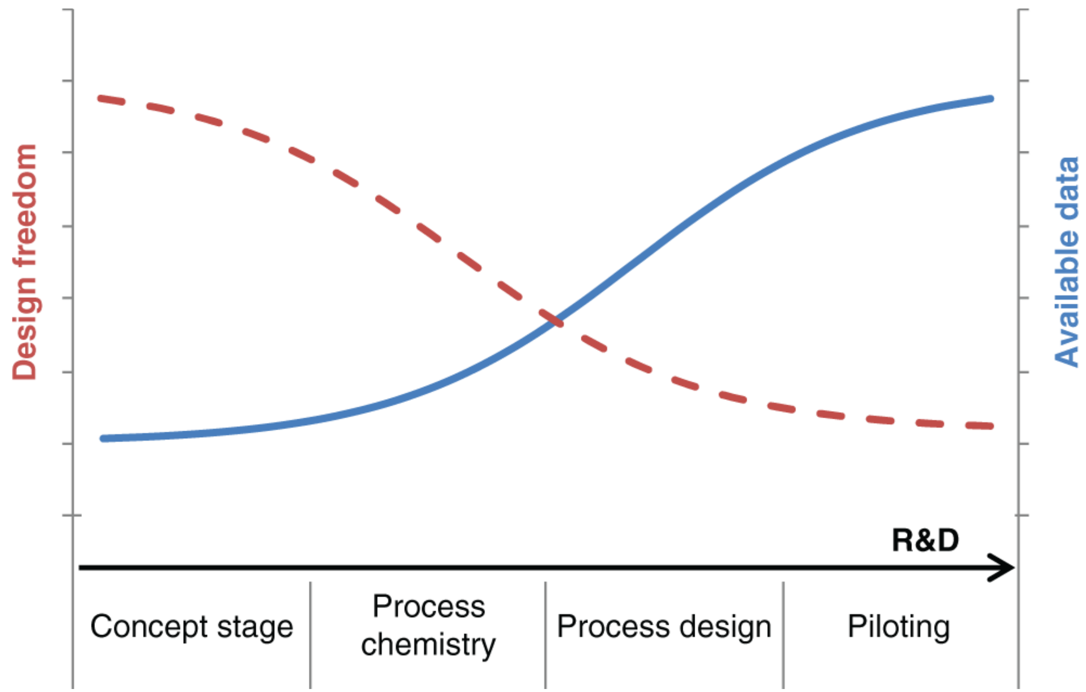
Key challenges for the economic and environmental evaluation of large biorefinery concepts

Prof. dr. Andrea Ramirez
Chair on Low Carbon Systems and Technologies
Delft University of Technology
c.a.ramirezramirez@tudelft.nl

TU Delft

The Challenge for ex-ante assessment



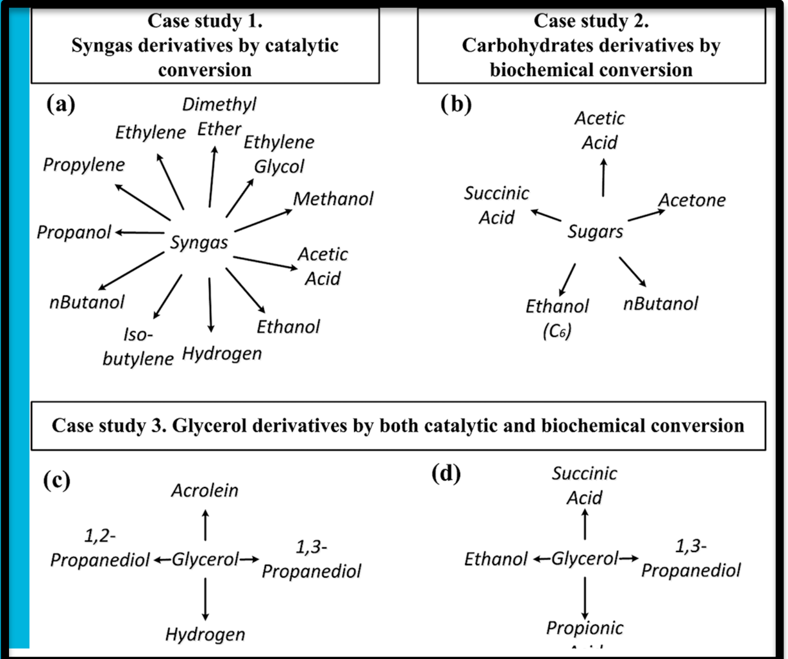
Source: Broeren et al., 2017

To provide useful information to technology developers and policy makers with limited information

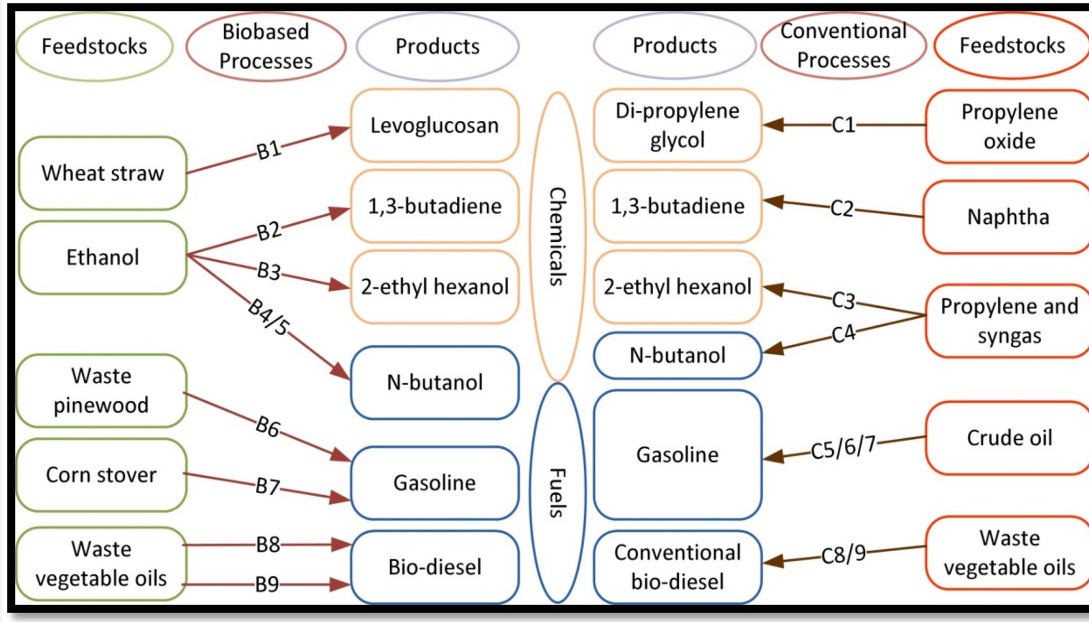
Types of ex-ante assessments

1 Screening studies

- Many technologies/configurations to be assessed
- Aim to identify significant differences (order of magnitude)- which ones could be potential winners?
- Limited time and resources
- High level of uncertainty: no necessarily a problem
- Multi-criteria approach

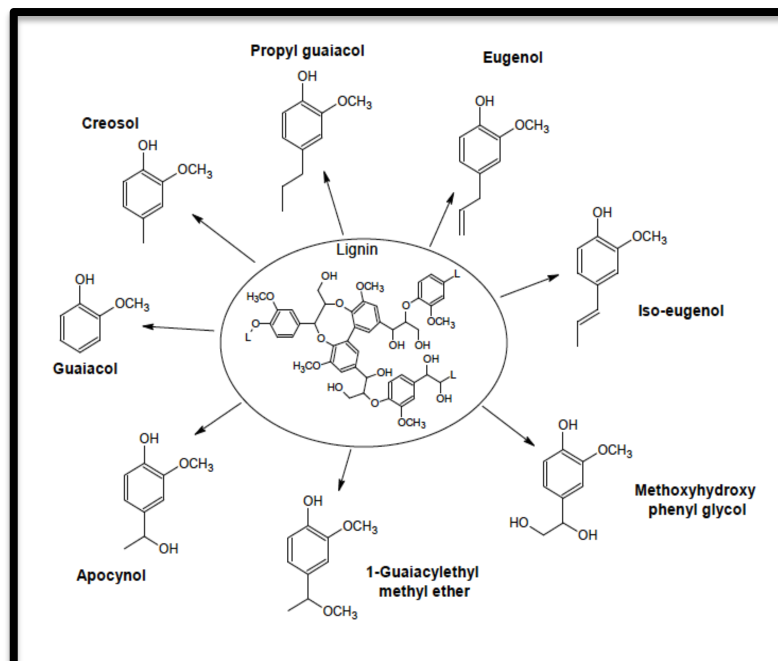


Moncada et al., Early-stage comparative sustainability assessment for potential configurations of intergrated biorefineries. Screening of biobased derivative from platform chemicals. Biofuels, bioproducts and biorefining 9, 6 (2015), 722-748



Patel et al., Early-stage comparative sustainability assessment of novel biobased processes, ChemSusChem, 2013, 6 (9), 1724-1736

Holladay et al., Top value added chemicals from biomass. Results of screening for potential candidates from biorefinery lignin, PNNL-16983, 2007



Overview of methods for env. ex-ante analysis biobased chemicals (source: Broeren et al., 2017)

Category	Method name/reference	Objective/description[a]	Indicators[b]	Life cycle scope	R&D phase(s)	Made for bio-based
Full assessment	PEF[29]	Product Environmental Footprint	14	Cradle-to- grave	N.a.	No
	ILCD[30]	International Life Cycle Data system handbook	13	Cradle-to- grave	N.a.	No
	Prosuite[31]	Prospective sustainability assessment of technologies	24	Cradle-to- grave	N.a.	No
	WBCSD[32]	Life cycle metrics for chemical products	22	Cradle-to- grave	N.a.	No
	BASF Eco-efficiency[33]	Eco-efficiency analysis	10	Cradle-to-grave	N.a.	No
	S2BIOM[34]	Life-cycle based environmental sustainability assessment of non-food bio-mass value chains	14	Cradle-to- grave	N.a.	Yes
Early-stage assessment – Multi-indicator	Sugiyama *et al.*[9]	Decision framework for chemical process design including environmental, health and safety assessment	4	Mixed	Concept–Process design	No
	EcoScale[6]	Semi-quantitative tool to select an organic preparation based on economic and ecological parameters	4	Gate-to-gate	Process chemistry	No
	Patel *et al.*[7]	Sustainability assessment of novel chemical processes at early stage	4	Mixed	Process chemistry	No
	GSK FLASC[35]	Fast Life Cycle Assessment of Synthetic Chemistry	8	Cradle-to-gate	Process chemistry	No
	Sheldon/Sanders[8]	Concise metrics for the production of chemicals from renewable biomass	3	Mixed	Process chemistry	Yes
	Cabezas *et al.*[36]	Pollution prevention with chemical process simulators	9	Gate-to-gate	Process design	No
	Young/Cabezas[37]	Designing sustainable processes with simulation	8	Gate-to-gate[c]	Process design	No
	Chen *et al.*[38]	Design guidance for chemical processes using environmental and economic assessments	9	Cradle-to-gate[d]	Process design	No
	Schwarz *et al.*[39]	Sustainability metrics to guide decision-making	10	Gate-to-gate	Process design	No
	Tugnoli *et al.*[40]	Quantitative sustainability assessment in the early stages of process design	16	Gate-to-gate	Process design	No
	Tabone *et al.*[41]	Sustainability metrics	11	Mixed	Process design	No
Early-stage assessment – Single-indicator	Atom economy[42]	Molecular weight of product / molecular weight of reactants	1	Gate-to-gate	Concept	No
	Reaction mass efficiency[43]	Mass of isolated product / total mass of reactants used	1	Gate-to-gate	Concept	No
	Mass intensity[44]	Total mass used in a process / mass of product	1	Gate-to-gate	Concept	No
	Environmental factor[45]	Total non-product or non-H_2O mass out of process / mass of product	1	Gate-to-gate	Concept	No
	Effective mass yield[46]	Mass of desired product / mass of all non-benign materials used in synthesis	1	Gate-to-gate	Concept	No
	Carbon efficiency[43]	Mass of carbon in product / mass of carbon in reactants	1	Gate-to-gate	Concept	No
	Specific process energy[43]	Total process energy / mass of product	1	Gate-to-gate	Process chemistry	No
	C-factor[47]	Cradle-to-gate kg CO_2 emitted / kg product	1	Cradle-to-gate	Process design	No
	Specific solvent use[43]	Total (gross) mass solvent / mass of product	1	Gate-to-gate	Process design	No
	Specific solvent recovery energy[43]	Total solvent recovery energy / mass of product	1	Gate-to-gate	Process design	No
	Persistency/bioaccumulation[43]	Total (persistent and bioaccumulative material) / mass of product	1	Gate-to-gate	Process design	No
	Weighted persistency/bioaccumulation[43]	Total (persistent and bioaccumulative material / (EC_{50} material / EC_{50} DDT control))[e]	1	Gate-to-gate	Process design	No
	Weighted hazard exposure[43]	Total (mass of material (kg) / permissible exposure limit for material (ppm))	1	Gate-to-gate	Process design	No
	Solvent ozone creation potential[43]	Total (mass of solvent * POCP value * vapor pressure) / (mass of product * vapor $pressure_{toluene}$ * $POCP_{toluene}$)[f]	1	Gate-to-gate	Process design	No
	Specific energy GHG emissions[43]	Mass of GHG emissions (CO_2 eq.) from energy / mass of product	1	Gate-to-gate	Process design	No
	Specific GHG emissions, excl. solvent[43]	Mass of GHG emissions (CO_2 eq.) ex. energy for solvent recovery / mass of product	1	Gate-to-gate	Process design	No

[a] For full assessment methods and multi-indicator early-stage methods, this column describes the method using (an excerpt of) the title of the original source with minor editorial changes. For early-stage single-indicator methods, a definition of the indicator is provided based on the reference with minor editorial changes for clarity.
[b] Note that this is the total number of indicators for environmental sustainability only; some methods include additional indicators for social, economic, or technical aspects. The indicators are reviewed in

http://onlinelibrary.wiley.com/doi/10.1002/bbb.1772/full

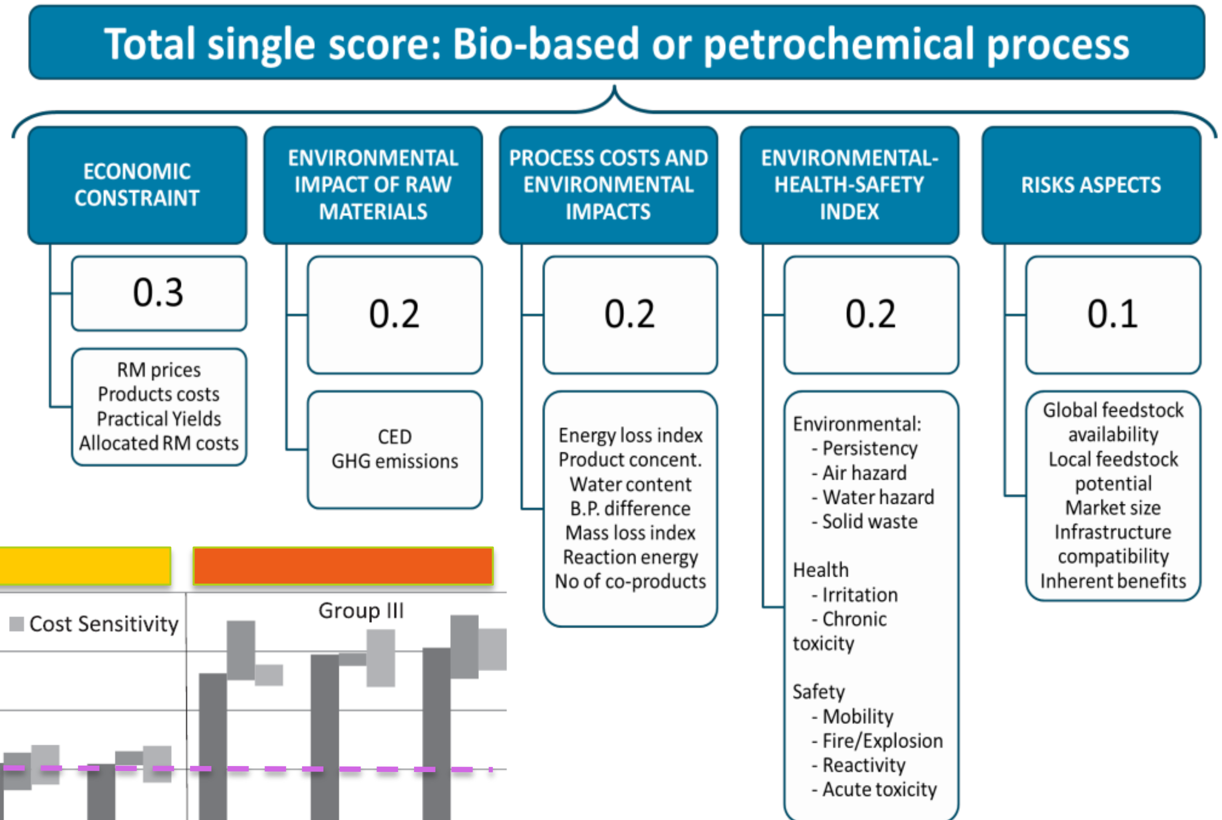
Technology status+economics….

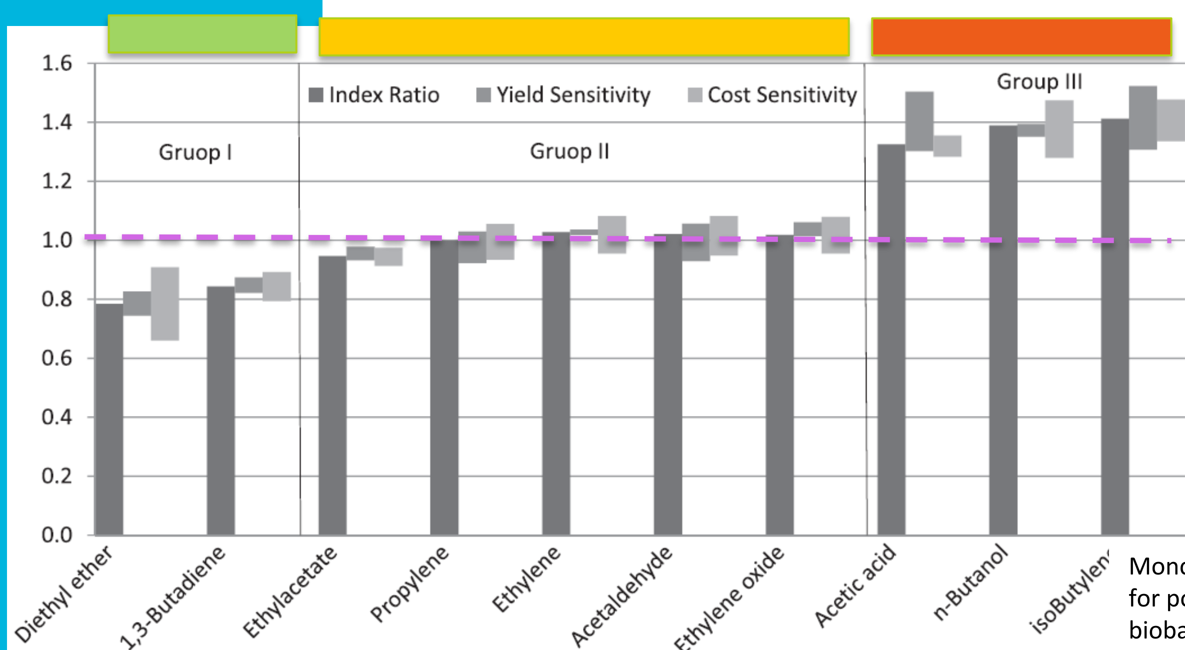
Lignin Derived Product	Current Technology Status from Lignin*	Expected Difficulty from Lignin*	Market Volume*	Market Value†	Market Risk*	Utility as Building Block*	Expected from Lignin as Mixture?
Process Heat & Power	H	L		$6/10^6 Btu	L	NA	NA
Syngas	H	L‡	H	Variable	L	H	NA
Syngas Products							
Methanol/Dimethyl ether (DME)	H	L	H	$0.80/gal	L	H or Fuel	Y
Ethanol/mixed alcohols	L	H	H	$1 - $3.5/gal	L - M	H or Fuel	Y
Fischer Tropsch Liquids	H	L	H	$1.5 - $2/gal	L - M	L	Y
Mixed Liquid Fuels	M	M	H	$1.3 - $2/gal	L	L	Y
By-product C1 to C7 gases, hydrocarbons, or oxygenates	L	M - H or as consequence of other transformations	NA	variable	L	Perhaps or use for reforming/ gasification	Y
Hydrocarbons							
BTX and Higher Alkylates	L - M	M		$2/gal	L	H	Y
Cyclohexane	L	M	H	$2.20/gal	L	M	Y
Styrenes	L	M-H	H	$0.70/lb	?	?	?
Biphenyls	L	H	L - M	?	?	L	Y?
Phenols							
Phenol	L-M	M	H	$0.55 - $0.65/lb	L	H	N
Substituted Phenols			M	$0.70 - $2.00/lb	M	M	Y
Catchols, cresols, resorcinols	L	H		>$1.5/lb	?	M	Y
Eugenol	L	H	?	M-H	?	?	Y

Holladay et al., Top value added chemicals from biomass. Results of screeing for potential candidates from biorefinery lignin, PNNL-16983, 2007

TU Delft

Tech+economics+env





Moncada et al., Early-stage comparative sustainability assessment for potential configurations of intergrated biorefineries. Screening of biobased derivative from platform chemicals. Biofuels, bioproducts and biorefining 9, 6 (2015), 722-748

2 Detailed studies

- Reduced number of technologies/value chains to be assessed
- Aim to assess competitiveness and environmental impacts of specific routes
- Comparison to petrochemical counterparts
- Depending on stage of development: uncertainty problematic

TU Delft

Feedstock → **Platform** → **Products**

Food crops
(i.e., classical processing)

Which feedstock performs better (for producing C6 sugars) from a technical, economic and environmental point of view?

Lignocellulosic biomass
(i.e., emerging alternative)

C6 sugars

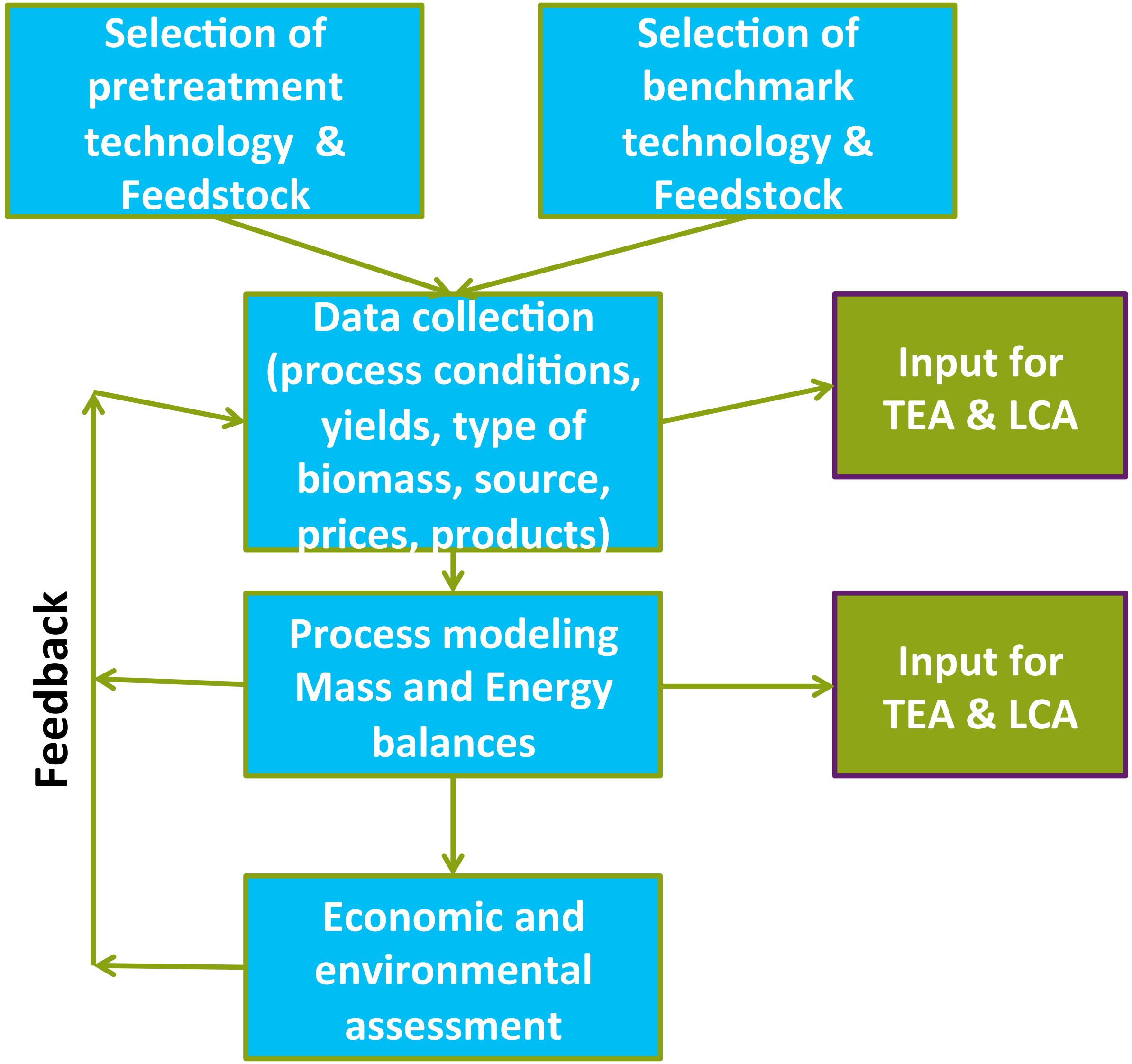
Butadiene

Caprolactam

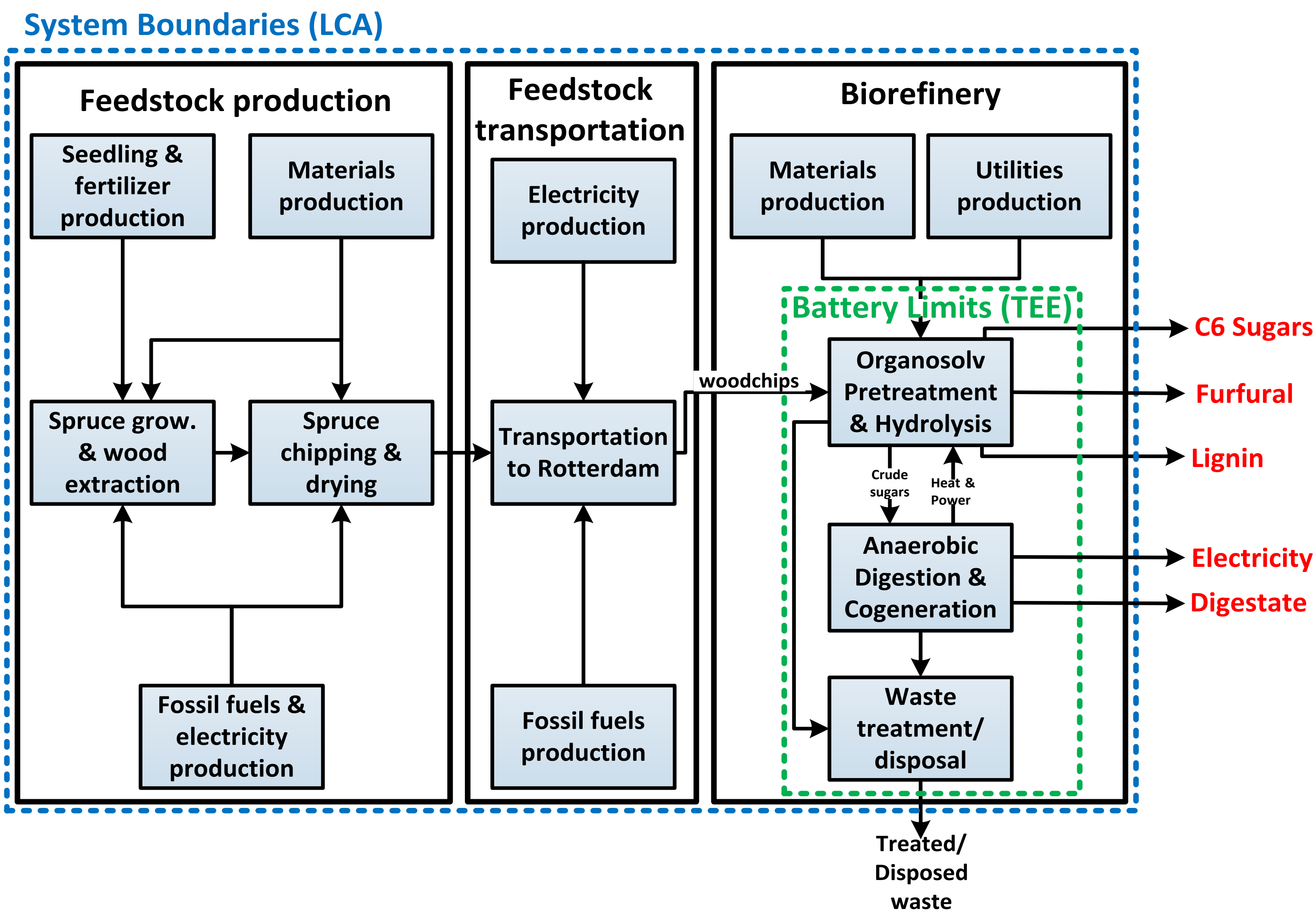
HMF

Which product shows the highest potential, from a techno-economic and environmental perspective?

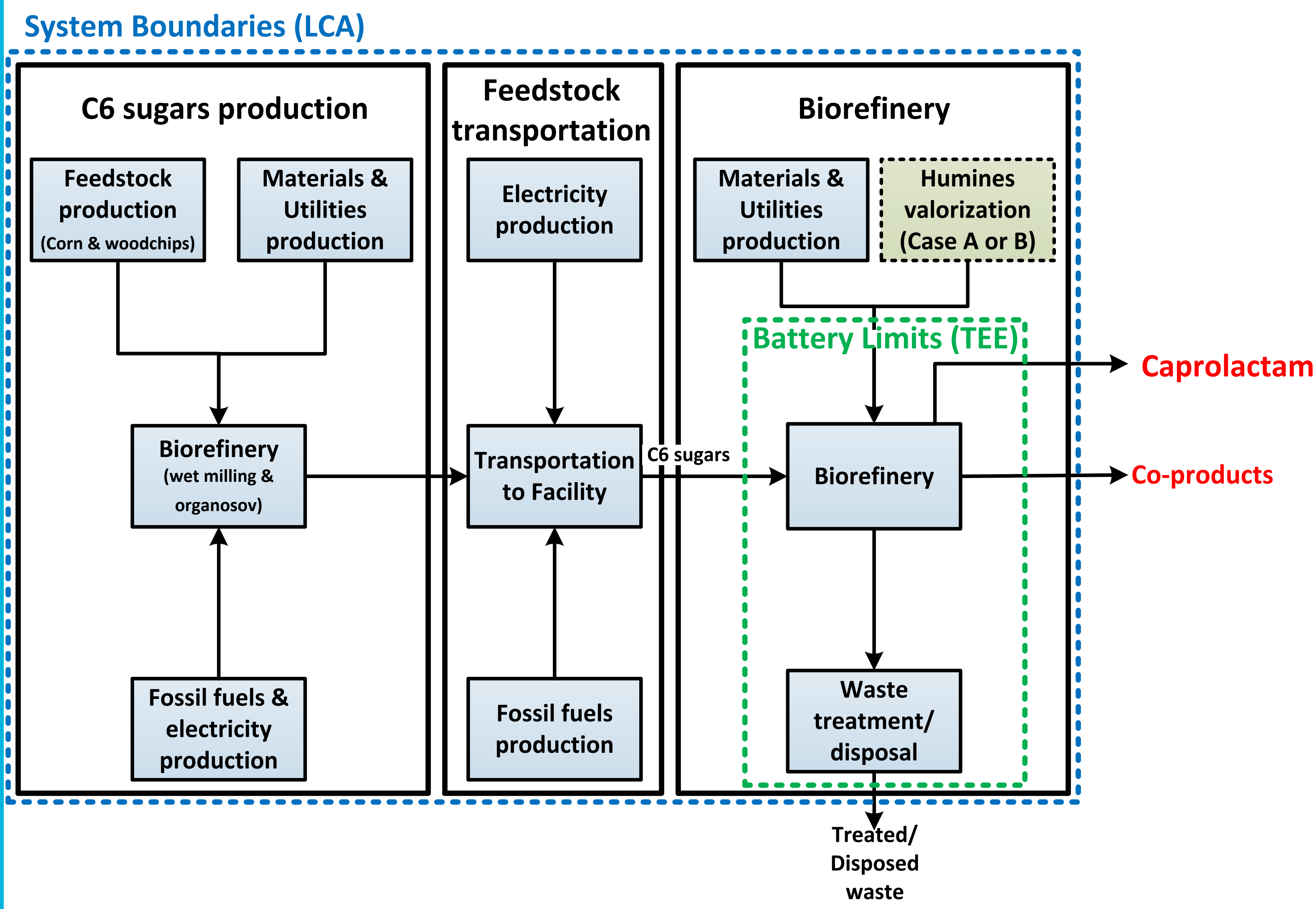
TU Delft


Selection of pretreatment technology & Feedstock
Selection of benchmark technology & Feedstock
Data collection (process conditions, yields, type of biomass, source, prices, products)
Input for TEA & LCA
Process modeling Mass and Energy balances
Input for TEA & LCA
Economic and environmental assessment
Feedback

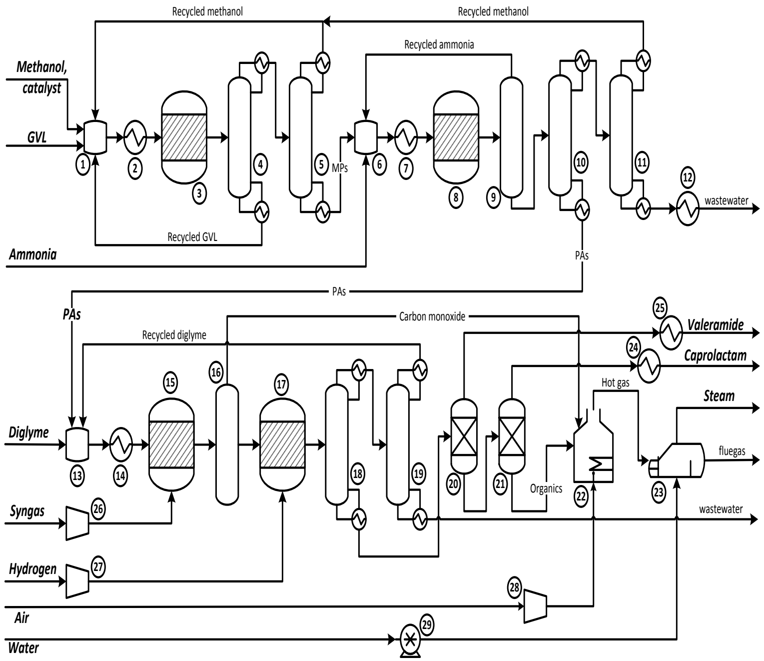
Differences in System boundaries between TEA and LCA



Example differences in System boundaries Caprolactam production



Modeling



Simplified flow diagram of the production of caprolactam from γ-valerolactone (one out three process sections in a briorefinery concept from c6 sugars to caprolactam)

- **Process flowsheeting**
  - Energy balances
  - Process flows
  - Feedstock and ancillary requirements
- **Equipment lists**
  - Bill of components and materials
  - Cost of material and components

Basis for

⇒ Estimation of costs (CAPEX & OPEX)

⇒ Estimation of Life cycle inventories

⇒ Use of costs to complement inventories

Synergies

TU Delft

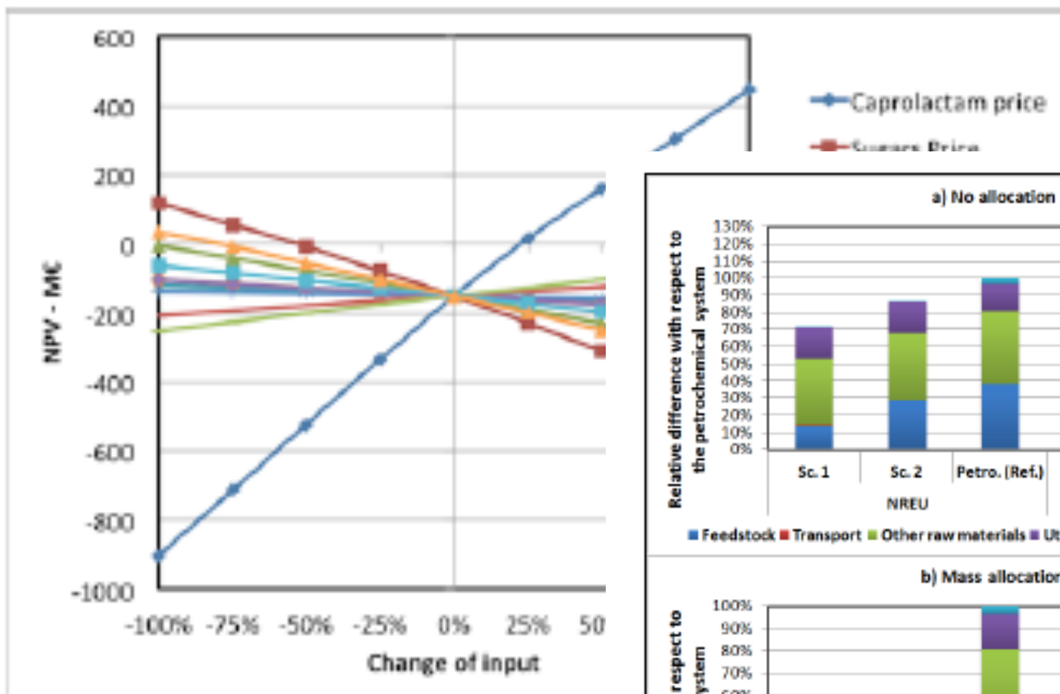
Results

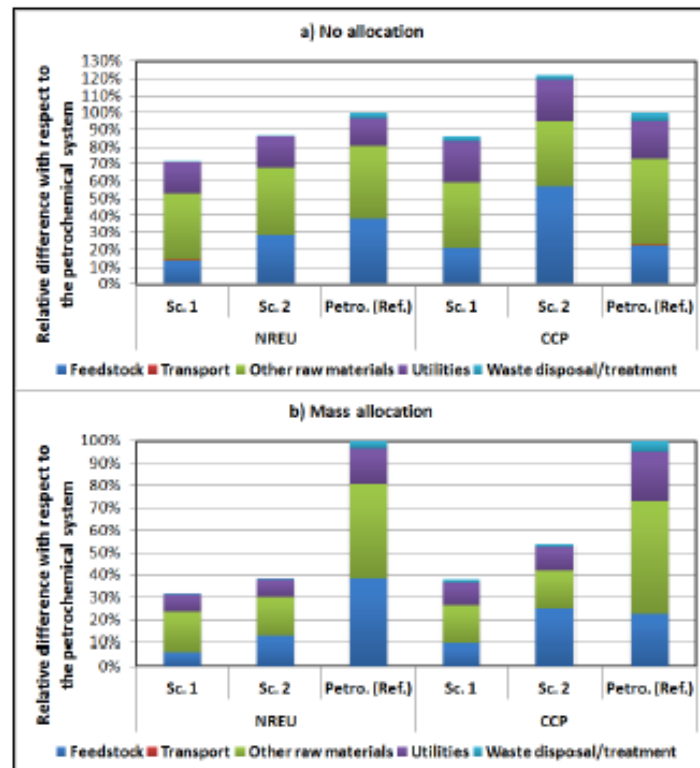
Table 10. Mass balances accounting for key material inputs and outputs of cases I and II of caprolactam production, expressed in ktonn

Cases	Case I	
Stream	Inputs – kt/y	Outputs – kt/y
Raw Materials		
C6 sugars [a]	170	-
Sulfuric Acid	$7*10^{-2}$	-
Dioxane	1	-
Hydrogen	2.5	-
Methanol	0	-
Water	39	-
Ammonia [b]	36	-
Diglyme	$4*10^{-1}$	-
Syngas [c]	22	-
Air	125	-
Demineralized water	153	-
Products		
Formic Acid	-	35
Water	-	17
Caprolactam [d]	-	47
Valeramide [e]	-	25
Lp Steam [f]	-	153
Waste streams		
Humines	-	31 (5.6 [g]
Waste water	-	99
Flue gas [h]	-	143
Total	**549**	**549**

Table 13. Annualized production costs, revenues and Net Present Value of case I of caprolactam production. Results include the assessment of humines valorization cases

Feature	No humines Valorization		Humines Valorization case A		Humines Valorization case B	
	M€/year	Share	M€/year	Share	M€/year	Share
Production costs						
Raw Materials	58.0	43%	58.0	43%	66.7	46%
Utilities	26.6	20%	26.1	19%	26.6	18%
Maintenance	8.6	6%	8.6	6%	8.6	6%





TUDelft

Some key challenges, specially for detailed ex-ante studies

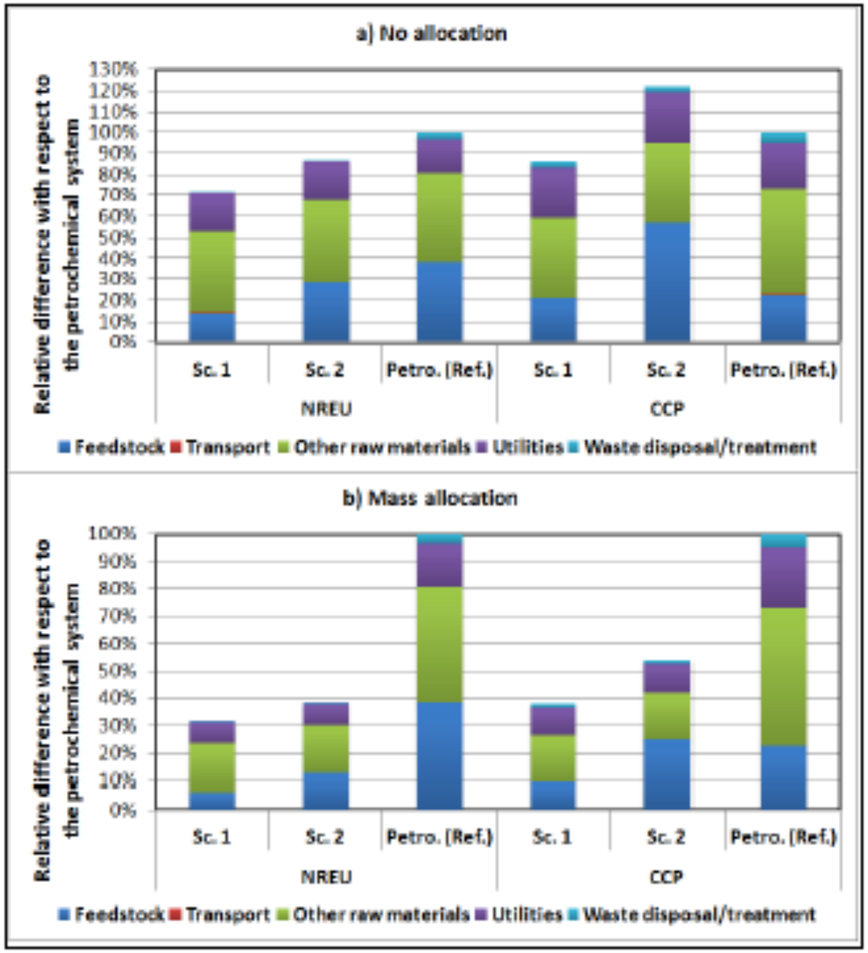
Comparability: functional unit

- Goal of a f.u is to ensure that the same function is fulfilled and that the comparison is meaningful
  – which product?
  – What about novel products? (do they compete with similar products?)
  – What if the function of a product is not comprehensively defined?

System boundaries and critical issues

- **Allocation**

  mass, volume, energy, market value



Products: caprolactam, formic acid and valeramide

System boundaries and critical issues

- **Displacement**

Gasoline

CO_2 based fuel

Biofuel

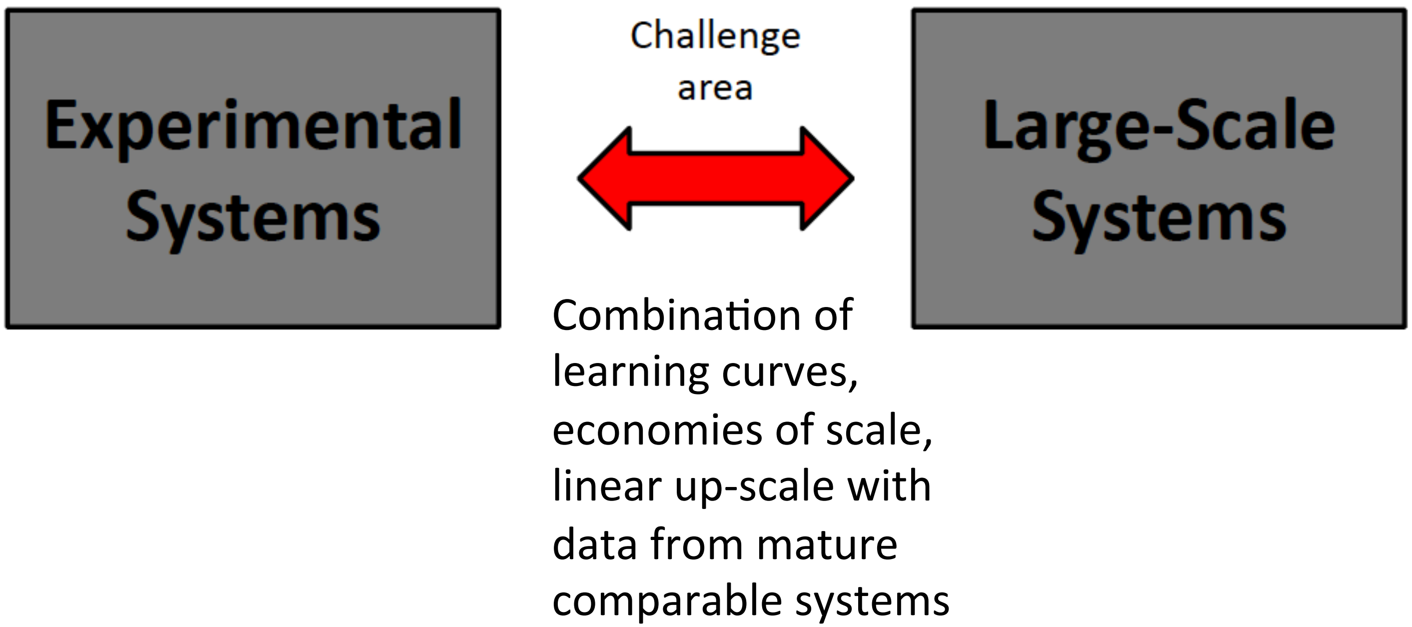
Hydrogen

Electric Vehicle

TU Delft

Effects of scaling up

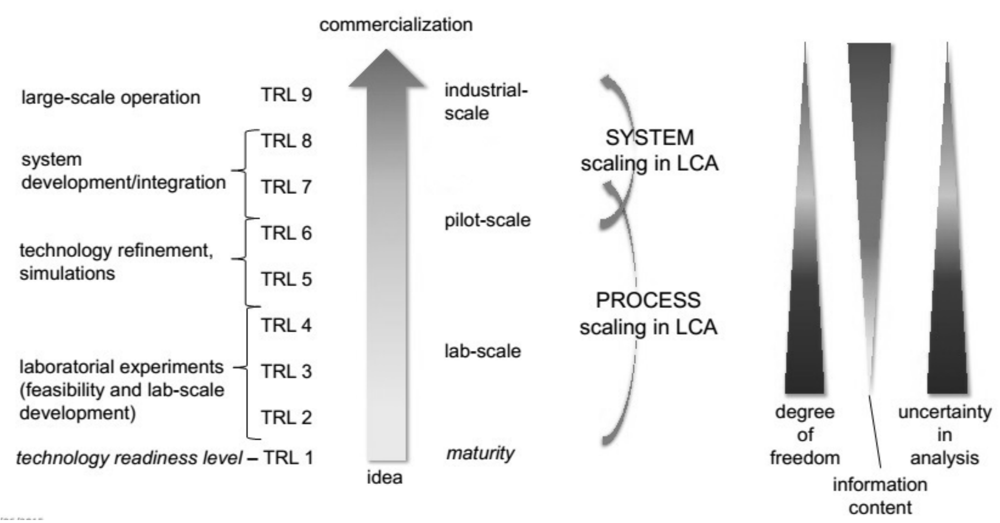
- Can affect the process themselves
  - Yields, energy use, type of energy supply, type and amount of waste, emission levels, batch continous?…)
- Process synergies (use of waste as heat or raw material in another process)
- Optimization and production capacity
- Process design and choices



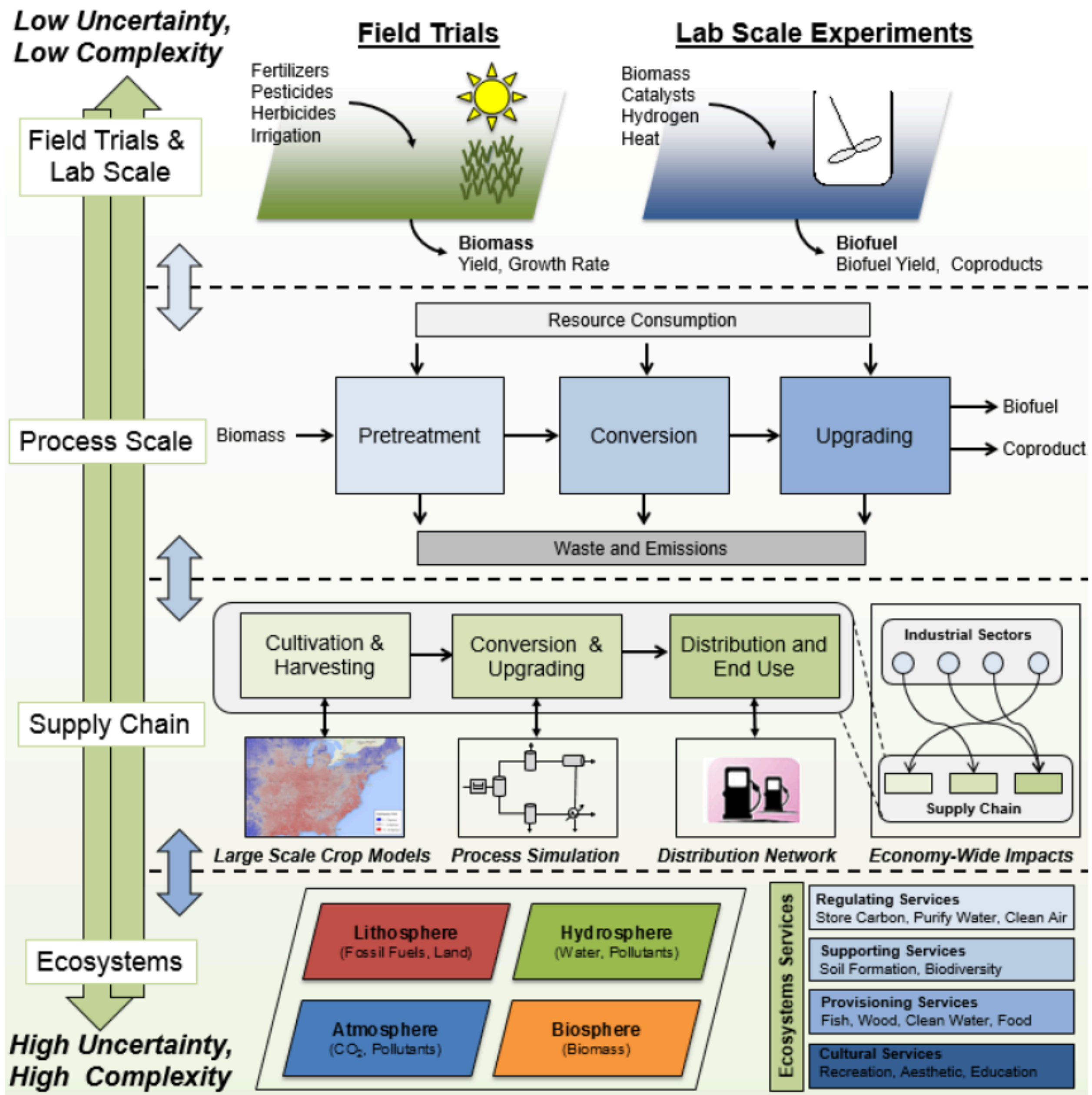
Scaling-up

Process scaling: how to obtain the mass, energy, emissions, equipment costs

System scaling: effects of the introduction of the scaled up product in the market and environmental impacts



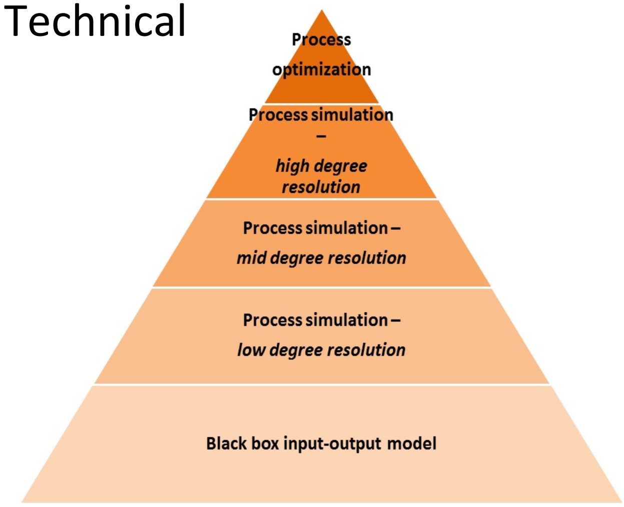
Source: Simon et al., 2016 (doi: 10.1002/ieam.1788)



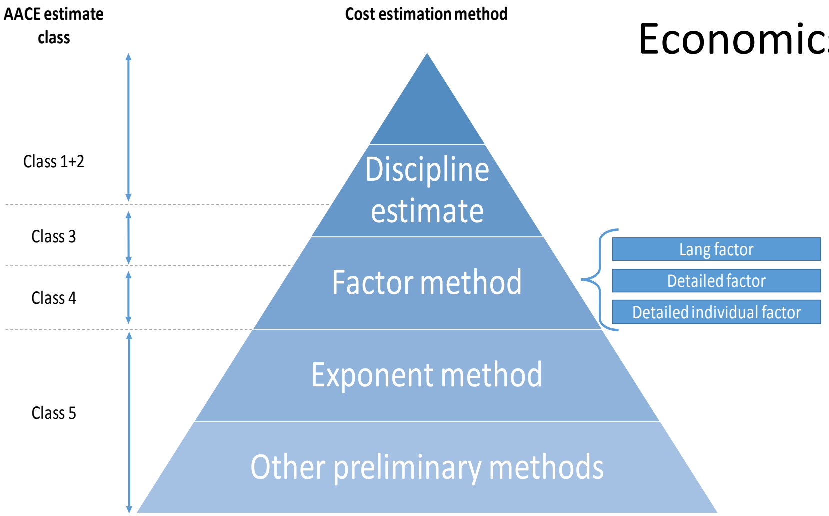
Source: Zaimes et al., 2015

What we know and we you do NOT know should guide model selection

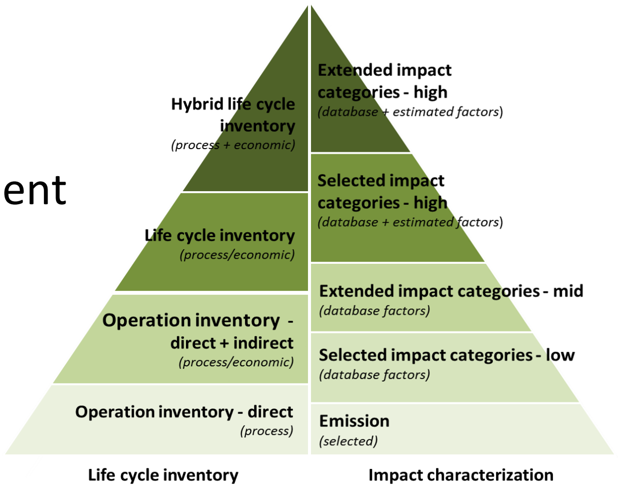
Technical



Economics



Environment

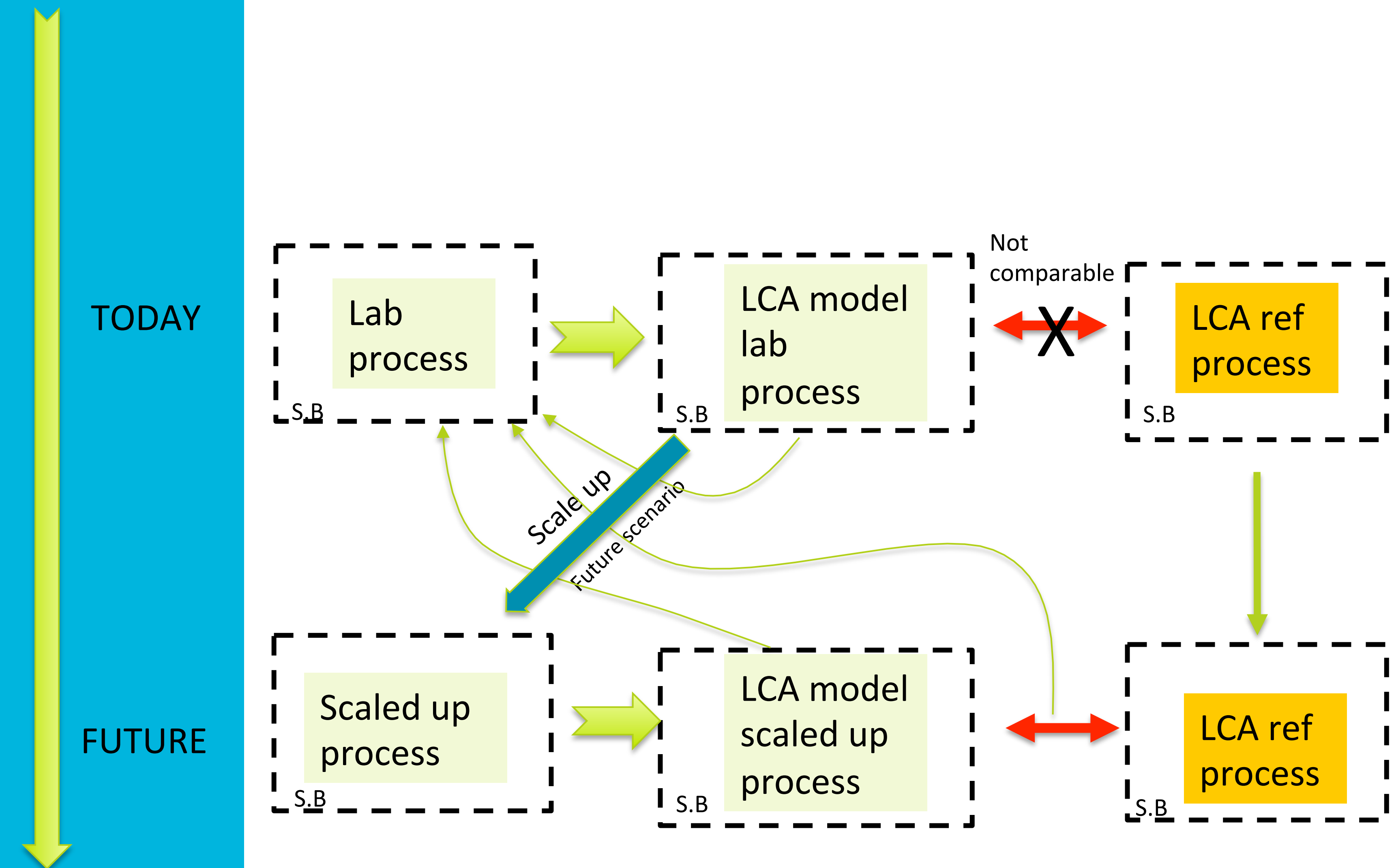


TU Delft

WHEN is the biorefinery deployed?

- Analysis takes placed in a supposed future scenario (Populations distributions, demand, regulatory requirements, market penetrations…)
- Scenario development is critical as can determine the results
- Time perspective
  - is the process already available-short time perspective- current conditions:
    - foreground changes but background can be assumed the same as today
  - process is at early stage (lab, pilot), time perspective in some years/decades; future conditions
    - foreground and background changes!

TU Delft



Villares et al, 2017. Doi: 10.1007/s11367-017-1270-6

Finally,

- Ex-ante is interdisciplinary research requires transfer of knowledge and data across research fields. Need for collaboration!
- TEE, LCA and LCC are heavily dependent on data (e.g., energy, raw materials, ancillary, operation conditions, life time, costs)
- Large uncertainties are inherent to ex-ante: it requires assumptions, simplifications and sensitivity analysis
- Complexity and uncertainty is reinforced by the unclear (or non-existing) socio-technical embedment of the technology
- Comparative and iterative approaches are needed. Results of ex-ante should not be considered deterministic outcomes and should not be used as such!

TU Delft

Thanks for your attention!

Email: c.a.ramirezramirez@tudelft.nl

TU Delft