# Modelling and Simulation for Evaluation of Biorefinery Processes:

# Experience at gISQP

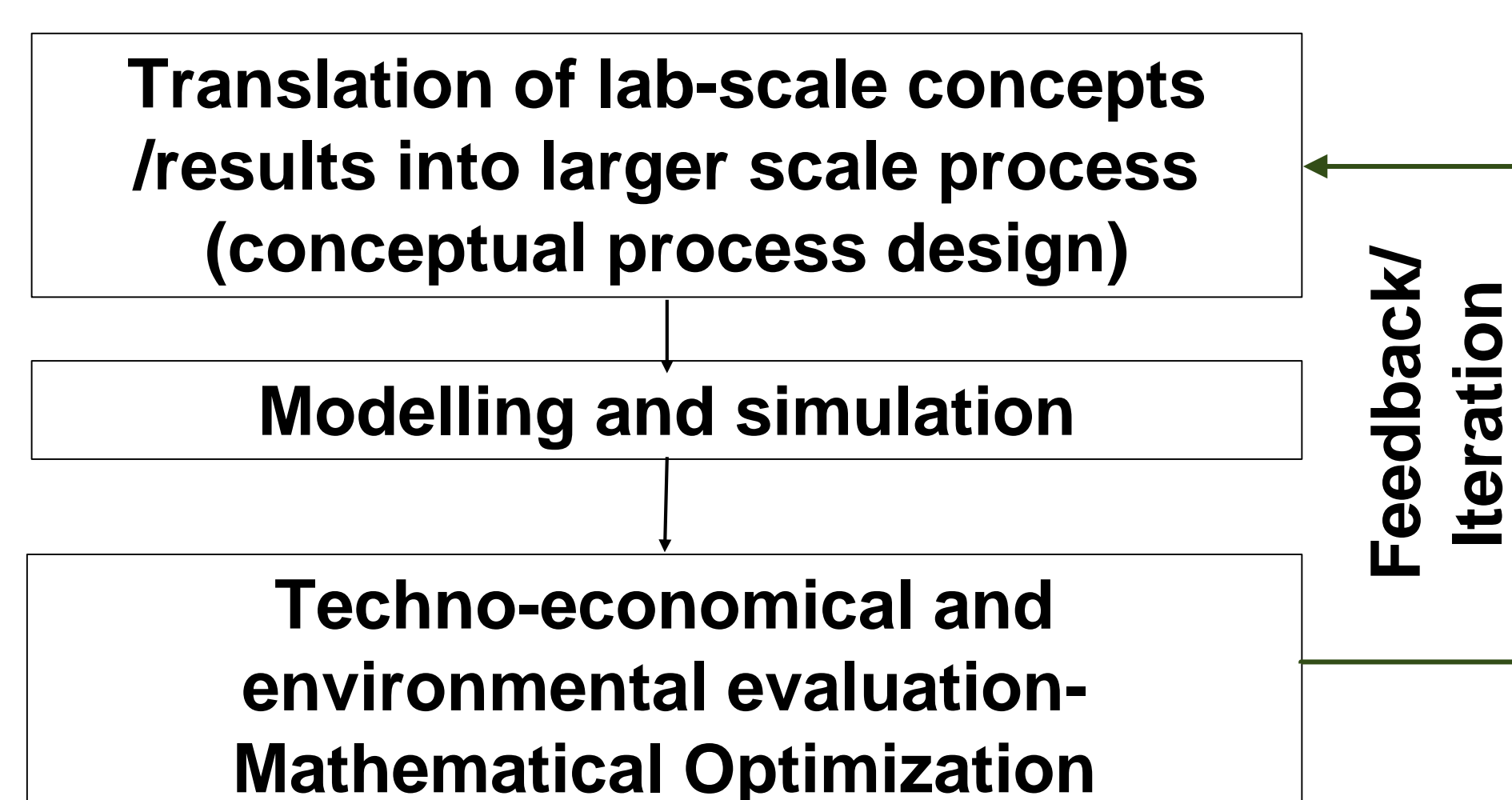## A. I. Torres, J. Ferreira, R. Kreimerman, C. Philippi, P. Ures, S. Gutiérrez

[a] grupo de Ingeniería de Sistemas Químicos y de Procesos – Instituto de Ingeniería Química – Facultad de Ingeniería – Universidad de la República
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## INTRODUCTION

- ▶ **Which products should a biorefinery produce?**
- ▶ **From which biomass?**
- ▶ **Which technologies should be used?**
- ▶ **Which are the production costs?**
- ▶ **Which are the bottlenecks?**

**FINDING ANSWERS TO THESE AND RELATED QUESTIONS IS THE CORE OF OUR RESEARCH AT gISQP**

▶ General methodology:

Translation of lab-scale concepts /results into larger scale process (conceptual process design)

Modelling and simulation

Techno-economical and environmental evaluation- Mathematical Optimization

Feedback/ Iteration

▶ Several levels of analysis:
- ▶ Unit operations
- ▶ Individual Processes
- ▶ Multi-product plants
- ▶ Networks of Processes/ Plants

## DYNAMIC SIMULATION OF EVAPORATORS FOR THEIR APPLICATION IN BIOREFINERIES (JF)
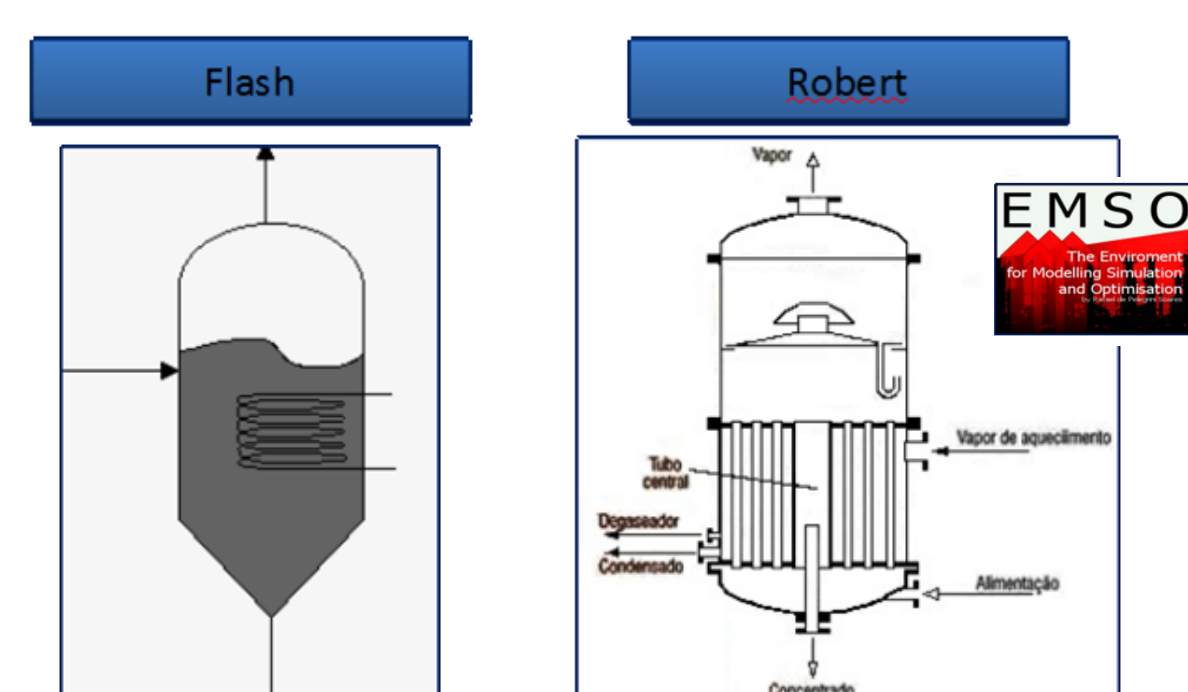
▶ **Background:** Level: Unit Operations

This work is part of a program whose goal is to model all the operations within sugarcane bagasse biorefineries

▶ **Objective:**

To develop a rigorous dynamic model for the operation of a real multi-effect evaporator

▶ **Methodology:**

- **Development and implementation of dynamic models for the operation of various evaporators in an EO software (EMSO)**
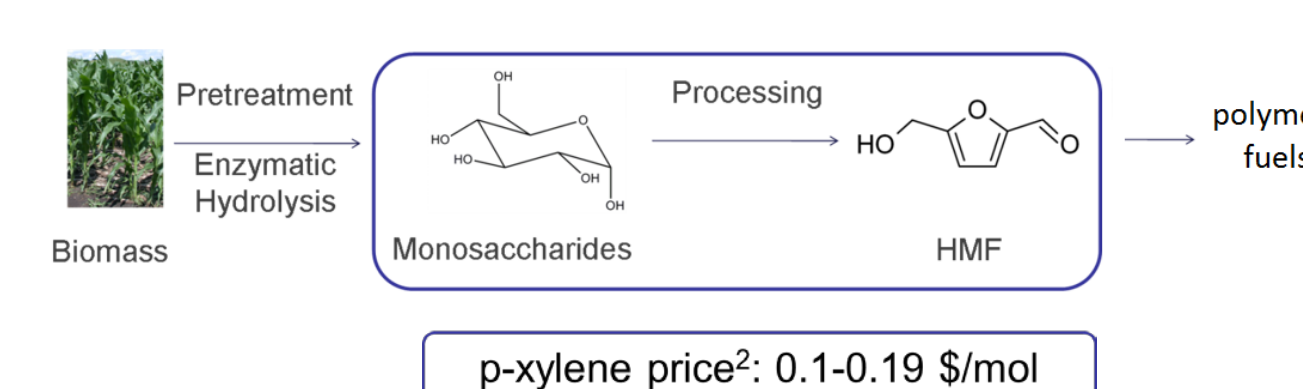- **Validation of the results against experimental data**



## DESIGN AND OPTIMIZATION OF PROCESSES FOR THE PRODUCTION OF 5-HMF FROM BIOMASS BASED SUGARS (AIT)

▶ **Background:** Level: Process Design

5-HMF is a furanic building block, it can replace p-xylene in the production of polymers



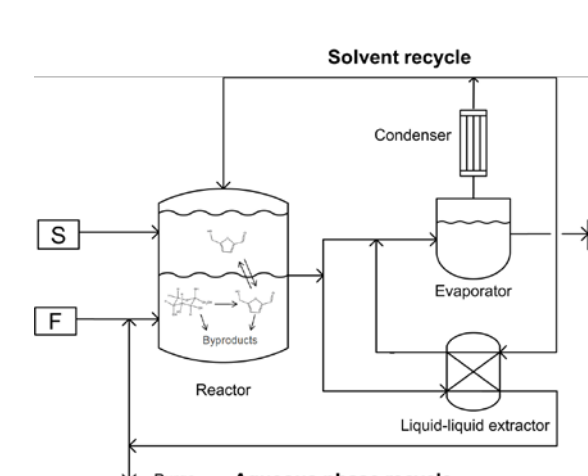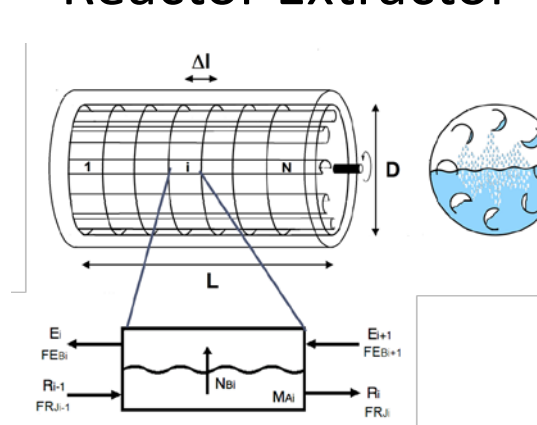p-xylene price[2]: 0.1-0.19 $/mol

▶ **Objective:**

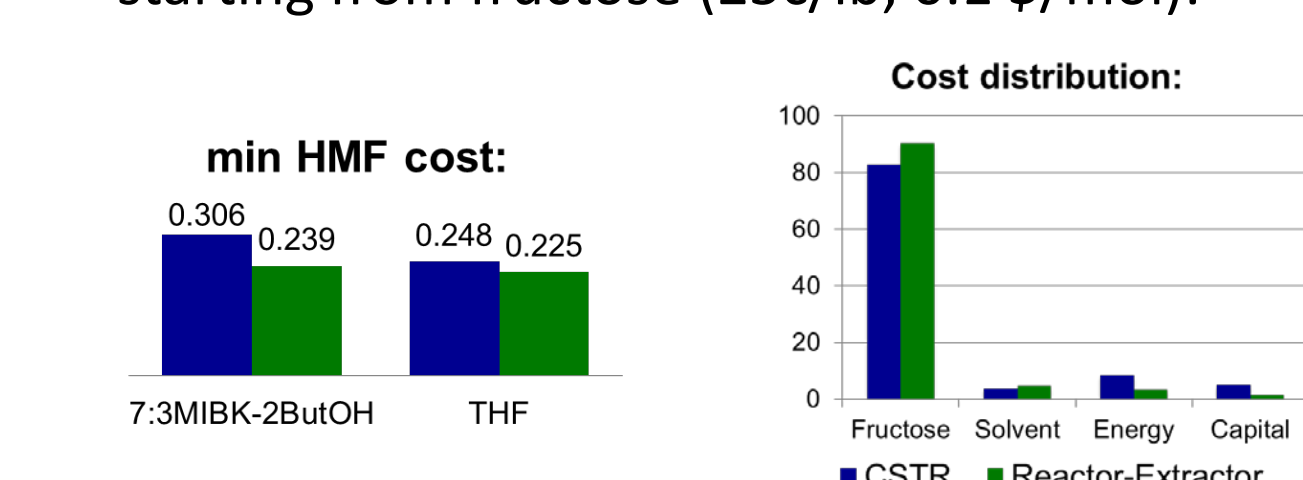Estimate minimum selling price for different processes

▶ **Results:**

CSTR-based process   Substitute CSTR for Reactor Extractor

- Simulations run for different extracting solvents, starting from fructose (25c/lb; 0.1 $/mol):

min HMF cost:   Cost distribution:

0.306  0.239    0.248  0.225

7:3MIBK-2ButOH   THF

Fructose  Solvent  Energy  Capital

CSTR   Reactor-Extractor



## DEVELOPMENT OF A MATHEMATICAL FRAMEWORK FOR THE DESIGN OF OPTIMAL MULTI-ACTOR BIOREFINERIES (AIT)

▶ **Background:** Level: Networks of processes

Akin to oil refineries conversion of biomass to fuels and chemicals is prone to be carried out by several actors
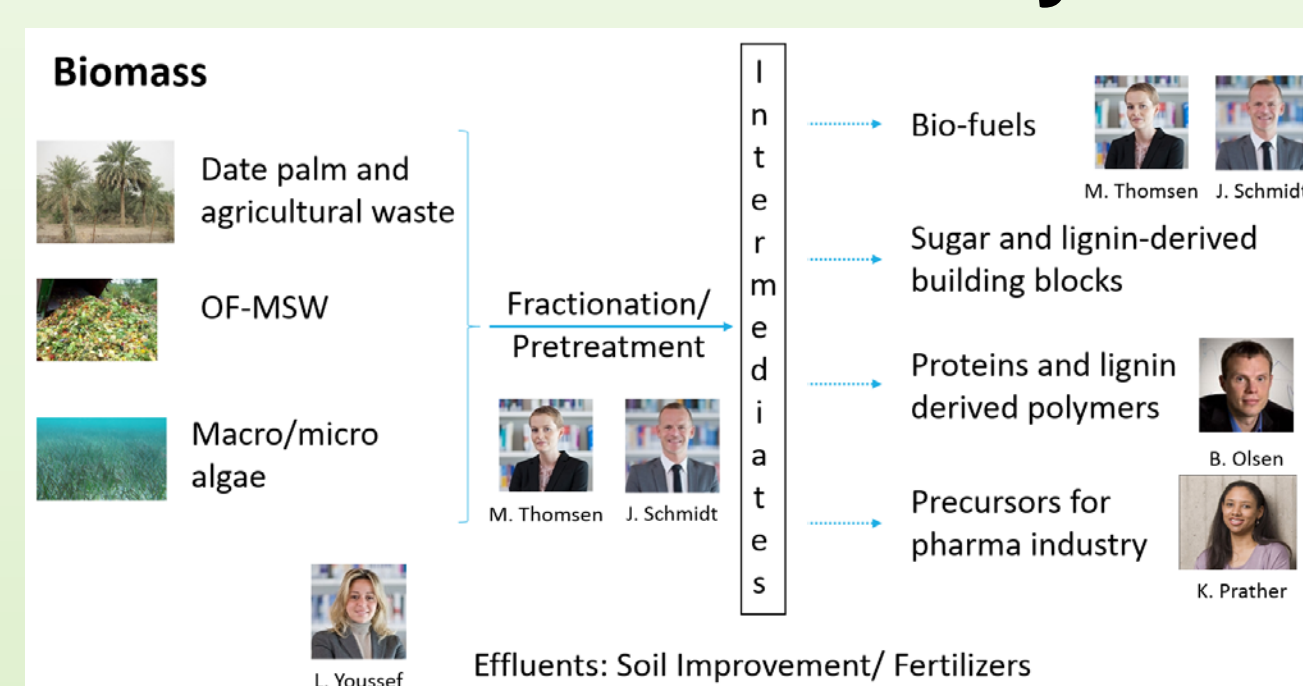
▶ **Objective:**

Develop a framework that guarantees network optimality as well as individual actor´s optimality

▶ **Methodology:**

- **Identify intermediates and actors (suppliers/ consumers)**
- **Each actor develops and optimizes its process**
- **Optimal network: Two-level Lagrangian approach**

▶ **Masdar-MIT biorefinery**



## TECHNO-ECONOMIC ANALYSIS OF BIOREFINERIES BASED ON AGROINDUSTRIAL AND FORESTRY RESIDUES (SG)

▶ **Objective:** Level: Multi-product plant design

Analyze viability of different biomass conversion technologies developed at Instituto de Materiales de Misiones

▶ **Methodology:**
- **Propose alternative raw material-technology-products scenarios**
- **Evaluate NPV and IRR**
- **Rank scenarios**

▶ **Other scenarios:**
- **Sugarcane bagasse to ethanol and or pellets**
- **Pine and Eucalyptus dust as RM**

▶ **Example: Sugarcane bagasse biorefinery**
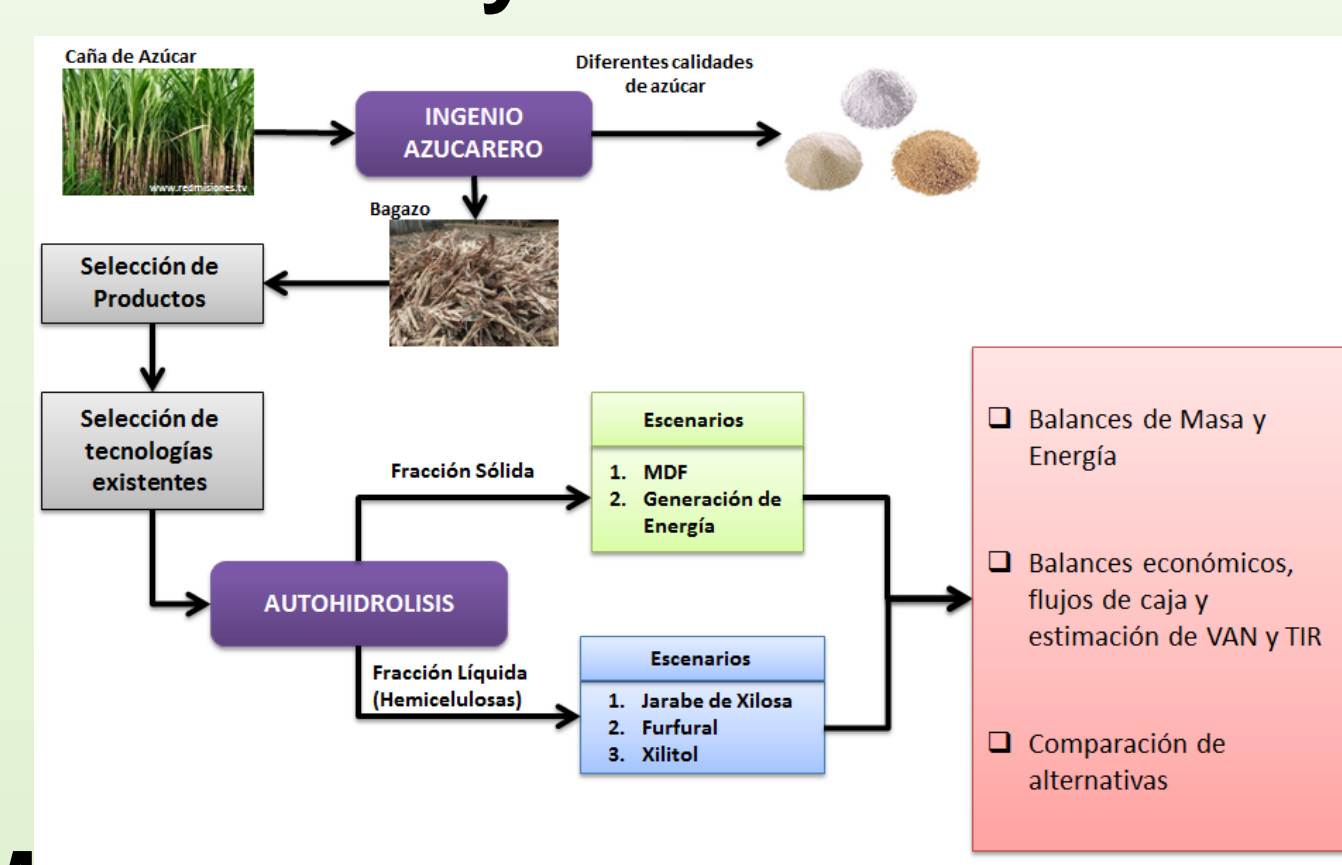


## BIOREFINERIES IN URUGUAY: TECHNOECONOMIC EVALUATION OF THE PRODUCTION OF BIOMASS BASED FUELS AND CHEMICALS FROM LOCAL FEEDSTOCKS ANII-FSE 1_2015_1_109976 (PI: AIT, co PI: SG, Consultant: RK, Researchers: CP, PU)

▶ **Background:**

Due its agricultural based economy, and lack of proven fossil fuels reserves, exploitation of biomass based resources for the production of fuels and chemicals is key for Uruguay´s development.

▶ **Objective:**

To develop a *systematic framework* for the analysis of biomass based products and technologies for their production

▶ **Within the project we aim to:**

- **Analyze possible raw materials (quantities, geographical distribution, chemical composition)**
- **Create an Aspen Plus database with models for a selection of the RM**
- **Propose evaluation criteria to screen possible candidate products**

- **Construct a repository of Aspen Plus models of RM- final product technologies**
- **Develop a mathematical programming code for the selection of optimal RM-technology-product pathways**