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The coupling of optimization techniques and LCA

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Department of Chemistry and Applied Biosciences

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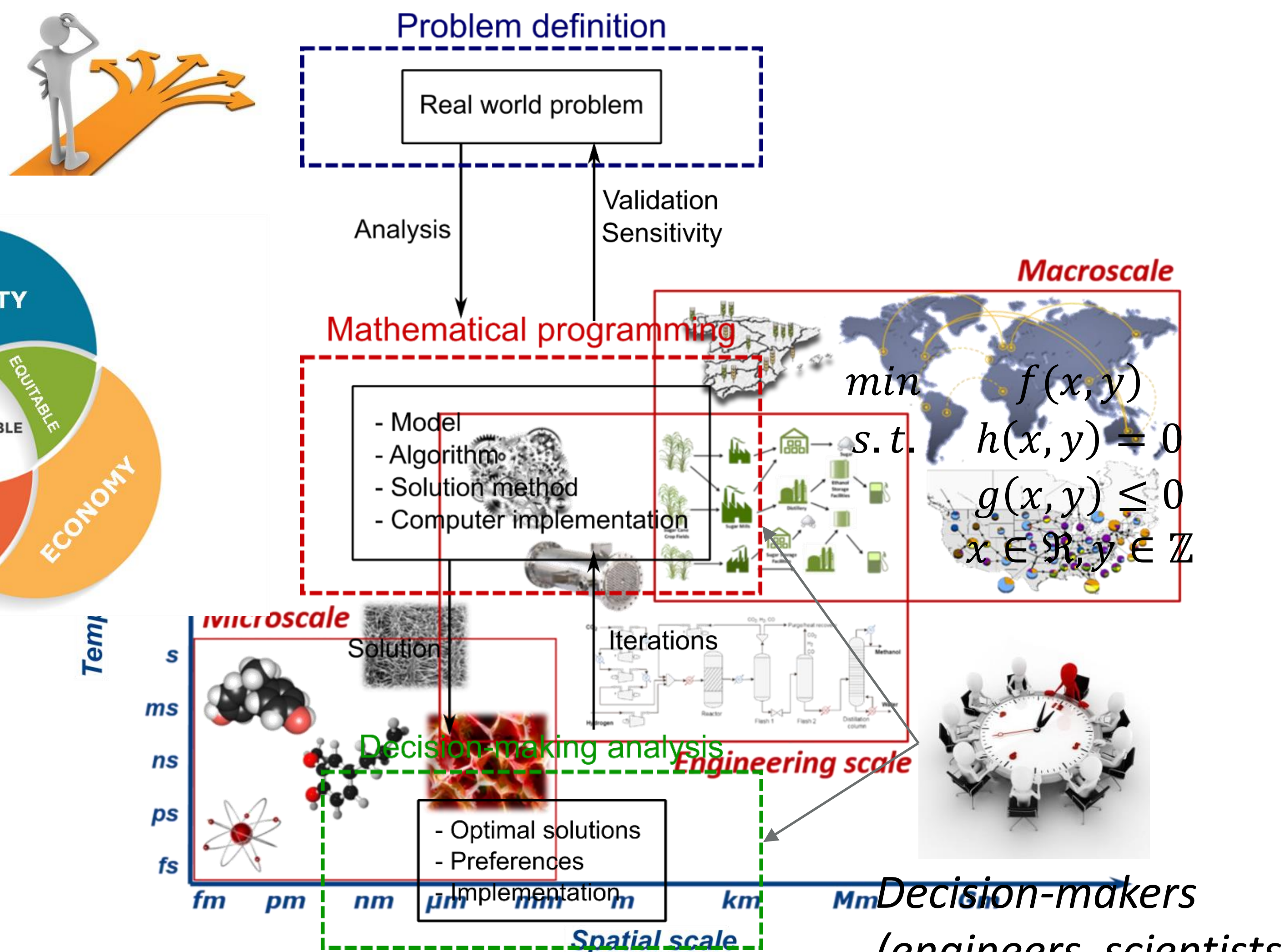
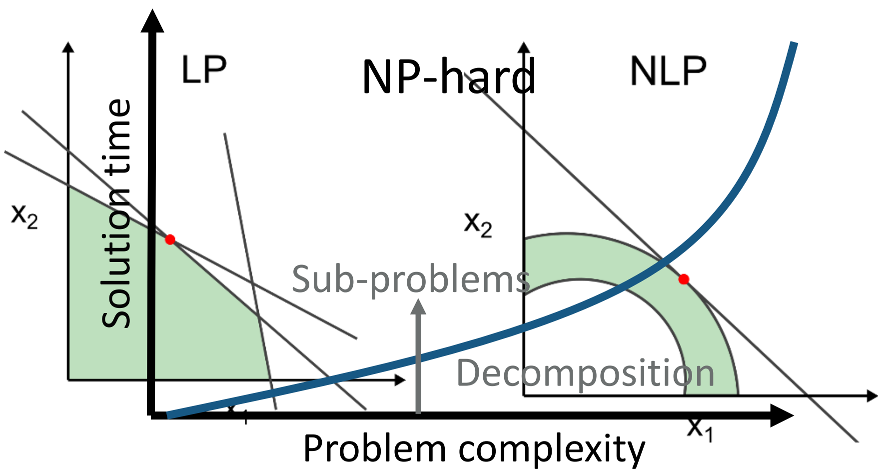
Sustainable decision-making process

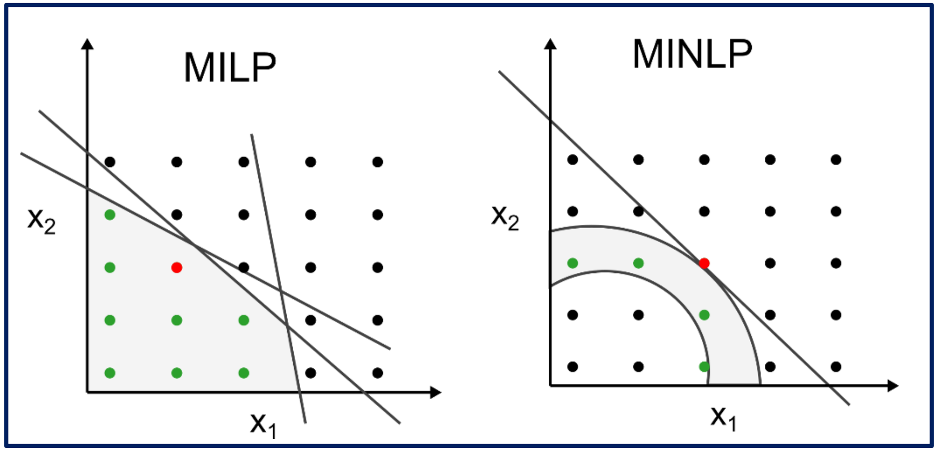


Mathematical programming

min	$f(x,y)$	Objective function (cost, environmental impact, safety, etc.)
$s.t.$	$h(x,y) = 0$	Process equations (mass & energy balances, etc.)
	$g(x,y) \leq 0$	Specifications
	$x \in \Re^n$	Continuous variables (pressures, temperatures, flows)
	$y \in \{0,1\}^m$	Discrete variables (logical decisions)

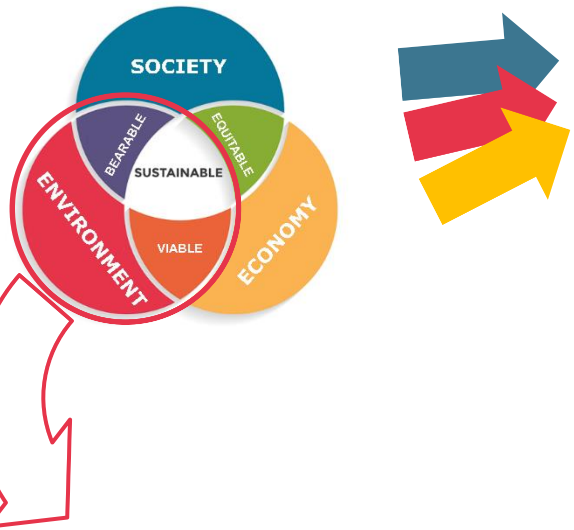
Types of mathematical programming problems





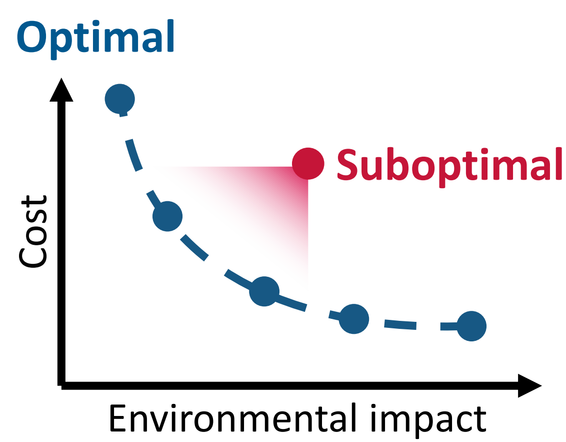
Multi-objective optimization

1. Several objective functions



$$\min \quad f_1(x,y), \dots, f_k(x,y)$$
$$s.t. \quad h(x,y) = 0$$
$$g(x,y) \leq 0$$
$$x \in \Re^n, y \in \{0,1\}^m$$

2. Life cycle sustainability assessment



3. Pareto optimal solutions

Azapagic, A., Clift, R. *Computers & Chemical Engineering,* 23 (10), 1509-1526, 1999.
Grossmann, I. E., Guillén-Gosálbez, G. *Computers & Chemical Engineering*, 34 (9), 1365-1376, 2010.

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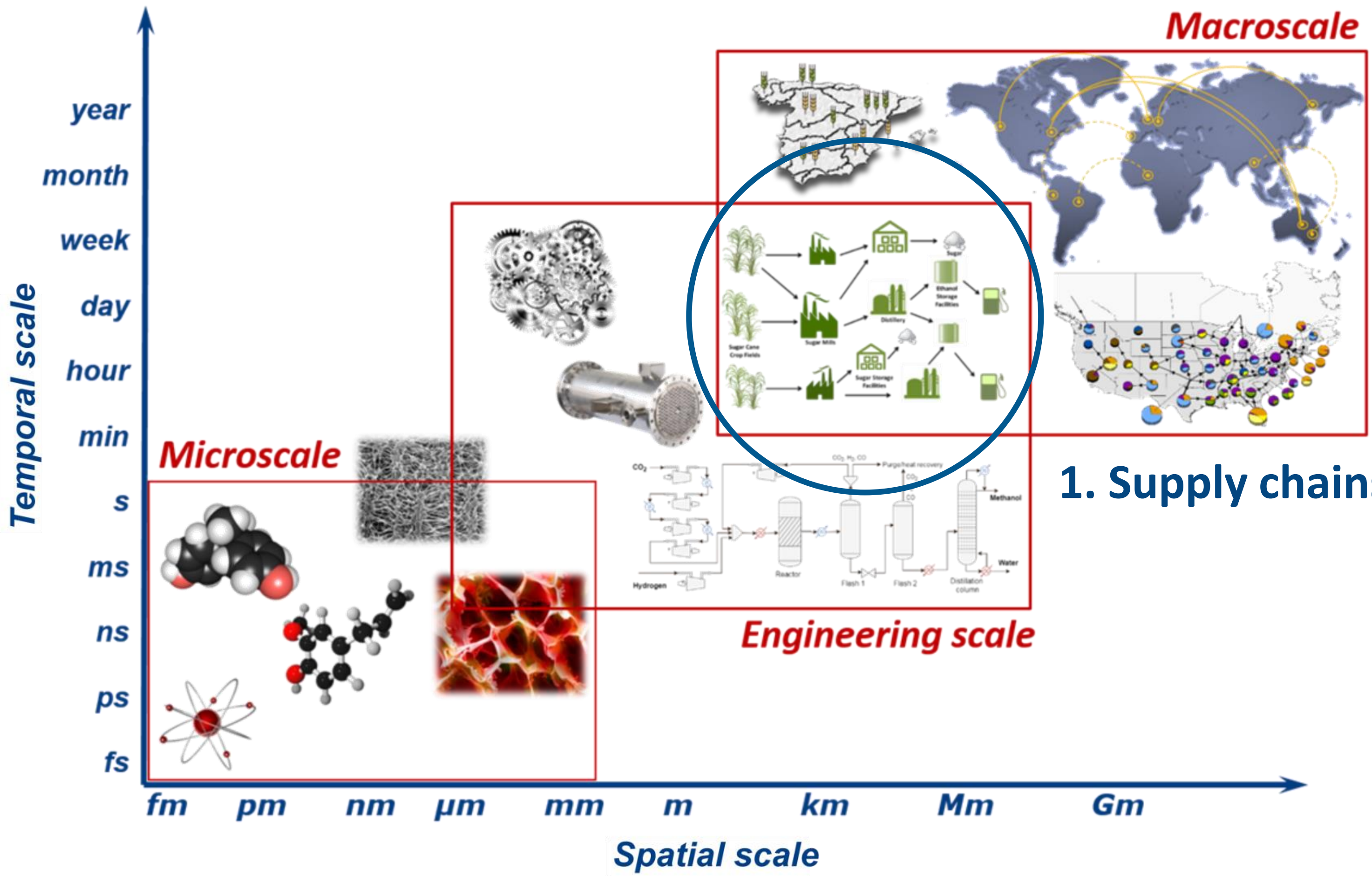

1. Supply chains

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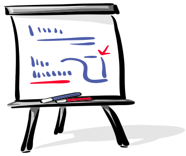
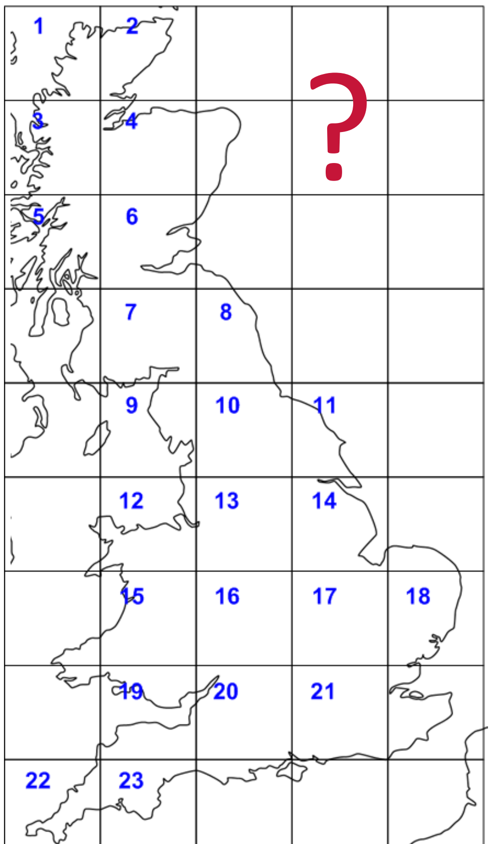
Supply chains: Hydrogen Supply Chains



Given are:

- Hydrogen demand
- Available technologies and potential locations (i.e. grids)
- Investment and operating costs
- GHG emissions



The task is to determine:

- The optimal SC in terms of cost & environmental impact

Production

- CH_4 reforming
- Coal gasification
- Biomass gasification

Transportation

- Liquid H_2
- Compressed-gaseous H_2

Storage

- Liquid H_2
- Compressed gas

Guillén-Gosálbez, G., Mele, F., Grossmann, I. E. *AIChE Journal*, 56 (3), 650-667, 2010.
Sabio, N., Kostin, A., Guillén-Gosálbez, G.*, Jiménez, L. *International Journal of Hydrogen Energy*, 37(6), 5385-5405, 2012.

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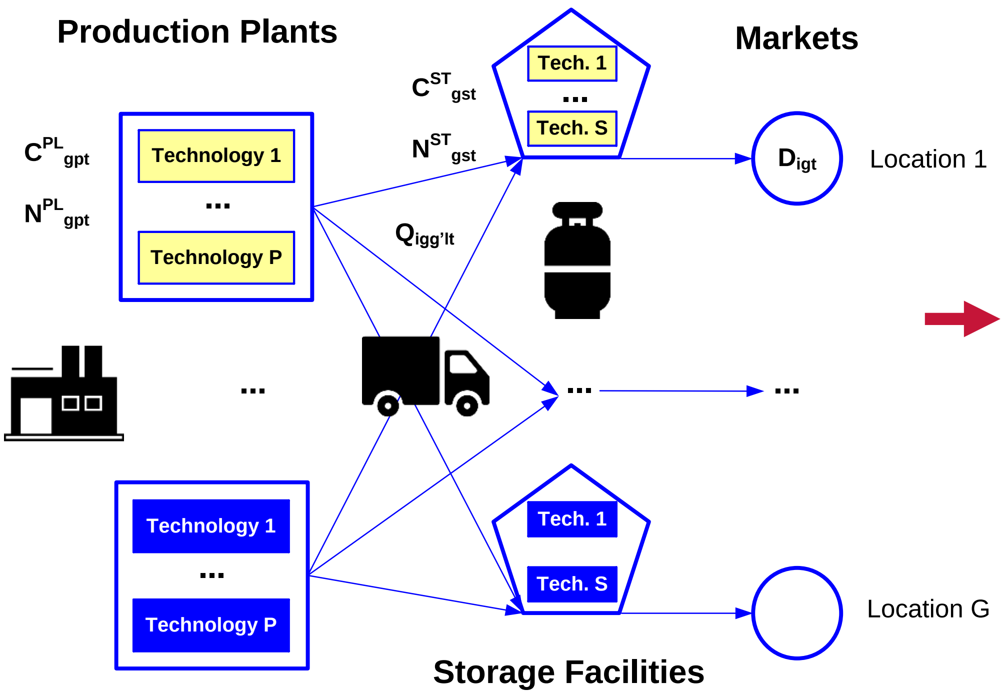
Superstructure: Mathematical representation that embeds all possible alternatives



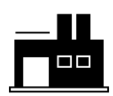
Multi-objective mixed-integer linear program (MILP)

- Mass balance equations
- Capacity constraints
- Objective function equations

1. Calculate the emissions and feedstock requirements: **LCI** from cradle to grave

$$LCI_b = \sum_i \sum_g \sum_p \sum_t PR_{igpt}(\omega_{bp}^{PR} + \omega_{bi}^{ST}) + \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in LI_i} \sum_t Q_{igg'lt}\omega_b^{TR} \quad \forall b$$

Production (raw materials, energy consumption and direct emissions)



Storage (compression of hydrogen)

Transportation tasks

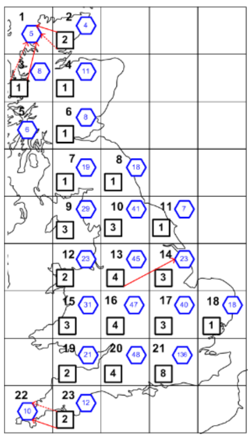
2. Translate LCI into damage (CML 2001, Recipe 2008, etc.): **Eco-indicator 99**, damage to human health caused by climate change

$$DAM = \sum_b \upsilon_b LCI_b$$

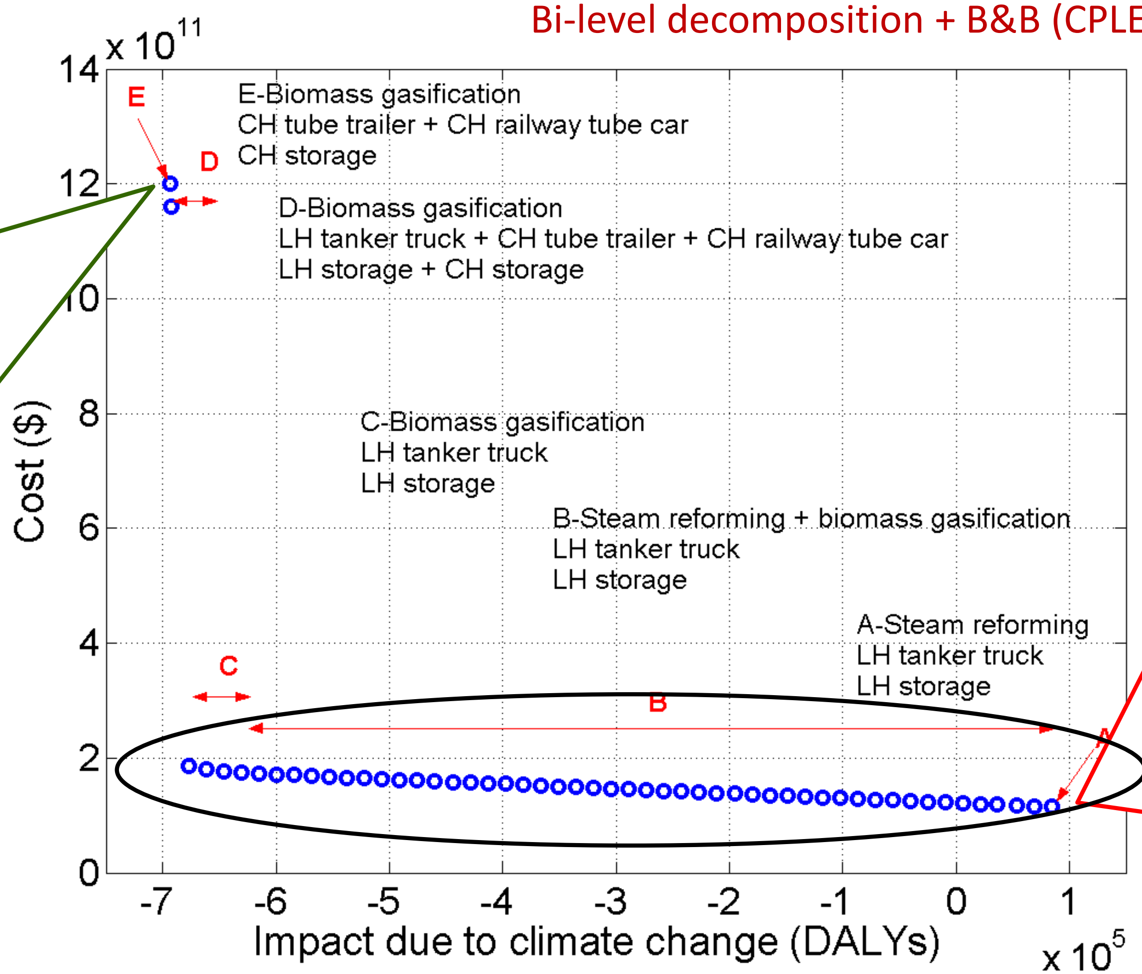
Damage factors translate life cycle inventory into impact

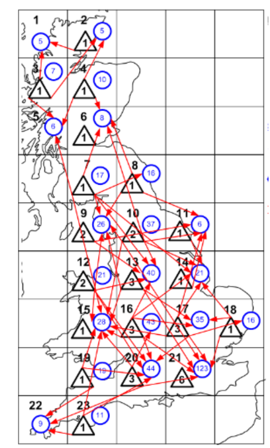
$$\min_{x,X,N}\left(TDC(x,X,N), DAM(x,X,N)\right)$$
$$s.t. \quad g(x,X,N) \leq 0$$
$$h(x,X,N) = 0$$
$$x \in \mathbb{R}, X \in \{0,1\}, N \in \mathbb{N}$$

MILP
Binary 10,580
Discrete 940
Continuous 12,701
Equations 35,491
Bi-level decomposition + B&B (CPLEX)



Minimum impact

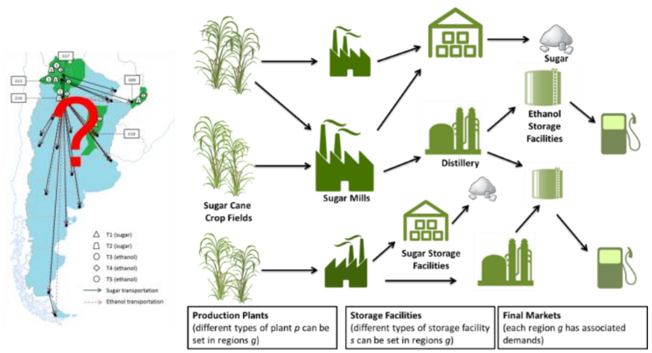




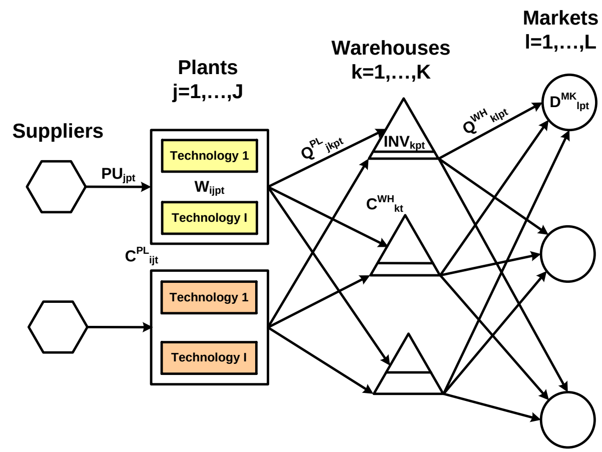
Minimum cost

Other applications

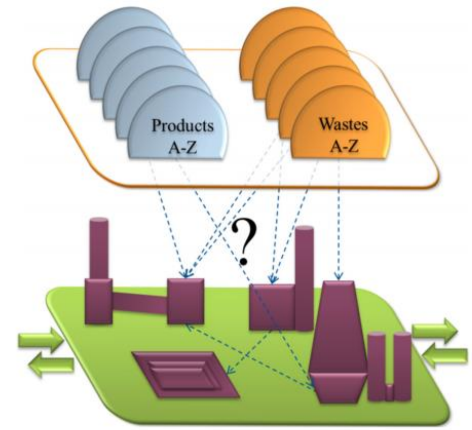
Biomass supply chains[1]



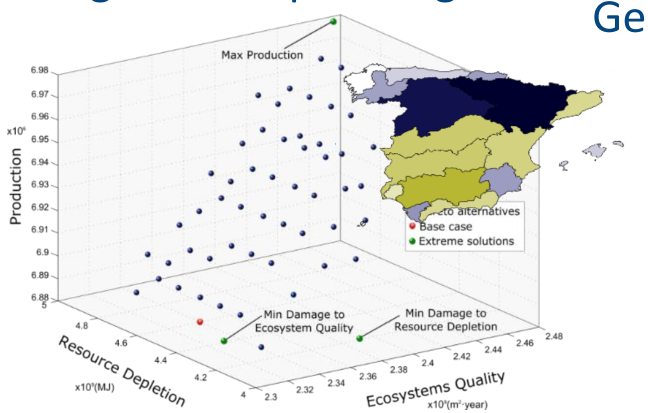
Petrochemicals[2]



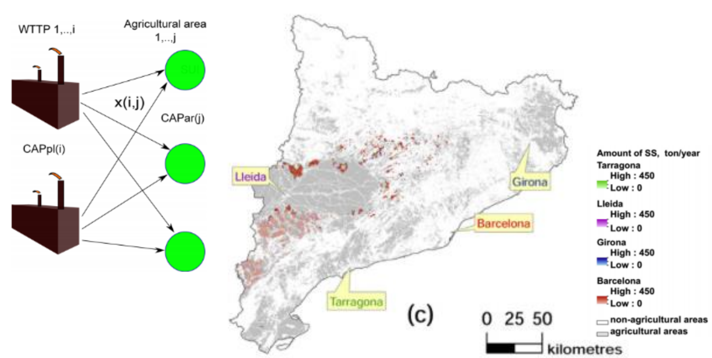
Waste management[3]



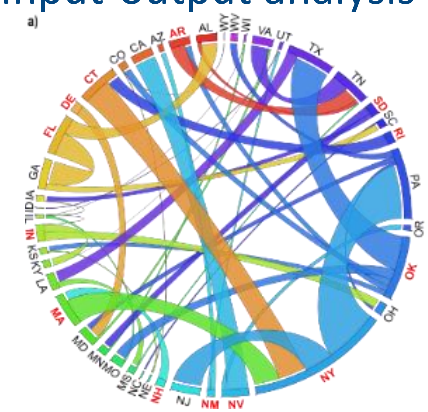
Agriculture planning[4]



Geographical Information Systems[5]



Input-output analysis[6]



1. Mele, F., Kostin, A., Guillén-Gosálbez, G. *, Jiménez, L. *Industrial & Engineering Chemistry Research*, 50 (9), 4939-4958, 2011.
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4. Galán-Martín, A., Vaskan, P., Anton, A., Jiménez, L., Guillen-Gosálbez, G.,*. *Journal of Cleaner Production*, 140, 816-830, 2017.
5. Vaskan, P., Passuello, A., Guillén-Gosálbez, G. *, Schuhmacher, M., Jiménez, L.. *Environmental Modelling & Software*, 46, 163-169, 2013.
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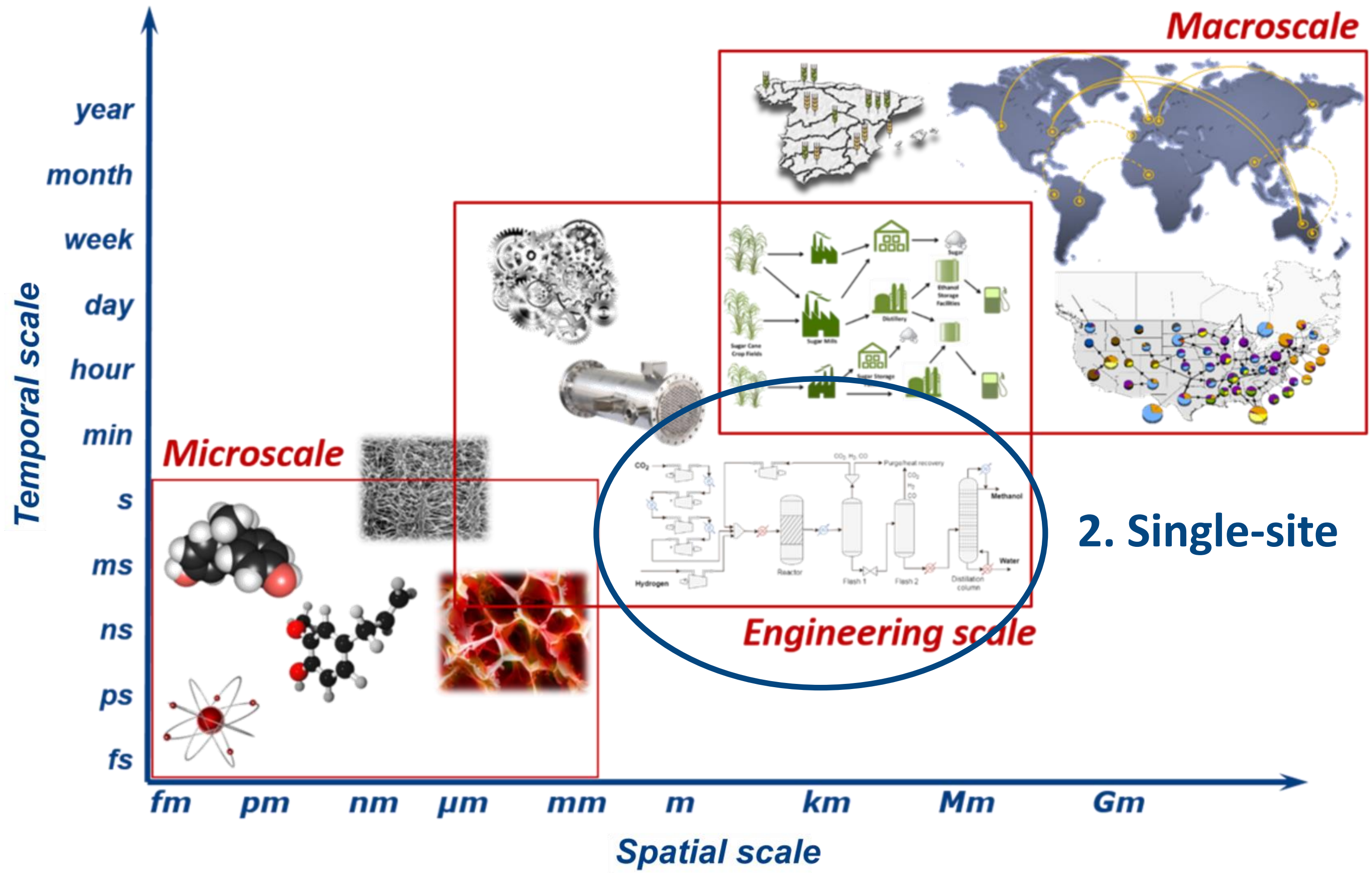
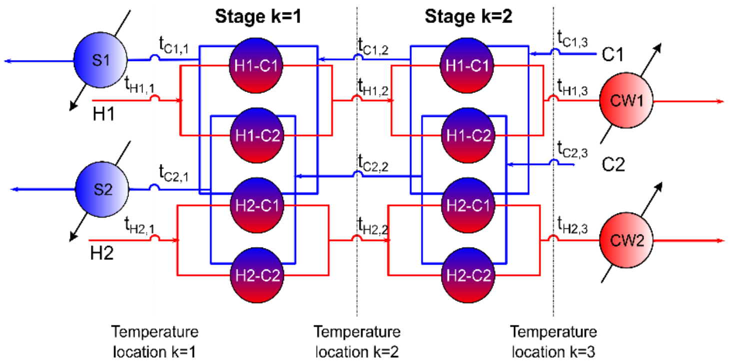
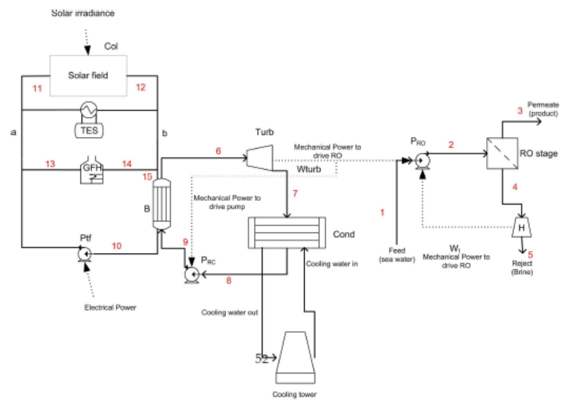

Macroscale
Microscale
Engineering scale
2. Single-site
Temporal scale
year
month
week
day
hour
min
s
ms
ns
ps
fs
Spatial scale
fm
pm
nm
µm
mm
m
km
Mm
Gm

Other applications

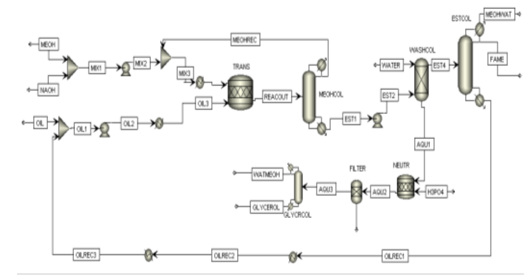
Heat exchangers[1]



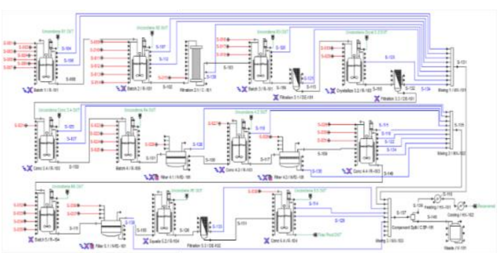
Thermodynamic cycles[2]



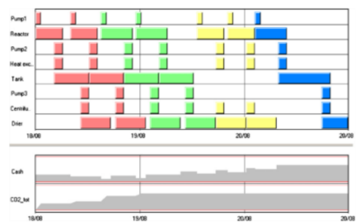
Biofuels[3]



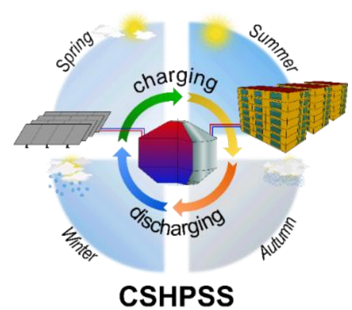
Pharmaceutical processes[4]



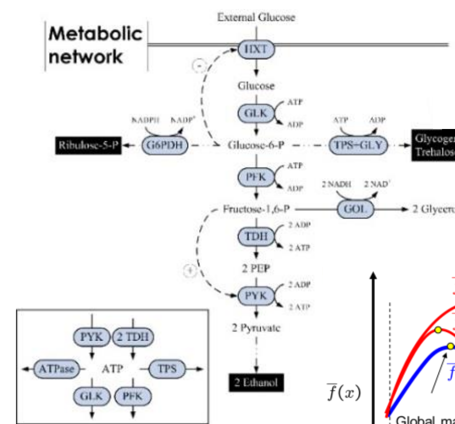
Scheduling[5]

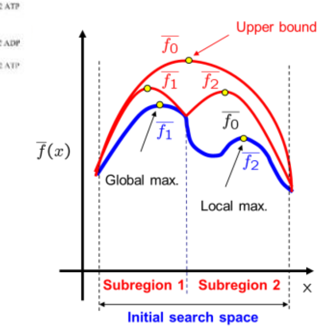


Buildings[6]



Systems biology[7]





1. Vaskan, P., Guillén-Gosálbez, G.*, Jiménez, L. *Applied Energy*, 98, 149-161, 2012.
2. Salcedo, R., Antipova, E., Boer, D., Jiménez, L., Guillén-Gosálbez, G.*, *Desalination*, 286, 358-371, 2012.
3. Brunet, R., Boer, D., Guillén-Gosálbez, G.*, Jiménez, L., *Chemical Engineering Research & Design*, 93, 203-212, 2015.
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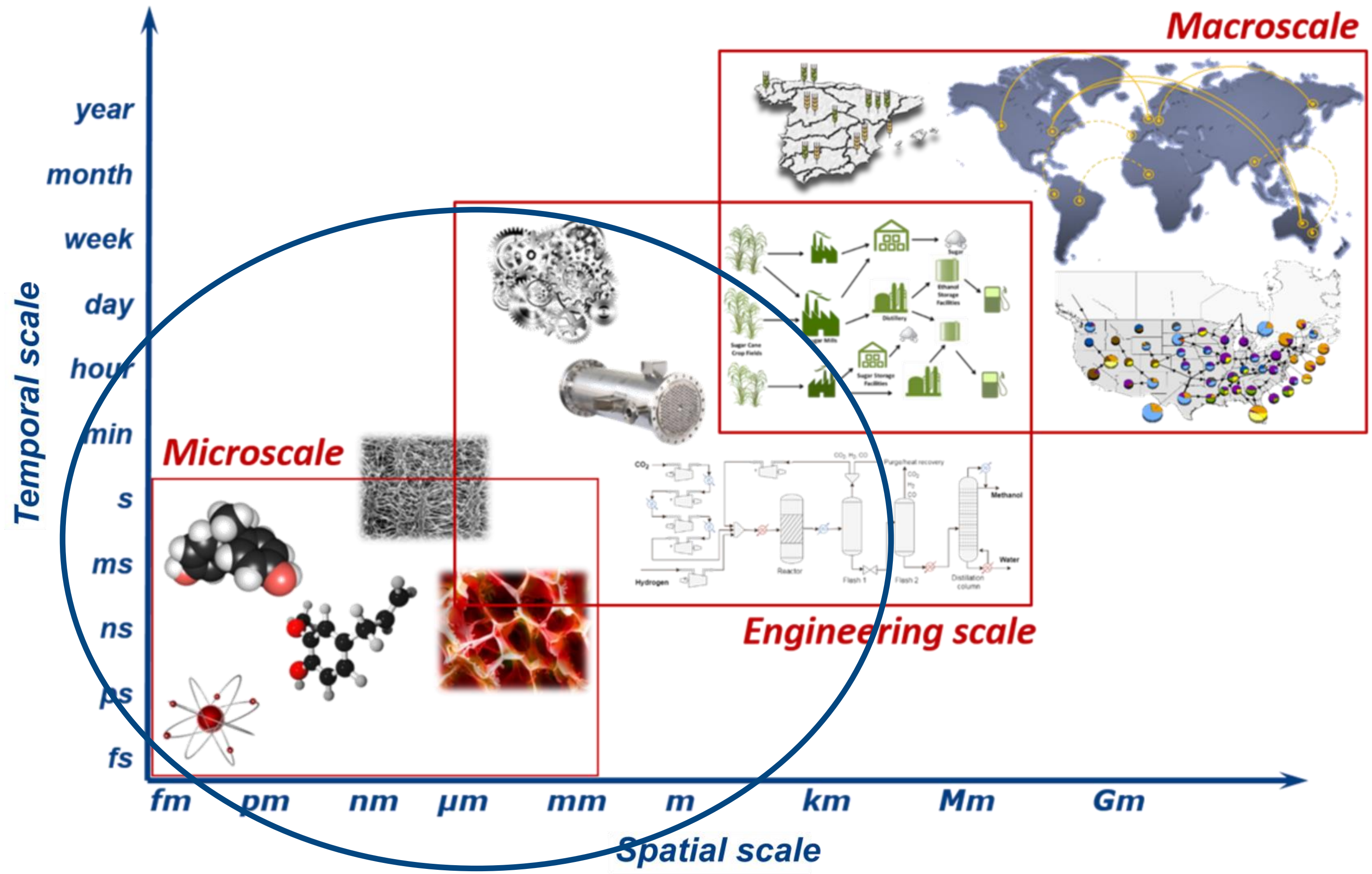
1. PSE tools to underpin the transition towards a more sustainable chemical industry



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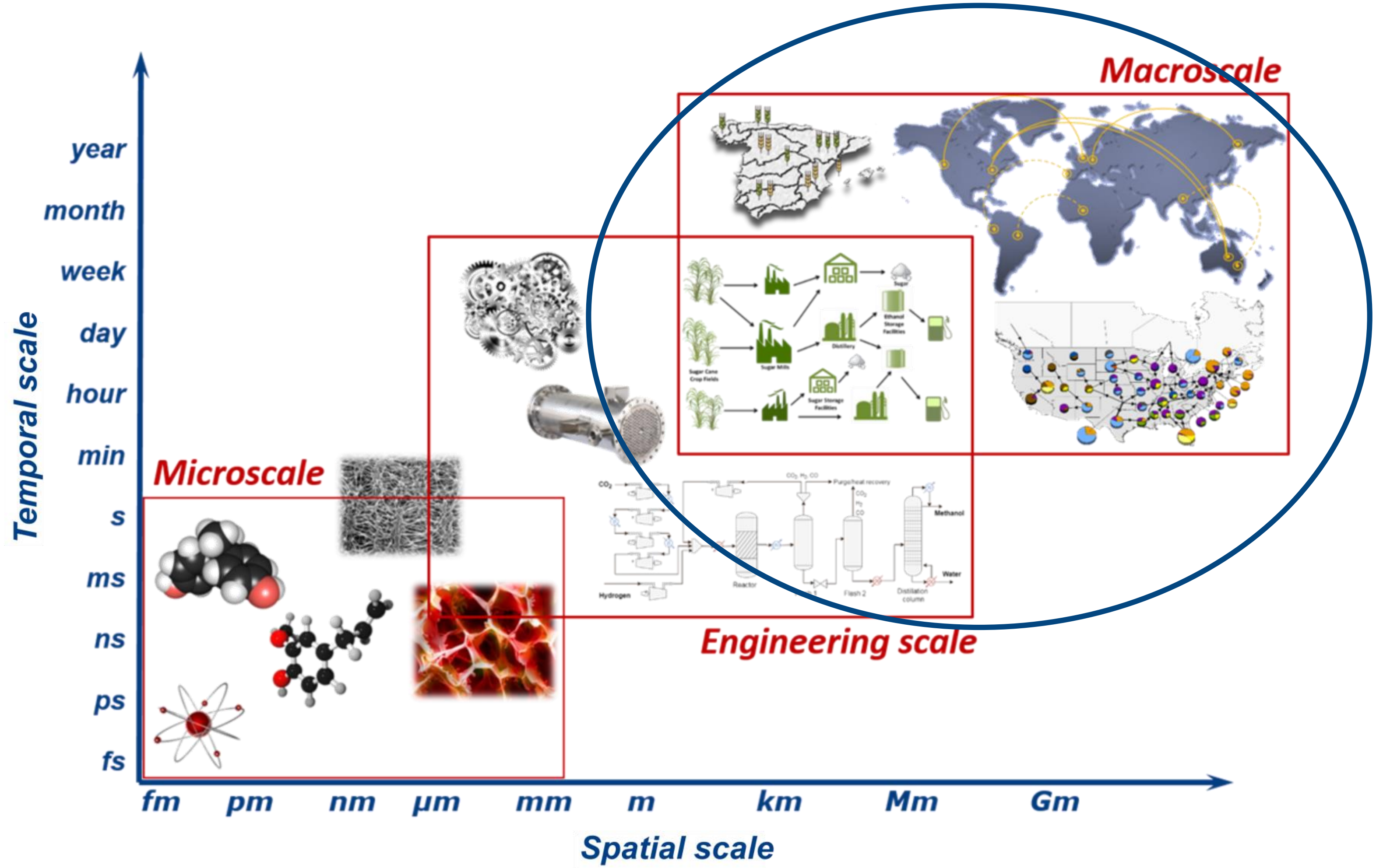
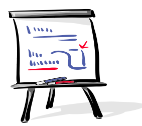
2. PSE to address global challenges in sustainability at the macro-scale level

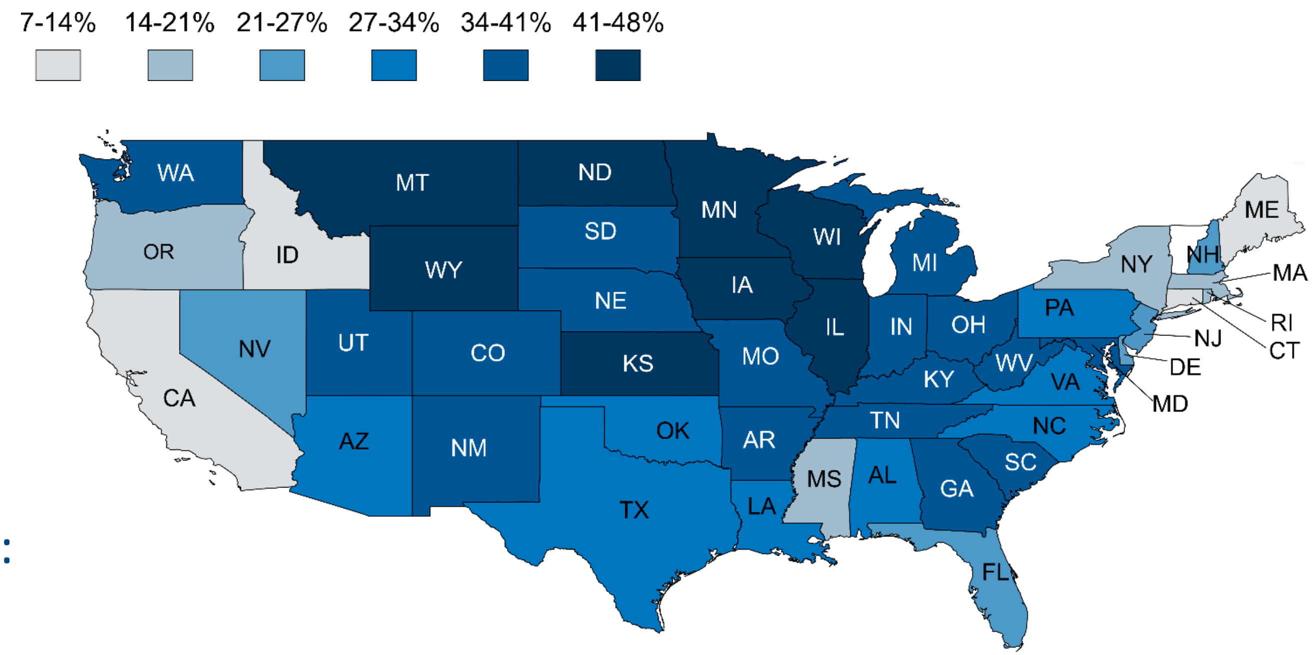


Motivation: Energy Systems Modelling (ESM)



Given are:

- Electricity demand
- Techno-economic data
- Carbon intensity



The task is to determine:

- Optimal electricity mixes

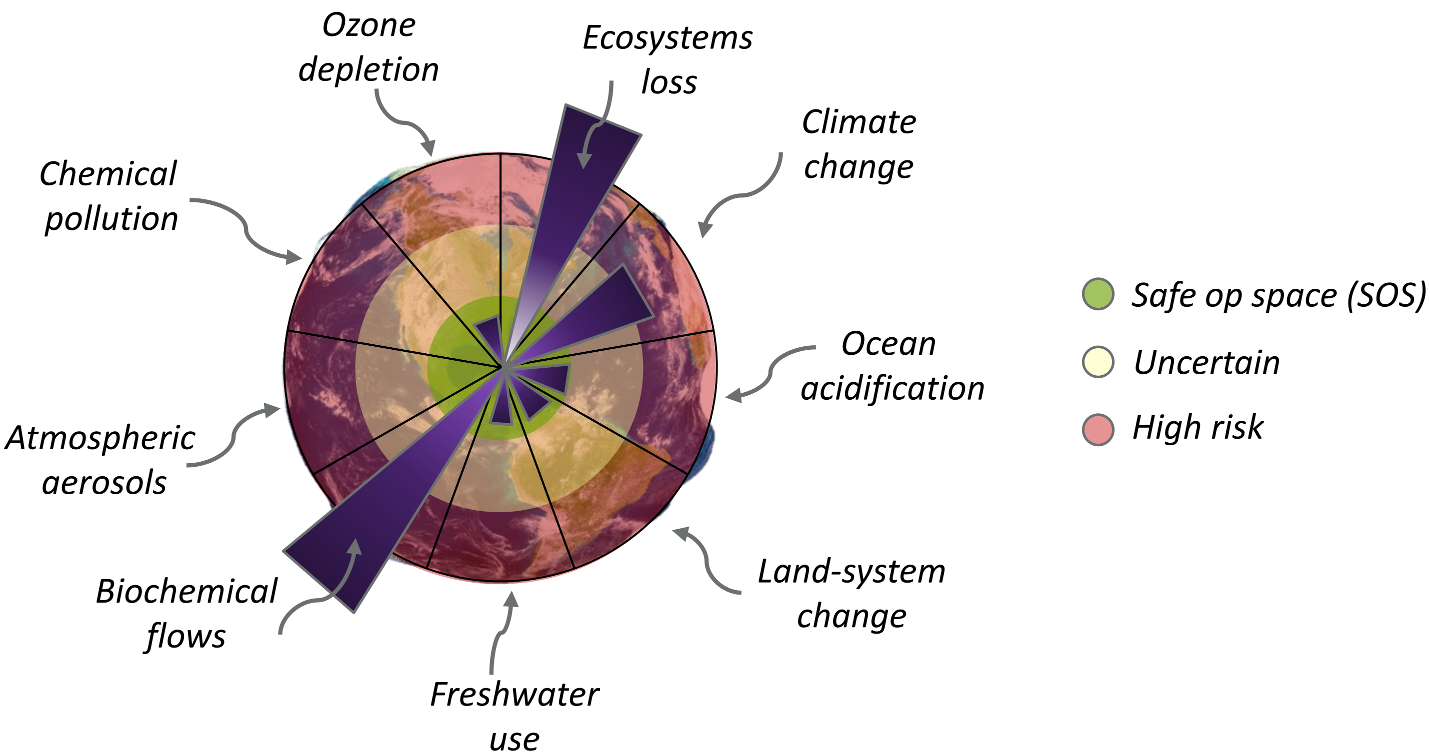
So as to:

- Minimise the total cost of electricity generation
- Minimise the environmental impact

Algunaibet, I., Pozo, C., Galán-Martín, A., Huijbregts, M., Mac Dowell, N., Guillén-Gosálbez, G.* *Energy and Environmental Science*, 12-6, 1890-1900, 2019.

Methodology: Planetary boundaries

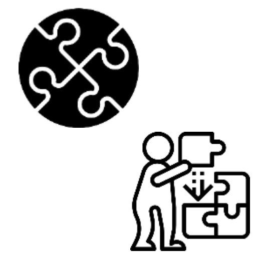
- Nine **Earth-System Processes (ESPs)** key for resilience*



*J. Rockstrom, W. Steffen, K. Noone, A. Persson, F. S. Chapin, E. Lambin, T. M. Lenton, M. Scheffer, C. Folke, H. J. Schellnhuber, B. Nykvist, C. A. de Wit, T. Hughes, S. van der Leeuw, H. Rodhe, S. Sorlin, P. K. Snyder, R. Costanza, U. Svedin, M. Falkenmark, L. Karlberg, R. W. Corell, V. J. Fabry, J. Hansen, B. Walker, D. Liverman, K. Richardson, P. Crutzen and J. Foley. *Ecology and Society*, 14, 32, 2009.

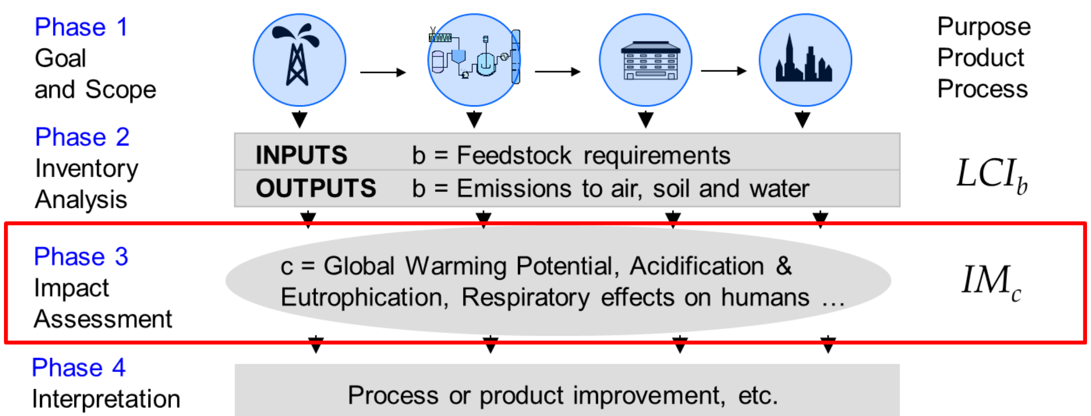
Methodology: Planetary boundaries

- Link electricity generation with the Earth's ecological limits:
  - **Downscale PBs** to regional and sectoral level



$$SOS_p \cdot \frac{POP^{US} ???}{POP^{World}} \cdot \frac{GVA^{USpower}}{GVA^{US}} = SoSOS_p \quad \forall p$$

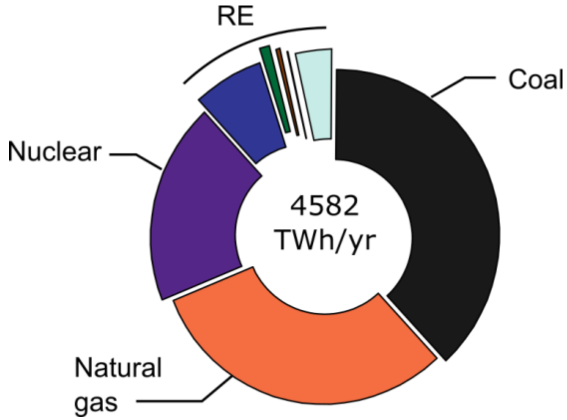
  - **Characterize environmental flows** in terms of ESP contributions

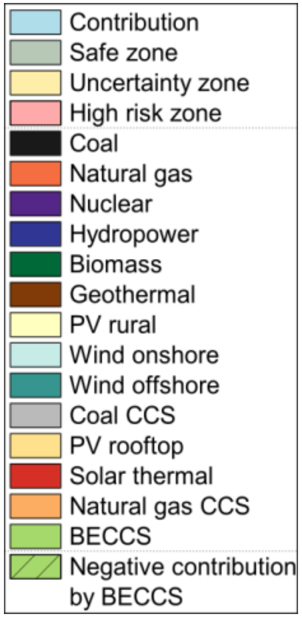


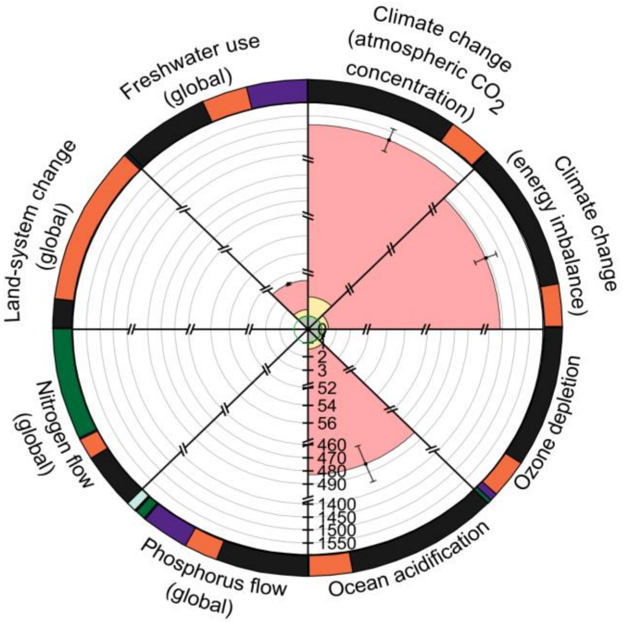
$$ESP_{pi} = \sum_l CF_{lp} LCI_{li} \quad \forall p, i$$

M.W. Ryberg, M. Owsianiak, K. Richardson, M.Z. Hauschild. *Ecological Indicators*, 88, 250-262, 2018.

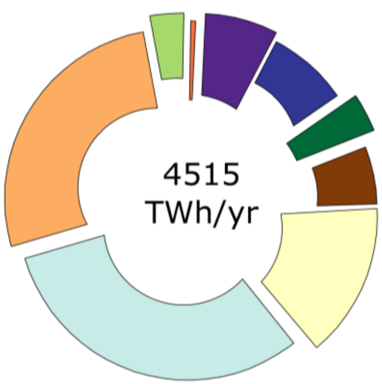
Business as usual

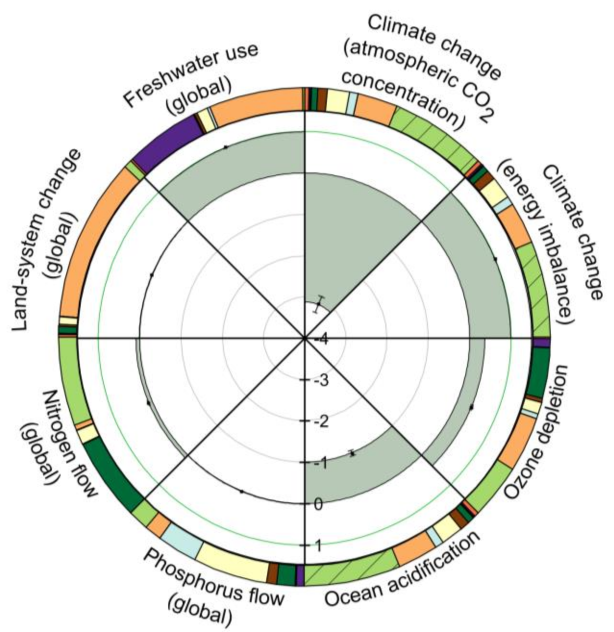






Minimum transgression solution





Conclusions

- Process Systems Engineering can be applied to solve a wide range of sustainability problems
- Main applications at the multi-site and single-site levels
- Improvements in sustainability can be attained by combining systems thinking, optimisation and life cycle thinking
- Future directions: provide decision-support tools to underpin the transition towards a more sustainable chemical industry & address global challenges

Take-home message

PSE concepts and tools provide a general framework to address a wide variety of relevant problems related to our sustainable development

Acknowledgements

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Diego Freire
Sebastiano D'Angelo
Iasonas Ioannou
Valentina Negri
Tim Forster

The coupling of optimization techniques and LCA

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Department of Chemistry and Applied Biosciences