BIOpt: A library of models for optimization of biofuel production processes

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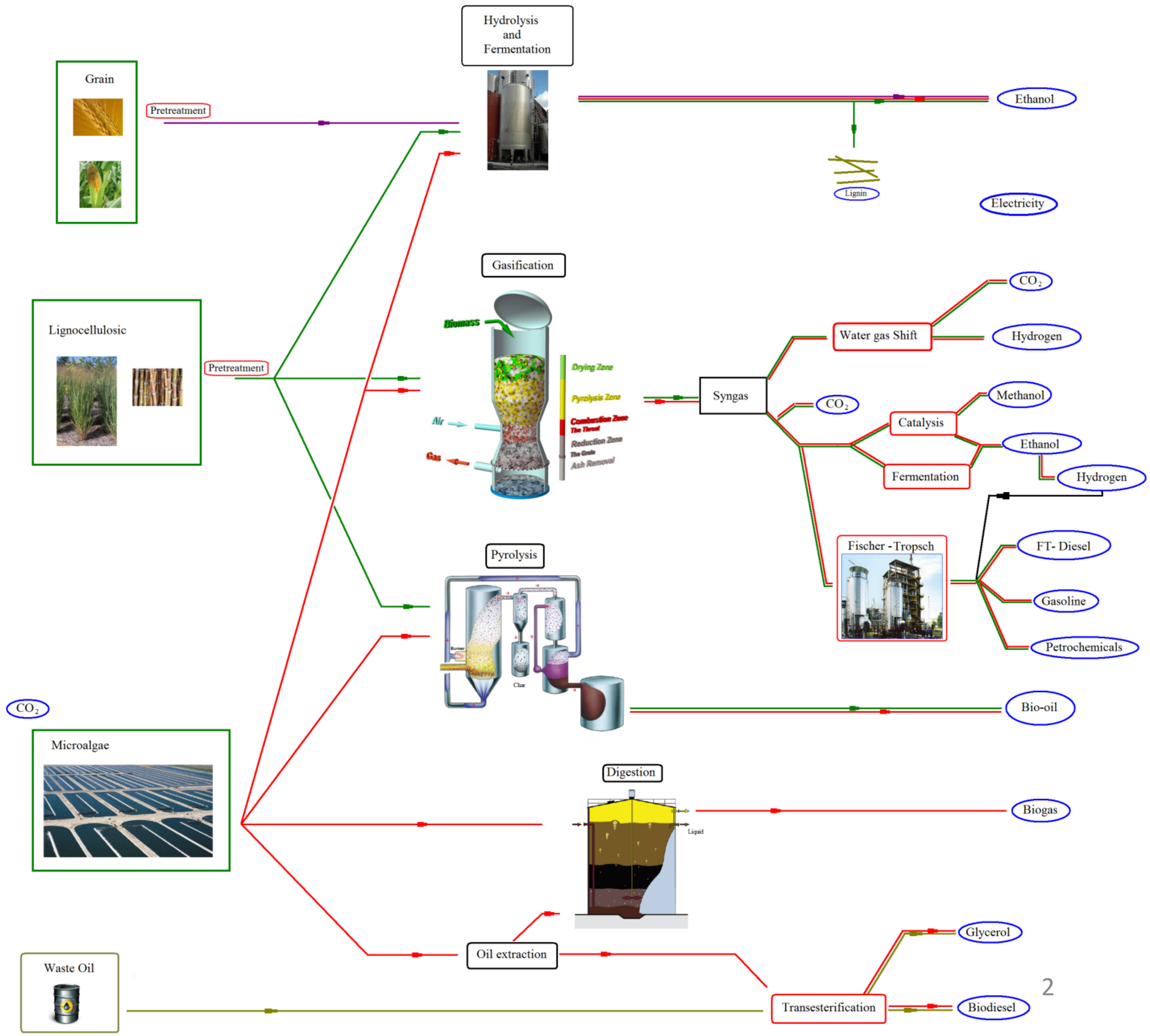
Introduction

We use mathematical programming techniques to accomplish the synthesis of the production of:

bioethanol, FT-diesel and hydrogen, from Switchgrass,

biodiesel from cooking oil or algae oil.



Approach

0.- Identify the alternative technologies (HUGE LITERATURE REVIEW)

1.- Develop special purpose models for the different units.

2.-Model the whole process: Superstructure

3.-Decide on the objective function

Cost, energy, environmental concerns (LCA)

4.-Propose solution strategy

5.-Evaluate the results.

Sensitivity analysis

Features and Models

Exothermic fermentation reactions that operate at low temperature and are not a source of heat as in traditional petrochemical plants.

Tend to require a **large amount of water or large energy demand** in distillation columns for separating highly diluted mixtures.

There is usually **lack of good understanding** of the biochemical reactors, pretreatments, etc. due to the presence of complex mixtures, lack of experimental information, and no commercial simulator has these units.

Models

1.- Short-cut

2.- Dimensional Analysis

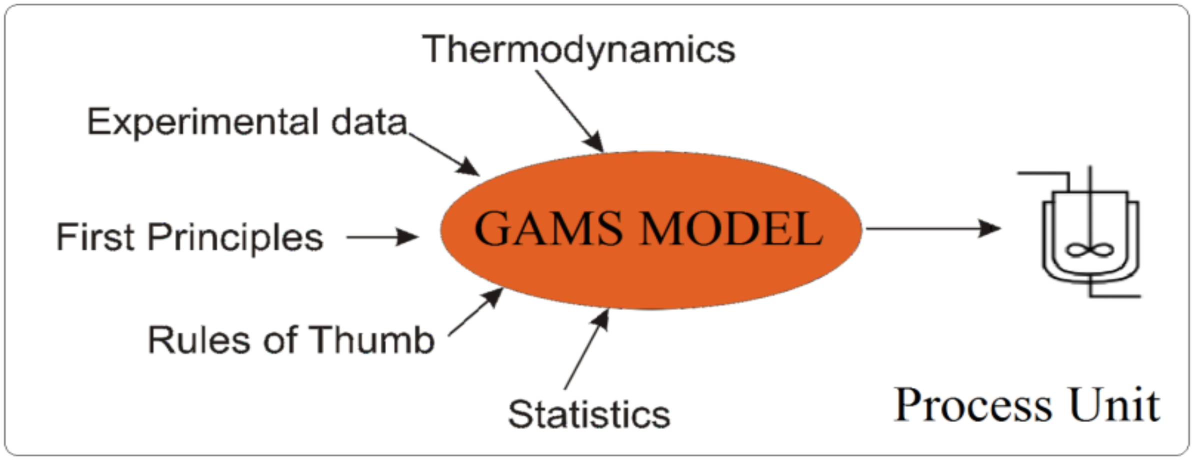
3.- Rules of Thumb

4.- Design of experiments

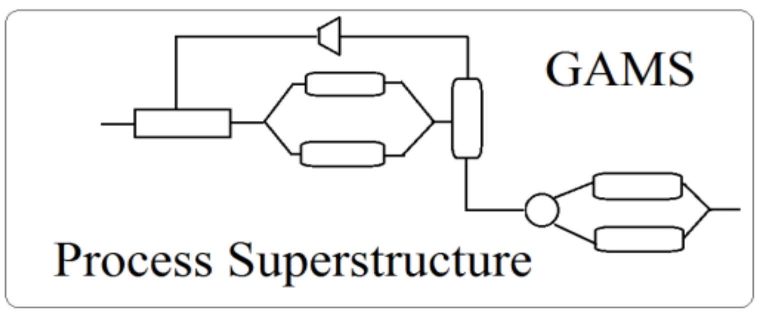
5.- Correlations

6.-Mechanistic modeling

Model the whole process: Superstructure



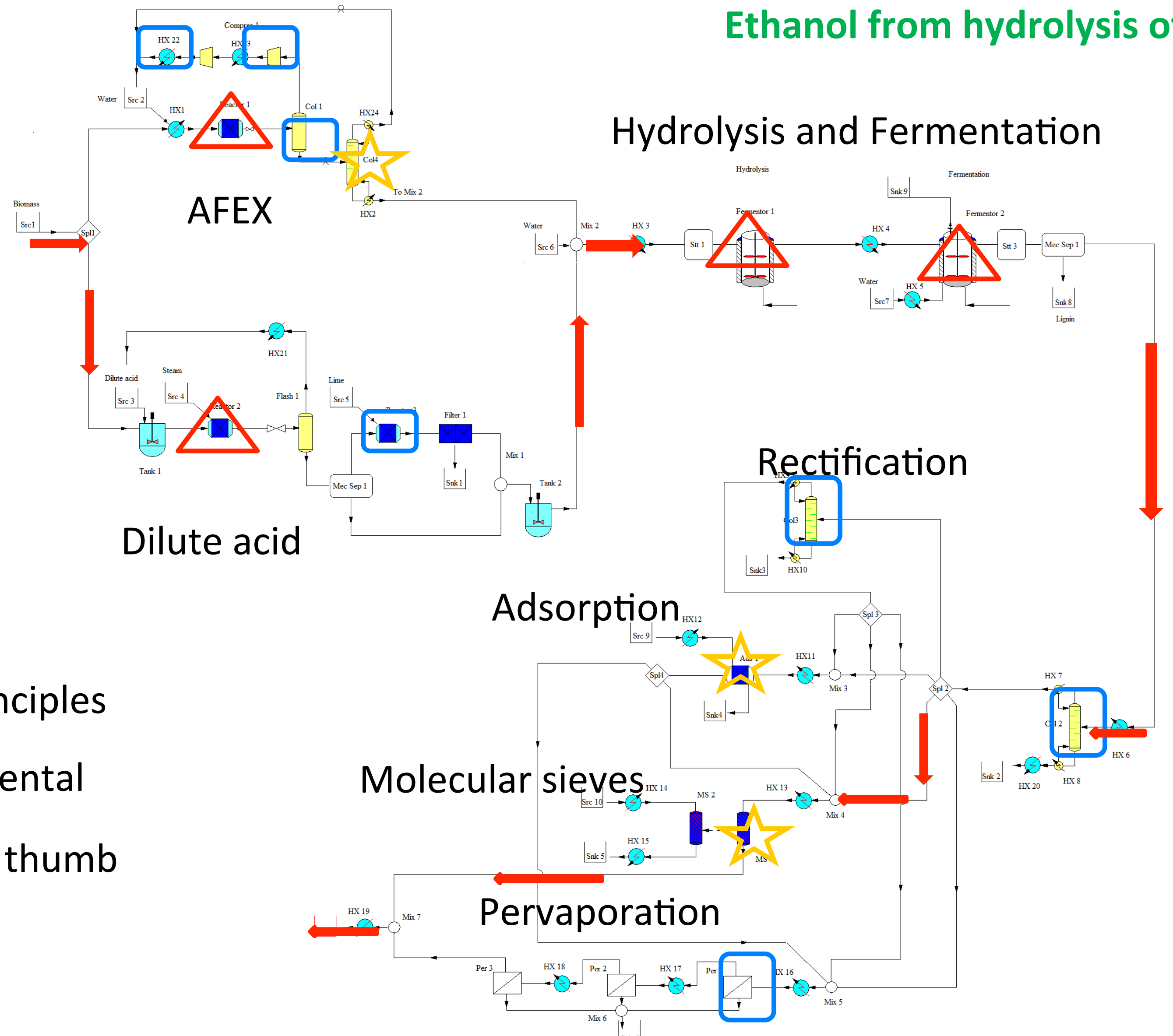
x N



Decide on the objective function

Results

Ethanol from hydrolysis of Switchgrass

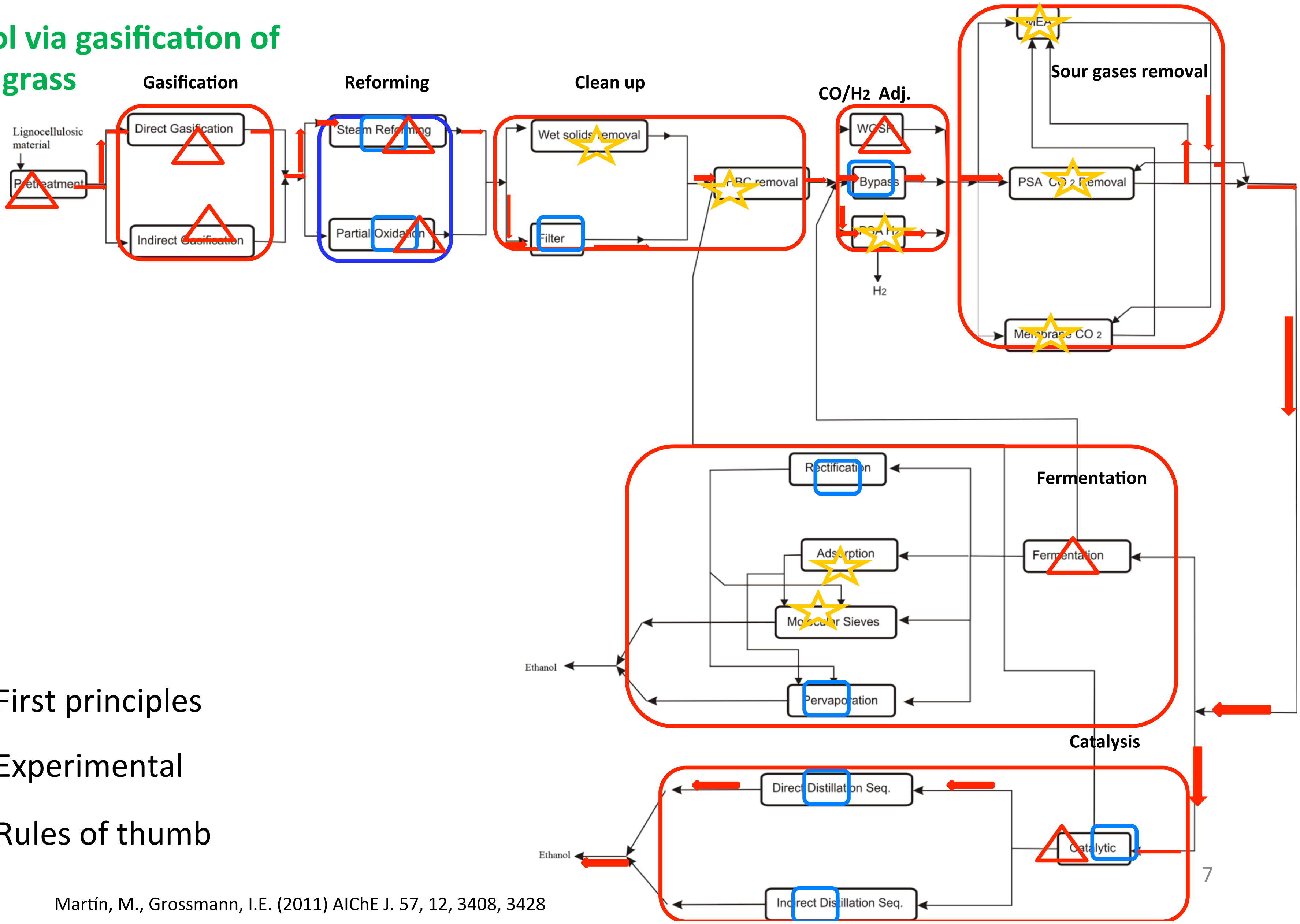


- First principles
- Experimental
- Rules of thumb

Martín, M., Grossmann, I.E. (2012) AIChE J 8 (5) 1538-1549

Results

Ethanol via gasification of Switchgrass



First principles

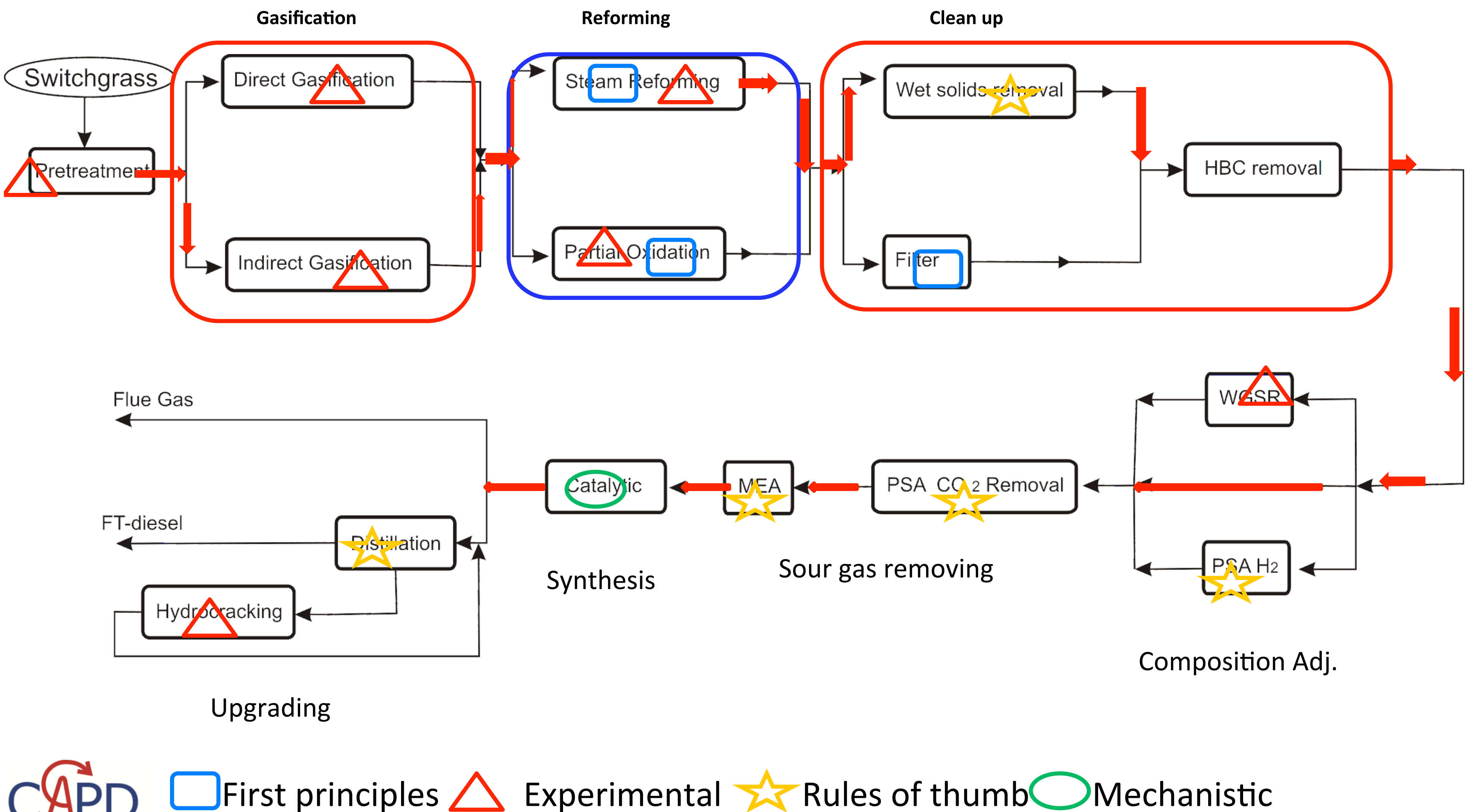
Experimental

Rules of thumb

Martín, M., Grossmann, I.E. (2011) AIChE J. 57, 12, 3408, 3428

Results

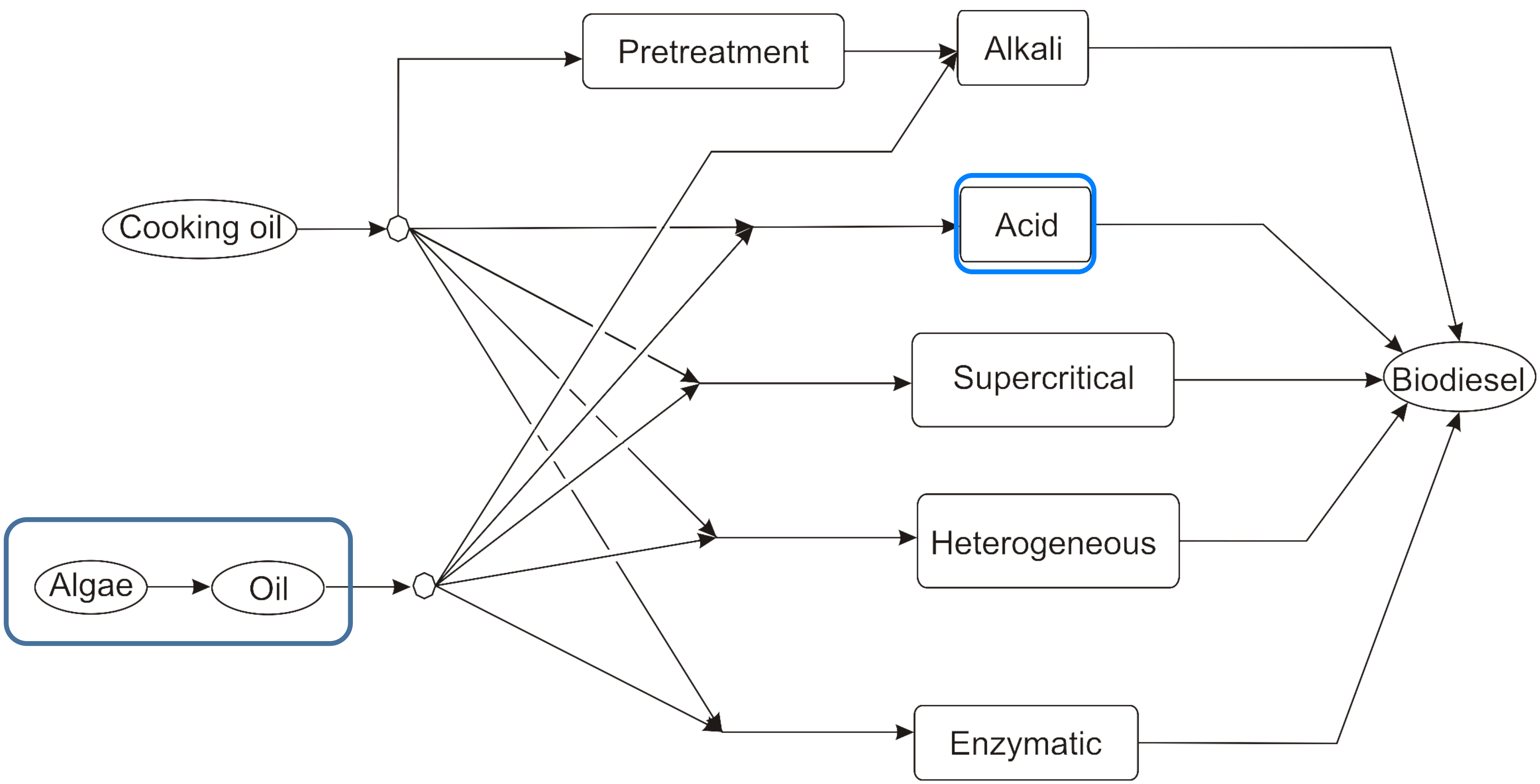
FT Diesel via gasification of Switchgrass



Martín, M., Grossmann,I.E (2011) Ind. Eng. Chem Res, *50* (23),13485–13499

Results

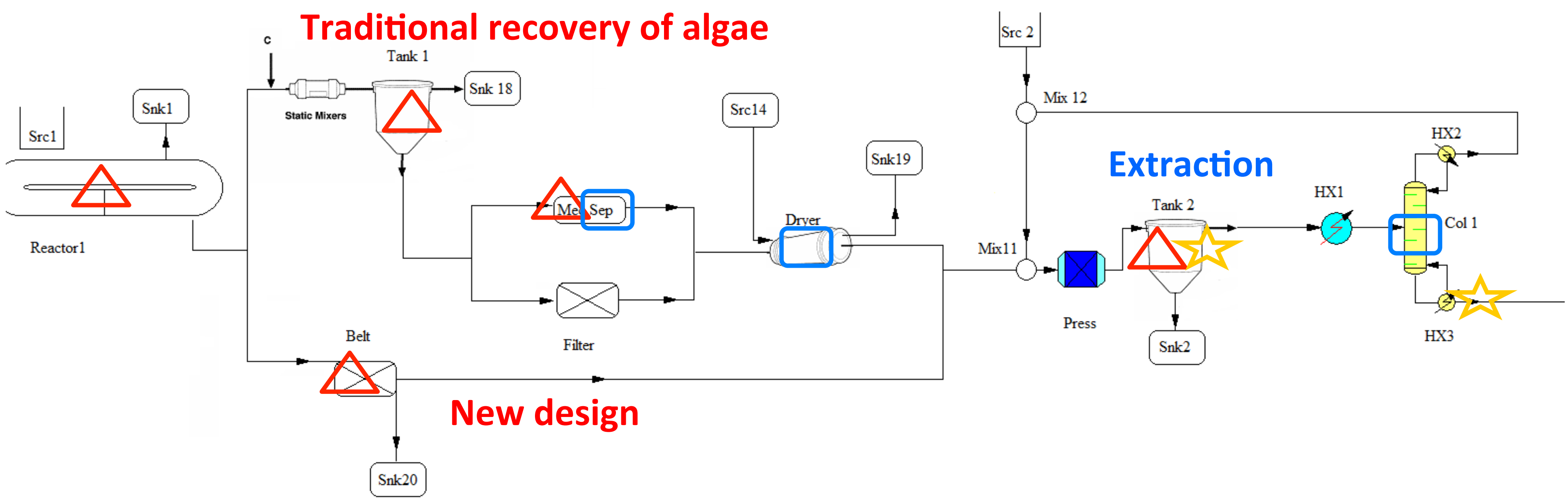
Superstructure flowsheet for the production of biodiesel



Martín, M., Grossmann, I.E. I&EC DOI. 10.1021/ie2024596

Results

Production of biodiesel from algae



First principles Mechanistic Experimental Rules of thumb

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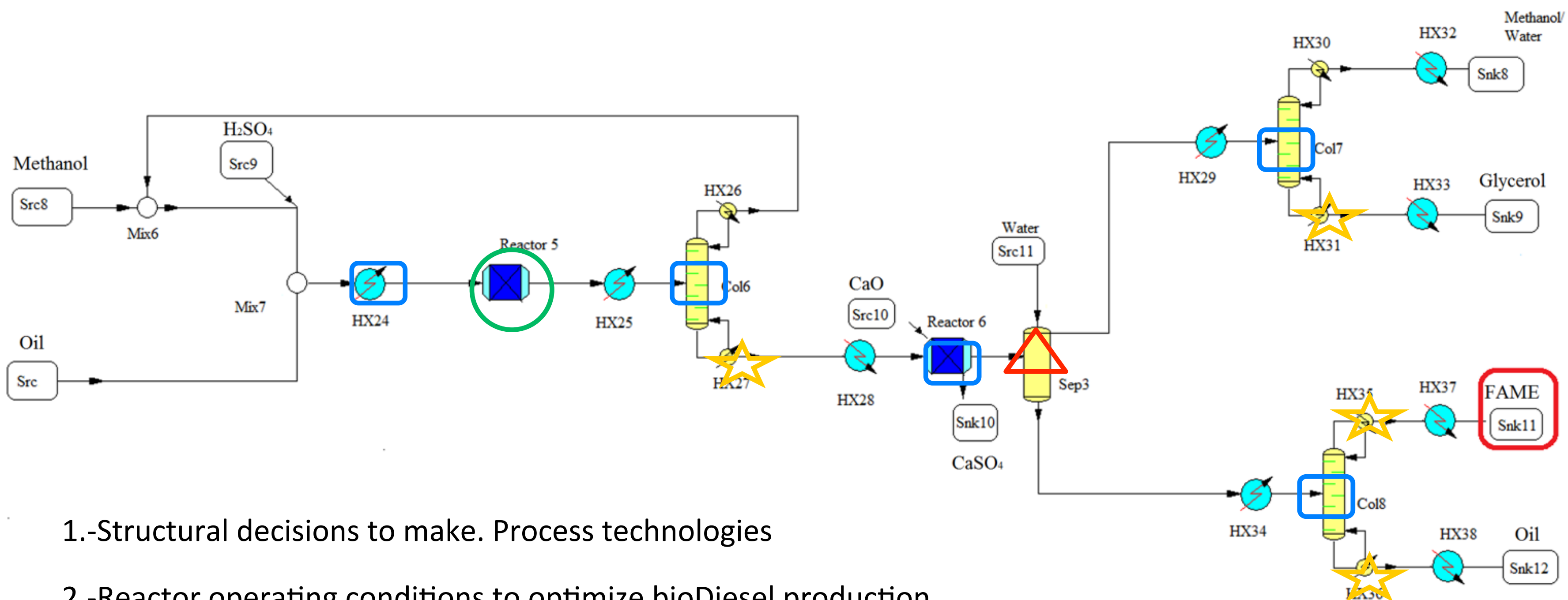
Results

Production of biodiesel



1.-Structural decisions to make. Process technologies

2.-Reactor operating conditions to optimize bioDiesel production

3.-Recycle of excess of methanol

Simultaneous optimization and heat integration of the process

First principles Experimental Rules of thumb DOE

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Summary of Results

	Ethanol (Hydrolysis)	Ethanol (Gasification & Catalysis)	Ethanol (Gasification & Fermentation)	FT-Diesel	H_2	Biodiesel (Cooking)	Biodiesel (Algae)
Total investment ($MM)	169	335	260	216	148	17	110
Capacity(MMgal/yr)	60	60	60	60	60*	72	69
Biofuel yield (kg/kg_{wet})	0.28	0.20	0.33	0.24	0.11	0.96	0.48
Production cost ($/gal)	0.80	0.41	0.81	0.72	0.68*	0.66	0.42
Water consumption(gal/gal)	1.66	0.36	1.59	0.15	--	0.33	0.60
Energy consump. (MJ/gal)	-10.2	-9.5	27.2	-62.0	-3.84*	1.94	1.94
ROI (%)	44.91	26.15	29.08	36.25	16.86	565.4	91.27
PayOut (yr)	1.02	1.66	1.51	1.24	2.40	0.09	0.52
Byproduct	Energy CO_2	Hydrogen Mix alcohols Energy CO_2	Hydrogen CO_2	Green Gasoline Energy CO_2	Energy CO_2	Glycerol	Glycerol Fertilizer

(*) For Hydrogen instead of gal, kg is used

Conclusions

--Mathematical programming techniques offer a powerful tool to synthesize bioprocesses to make them economically attractive and environmentally friendly.

--Biomass and waste are promising raw material for biofuels.

--The range of biofuels is broad: hydrogen, bioethanol, biodiesel, green gasoline and diesel, biomethanol....

--It is feasible to produce second generation of biofuels but further development is required in purification and reaction technologies to increase water recycle and reuse and increase the yield of the processes.