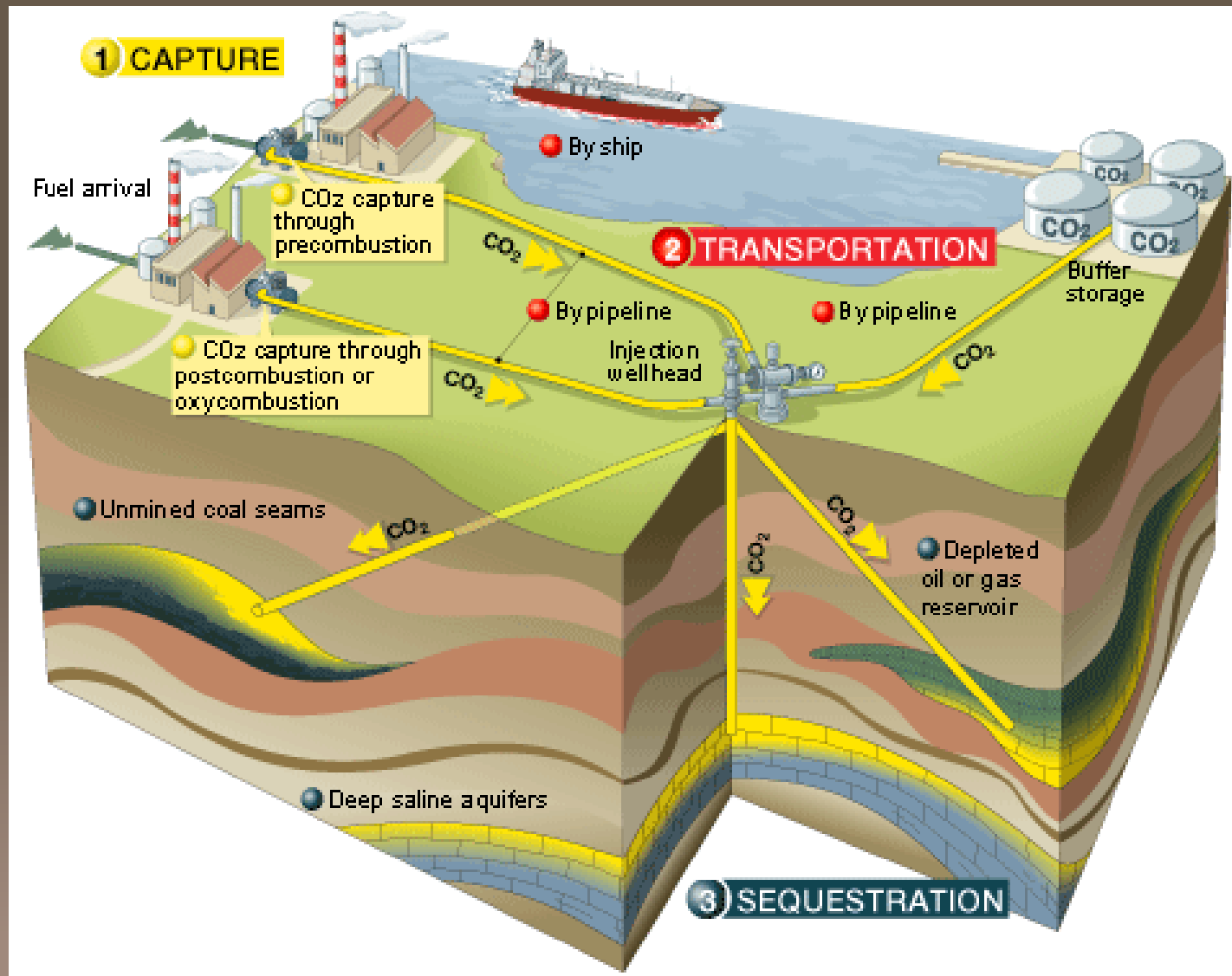


CO₂ capture

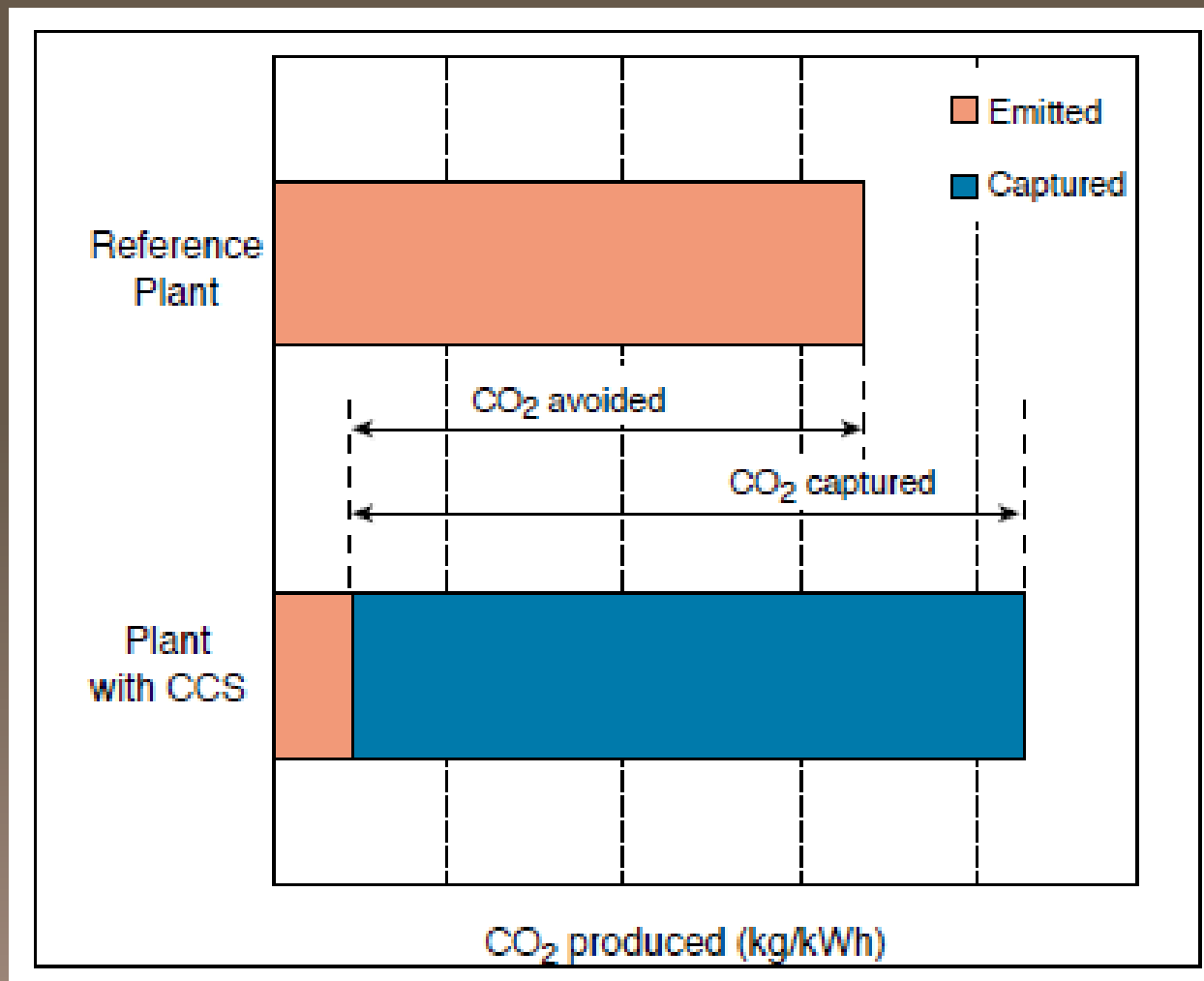
Industrial needs for simulation tools

Jing ZHAO, Total E&P

CCS (Carbon dioxide Capture and Sequestration)



CO₂ Capture



Source : IPCC Special Report on Carbon Dioxide Capture and Storage

CO2 Capture– two different application cases

	Post combustion	Natural gas
Specifications	% removal rate	50ppm – 2%
Pressure range	Low pressure	Low – High pressure
Constituents	O ₂ , N ₂ , SOX, NOX	Hydrocarbons, sulfur compounds
Techniques	Solvent (MEA)	Solvent (DEA, MDEA+X) Membrane etc.

Other technologies :

- ☐ Pre-combustion
- ☐ oxy-combustion
- ☐ chemical looping combustion

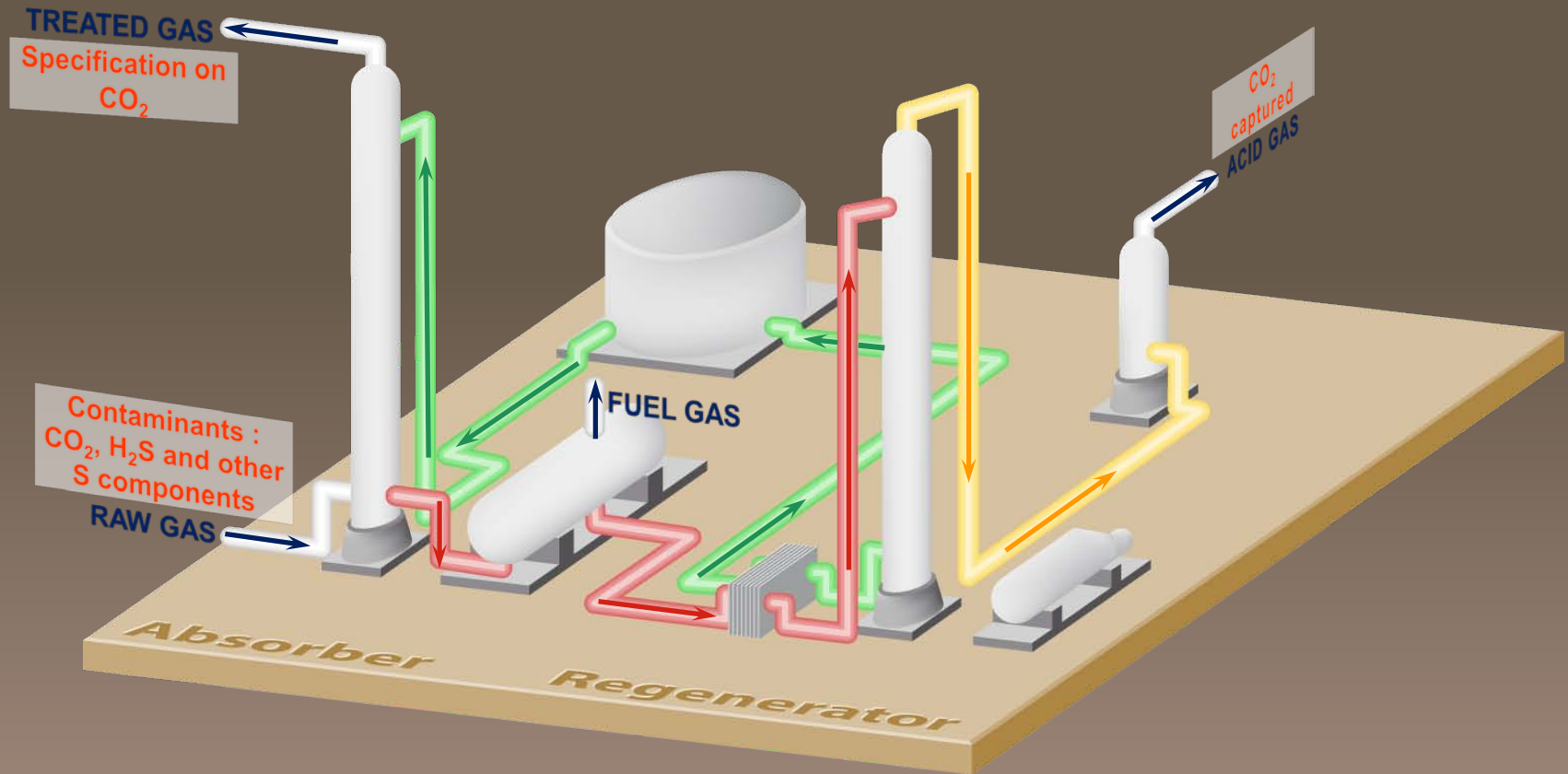
MEA



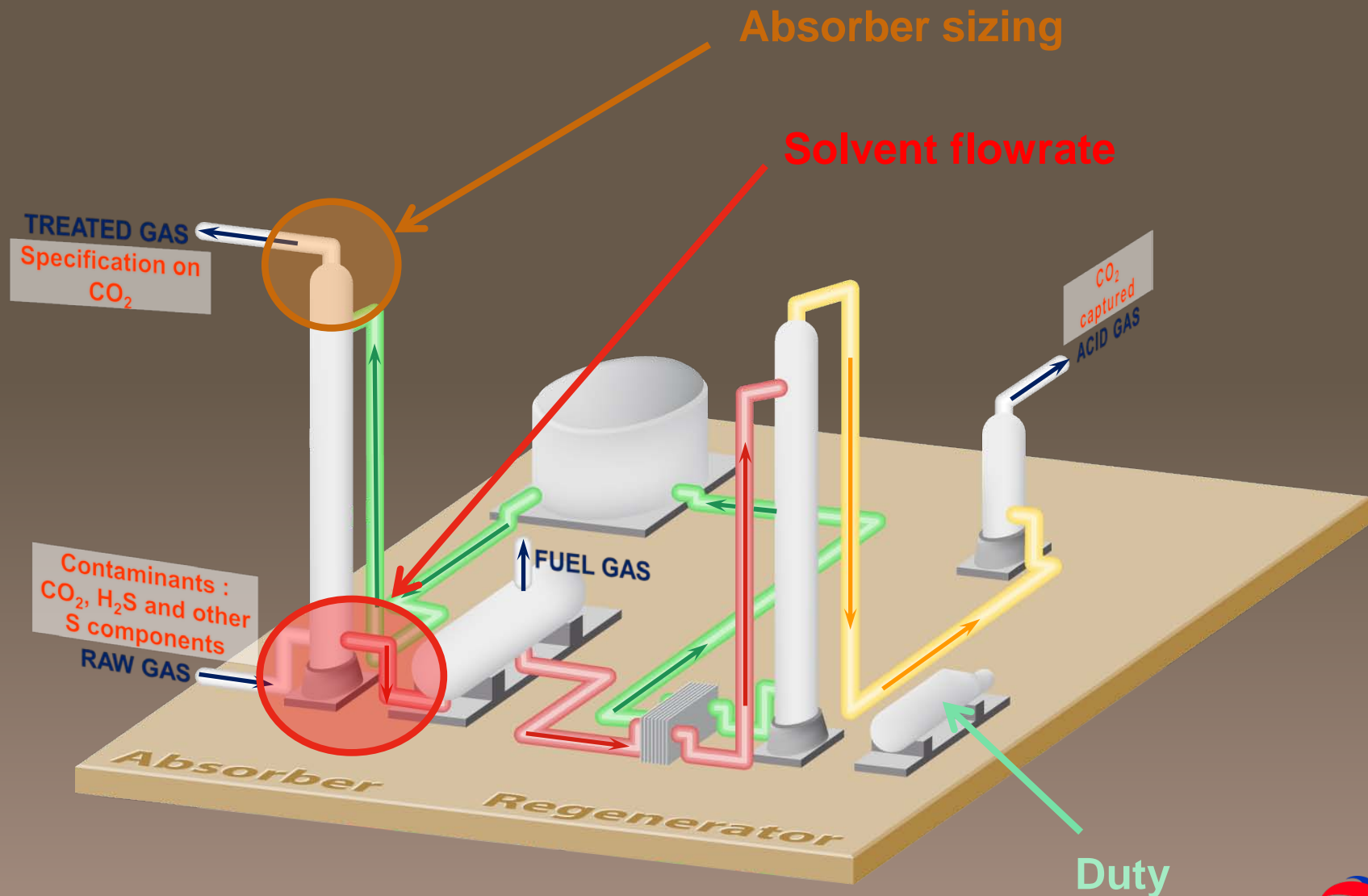
DEA



CO₂ capture by amine



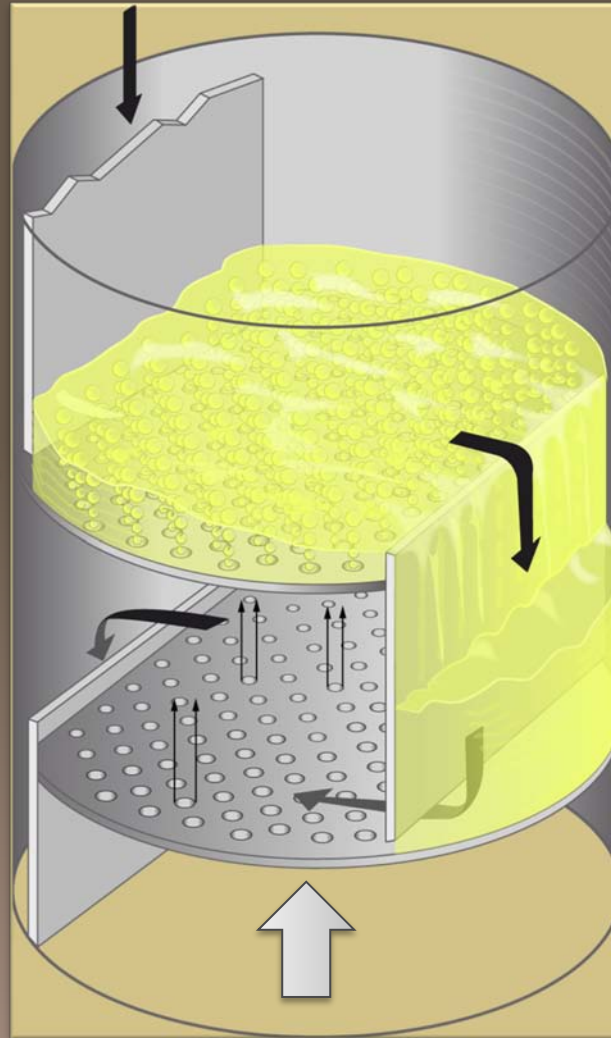
Process design needs



Column inside

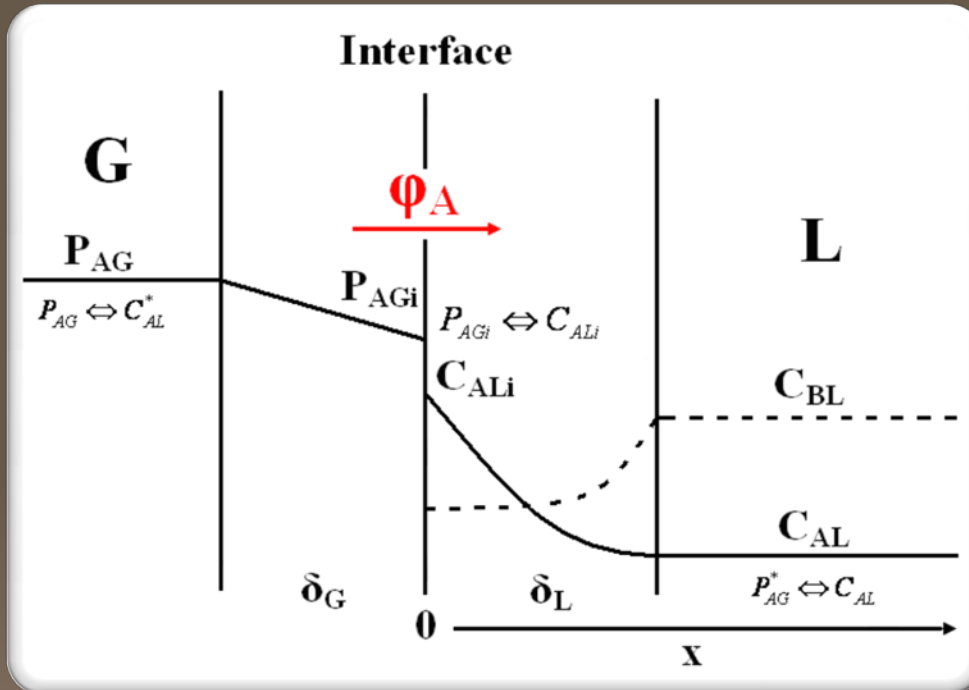
Solvent flow

Contact zone



Gas flow

Mass transfer with chemical reaction



Thermodynamics

$$EM = 1 - \frac{1}{\exp \left[\left(\frac{1}{k_G} + \frac{H_{\Lambda}^{Liq}}{E k_L} \right)^{-1} a \frac{P_{\Lambda}^{Gaz}}{Q_{\Lambda}^{Gaz}} \right]}$$

Kinetic

- Chemical reactions

Arrows in the diagram point from the terms in the equation to their respective categories: k_G and k_L are kinetic; H_{Λ}^{Liq} and a are thermodynamic.

Contactor parameters

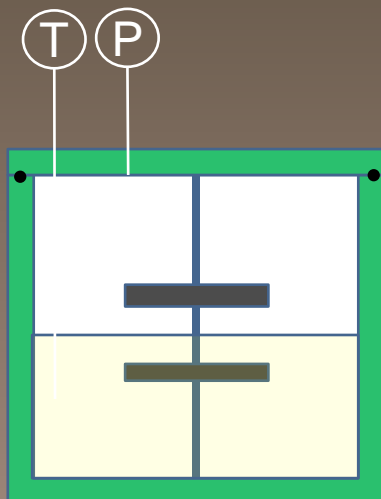
- Hydrodynamic
- Liquid/gas properties

Mass transfer efficiency calculation

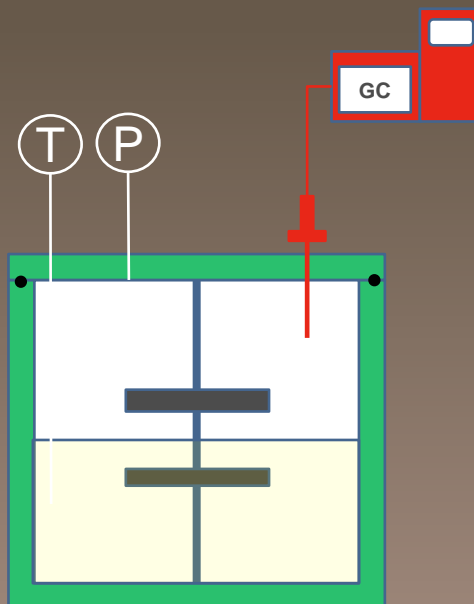
- Complex because of chemical reactions along with mass transfer
- Multi-components
- No classical values available

A good tool is half a job

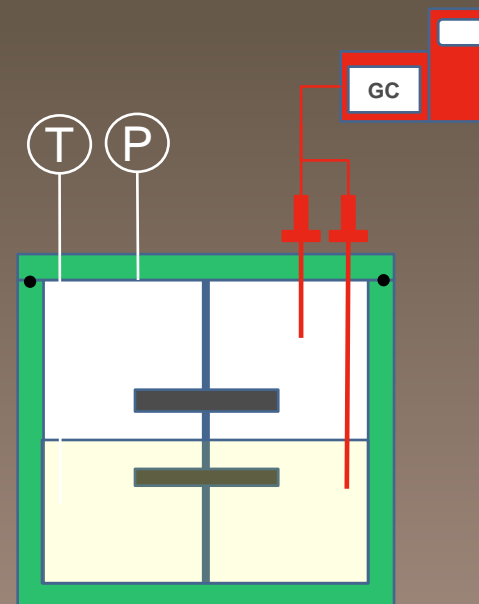
Synthetic method
(Mass balance)



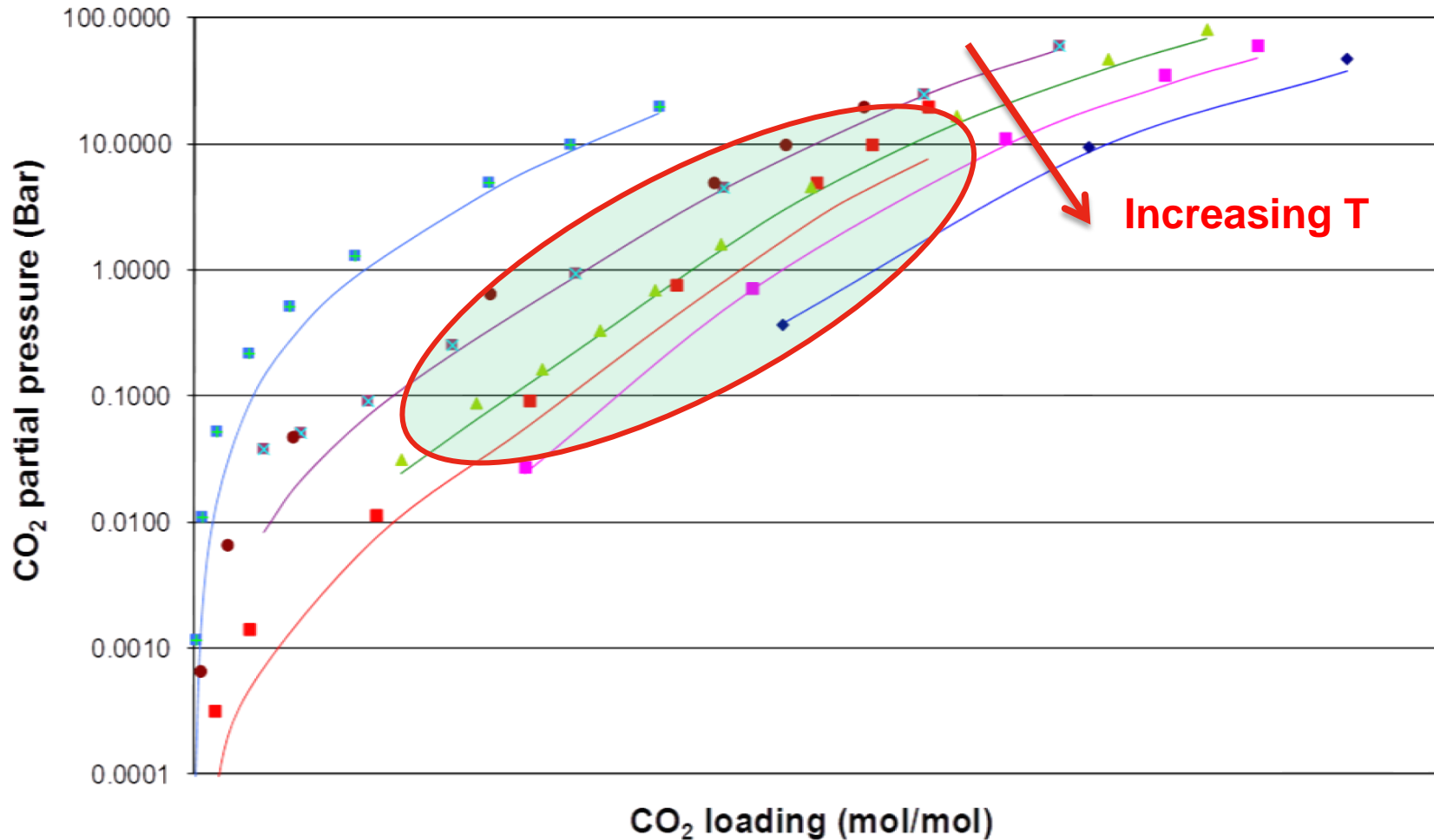
Synthetic-analytic method
(Gas analysis & Mass balance)



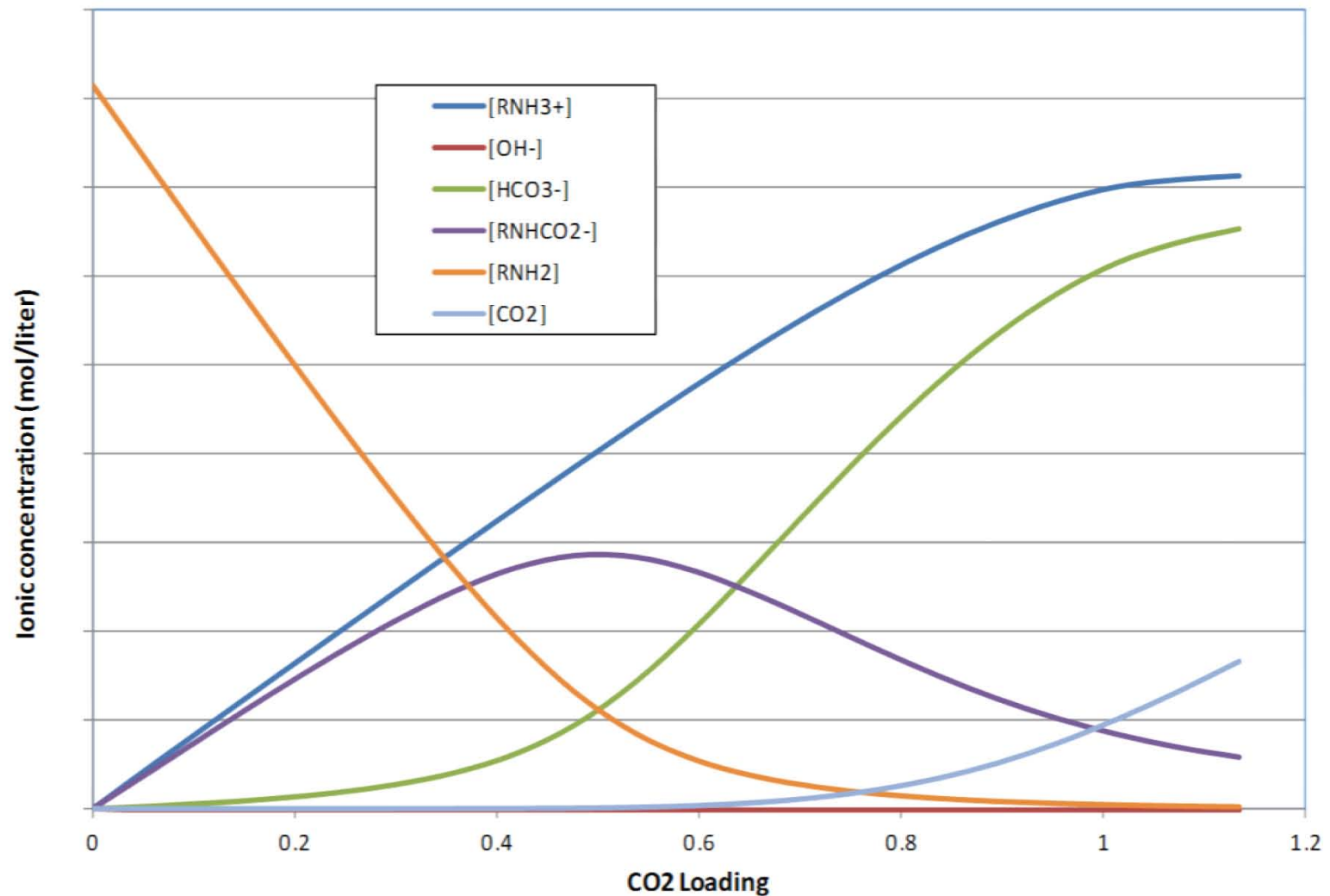
Analytic method
(Gas & liquid analysis)



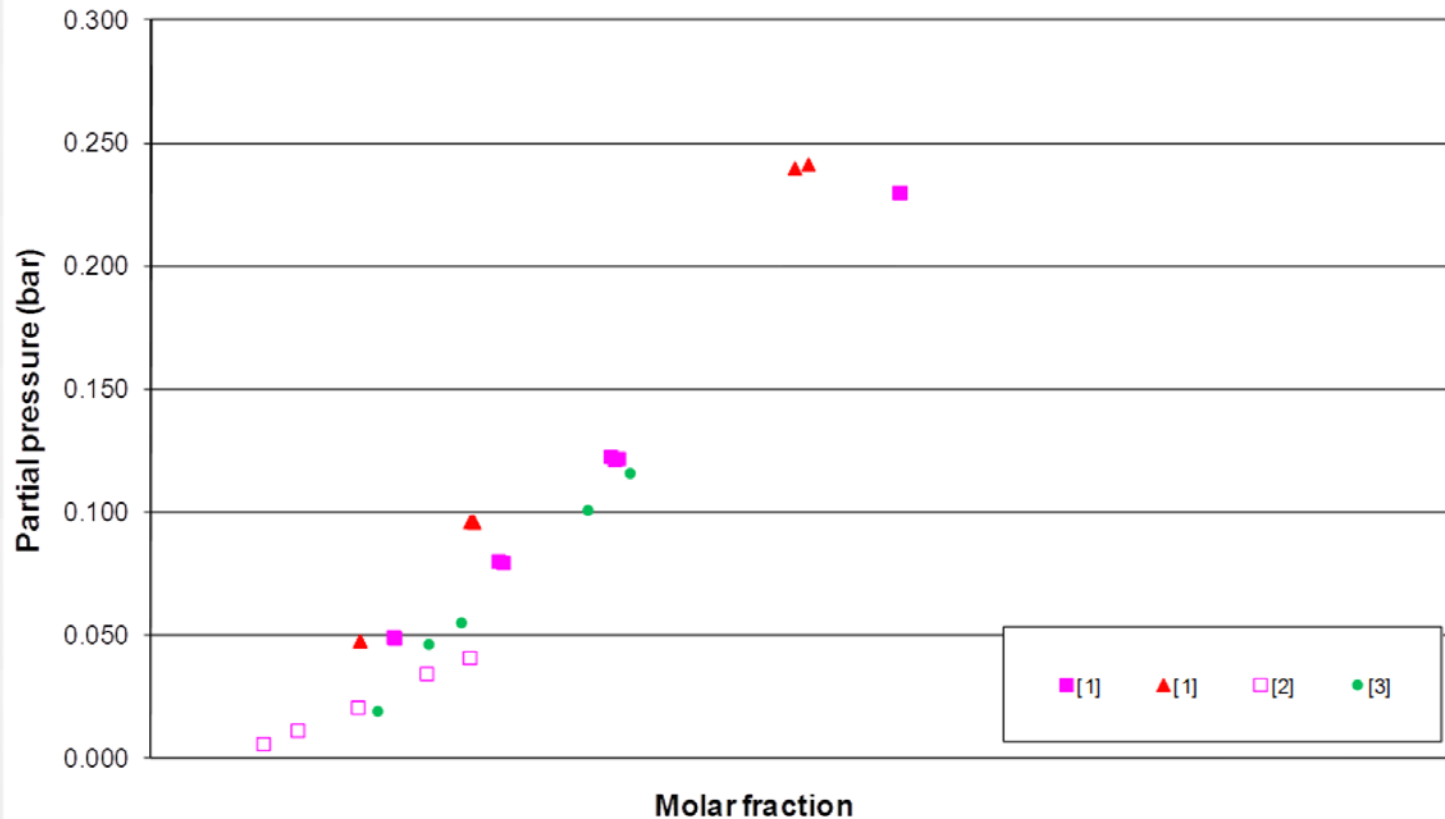
What kind of precision we need?



What kind of precision we need?



What kind of precision we need?



Conclusion

Process engineers' challenges and needs :

- ☐ **Experimental challenge to face the more stringent demand**
- ☐ **More precise modeling is necessary to reduce design margin and optimize the operations**
- ☐ **Fast, robust and flexible models**

“Without CCS, the long term role of gas may be limited to a flexible back-up and balancing capacity where renewable energy supplies are variable.”

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