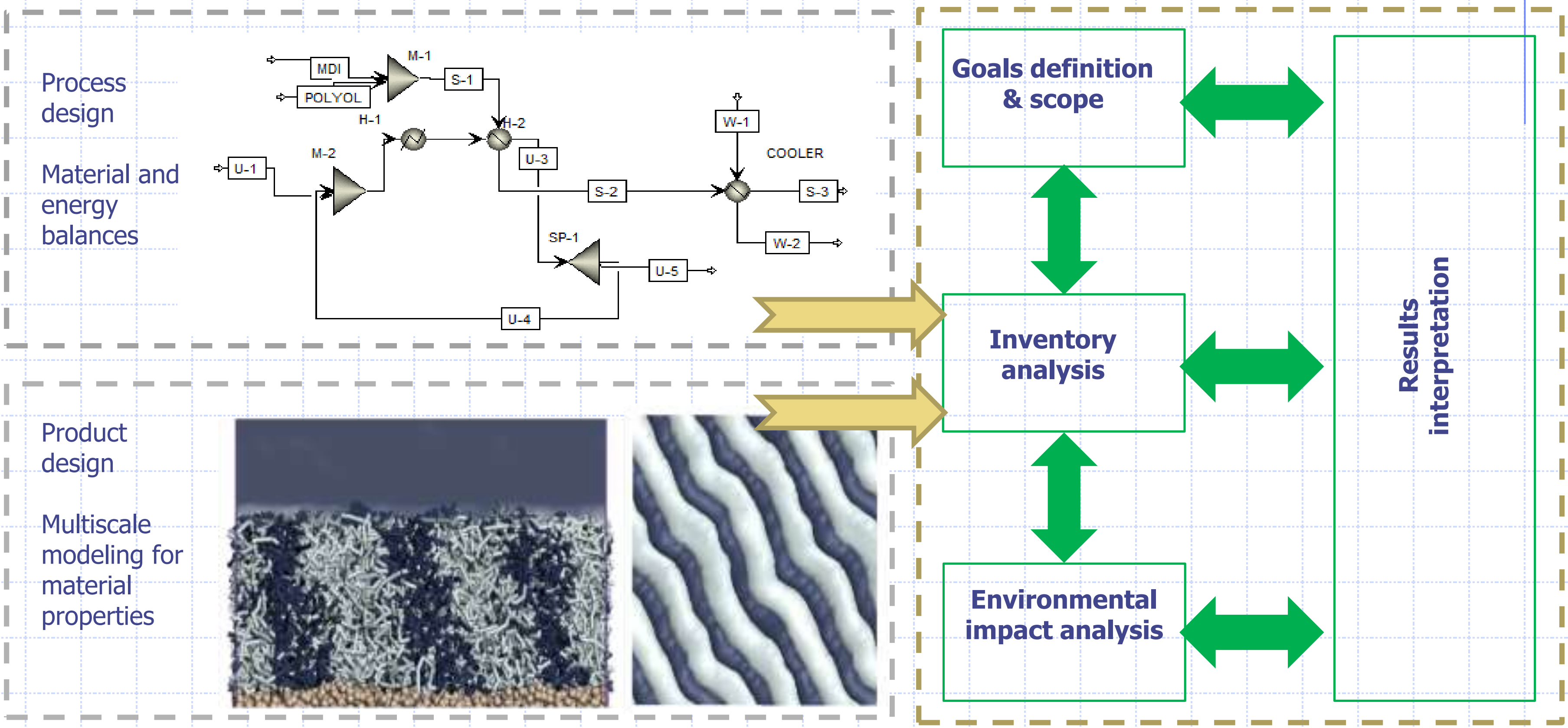
Source: http://read.nxtbook.com/wiley/plasticsengineering/may2014/processengineeringforrecycled.html

Why LCA?

- In “meeting needs of present without compromising our ability to meet future needs”, we are faced with obstacles and complexities
  - Corporate pressure
  - Social pressures
  - Regulatory gaps, overlap and barriers
  - Uncertain objectives/goals
  - Lack of tools to measure progress

- Intuition not a sufficient framework for analysis!
- LCA = systematic and quantitative method for comparing and improving products and policies

Process simulation, multiscale modeling and life cycle assessment



Objectives

- To provide theoretical and applied competences **to set up and solve process design and simulation** using **professional software**, analysis and synthesis.
  - **D1 - Knowledge and understanding skills:** to provide the theoretical expertise required to develop chemical process simulation.
  - **D2 - Ability to apply knowledge and understanding**: to develop complex chemical process simulations using commercial software.
  - **D3 - Autonomy of judgement**: to select the most appropriate strategy to simulate different chemical processes.
  - **D4 - Communicative skills**: to expose, by means of a written, oral and graphical exposition, the results coming from the simulation of a chemical process.
  - **D5 - Learning skills**: to identify the information required for the model adopted and will know how to obtain data from scientific literature databases, manuals and textbooks.

Course program

- Introduction
  - Process simulation motivation
  - Process design principles
- Process simulation fundamentals
  - Degrees of freedom analysis
  - Steady state process simulation
  - Solution of material and energy balances
  - Sequential modular approach and equation oriented approach
  - Introduction to dynamic simulations
  - Cape-Open standard
  - Process simulation perspectives
- Data banks and thermophysical properties
  - Data banks
  - Transport properties
  - Thermodynamic of phase equilibrium: G^E models and equation of state
  - Thermodynamic models: selection criteria and utilization
  - Model selection procedure
- Process simulation software (Aspen+, Coco,…)
  - Basic unit operations: streams, mixer, splitter, separators, pumps, heaters, heat exchangers, …
  - Complex unit operations: reactors, separation columns, liquid-liquid extractors, …
- Use of process simulators
  - Base case, design specifications, sensitivity analysis, optimization.
  - Energy analysis and optimization: pinch technology (hints)
  - Economic analysis (hints)
- Hands on process simulators Aspen+ and Coco

Teaching methodology

- Classroom lectures, demo and hands-on sessions on process simulators usage.
  - PPT slides available in MOODLE: https://moodle2.units.it//
  - Class exercises: process simulation projects to be done in class
  - Home work: process simulation projects to be done in autonomy
- Timetable
  - Tuesday 18-20
  - Thursday 17-20
- Demo of user interface of commercial SW
  - Aspen Properties
  - Aspen plus steady state
  - COCO
- Hands on (hybrid mode)
  - Simulation environment set up
  - Thermodynamics, physical properties and phase equilibria
  - Unit operations
  - Simulation and optimization of chemical processes

Text books

- Haydary J., Chemical Process Design and Simulation: Aspen Plus and Aspen Hysys Applications, Wiley, New York (2019)
- Turton R., Shaeiwitz J.A., Bhattacharyya D., Whiting W.B., Analysis, Synthesis and Design of Chemical Processes. Pearson Education International (2018), 5th Ed.
- W.D. Seider, D.R. Lewin, J. D. Seader, S. Widagdo, R. Gani, Ka Ming Ng, Product and Process Design Principles: Synthesis, Analysis and Evaluation, (2016) 4th Edition
- Aspen+ manuals
- Super Pro manuals
- COCO-COFE manuals

Exam methodology

- Home works (process simulation projects)
  - Assigned in class, in some cases continuation of exercises started in class
  - To be sent BEFORE a given deadline (weekly) via email; in case of unjustified delay the exercise is not considered in the evaluation
- Exam (at the end of the course)
  - Team work on the simulation of a given process
  - To be presented as a team …
  - … in a professional way.