Integrated, High Fidelity, Multiscale Process Models for the Process Industries

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Presented at Annual AIChE Meeting
November 7-12, 2010
Salt Lake City, Utah

enterprise level. Major difficulties in developing mathematical models that integrate the various parts of the chemical supply chain result from the huge differences in length and time scales in the supply chain and the number of chemical species considered at each level. Furthermore, at the longer scales, new situations can arise that may not be reliably predicted from the basic models.

Process Simulation: A Revolution

Process simulation, which emerged in the 1960s, has become one of the great success stories in the use of computing in the chemical industry. For instance, steady-state simulation has largely replaced experimentation and pilot plant testing in process development for commodity chemicals, except in the case of reactions having new mechanisms or requiring new separation technologies. Tools for steady-state process simulation are nowadays universally available to aid in the decisions for design, operation, and debottlenecking; they are part of every process engineer's toolkit. Their accuracy and predictive ability for decision-making is widely accepted to make routine plant trials and most experimental scale-up obsolete in the commodity chemicals industry.

The Process Industry Value Chain

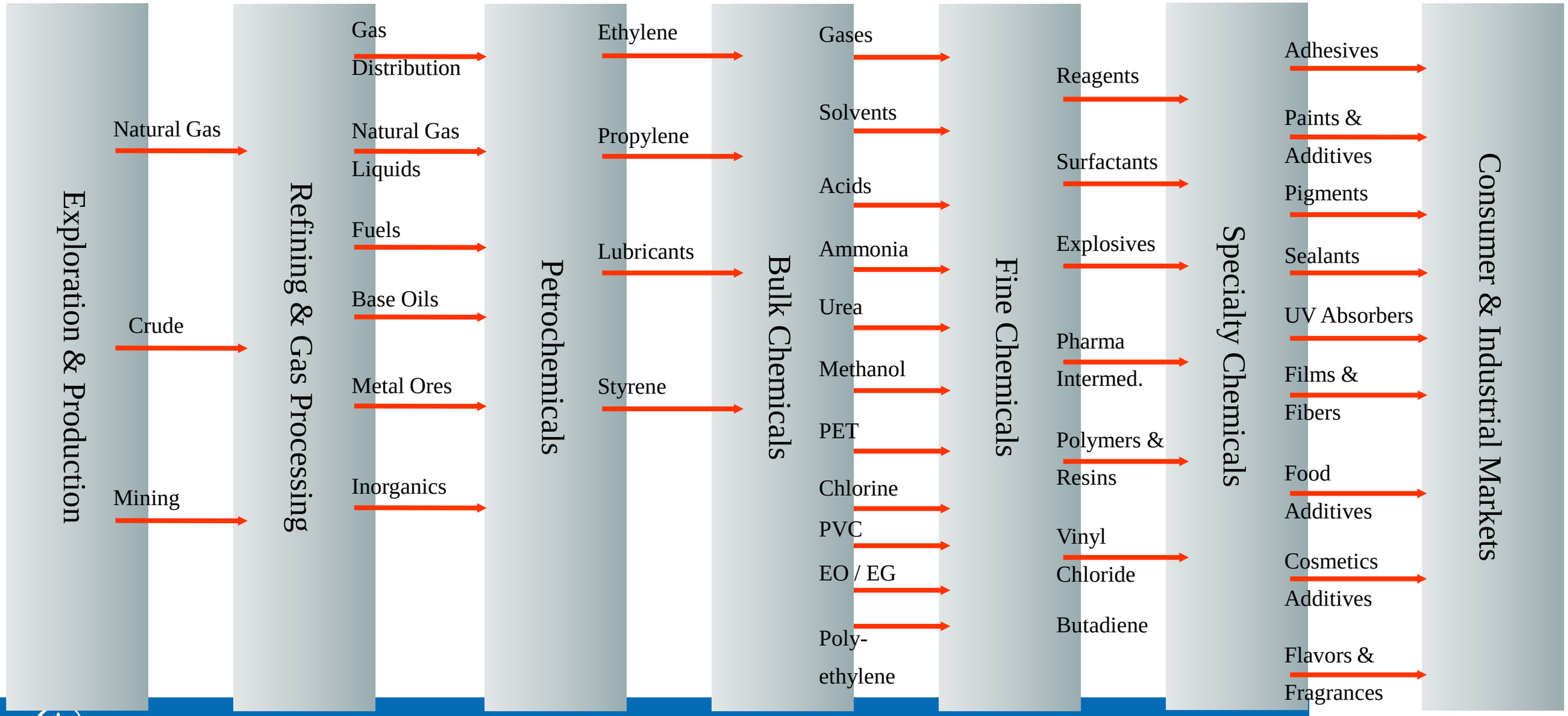
E&P

R&M

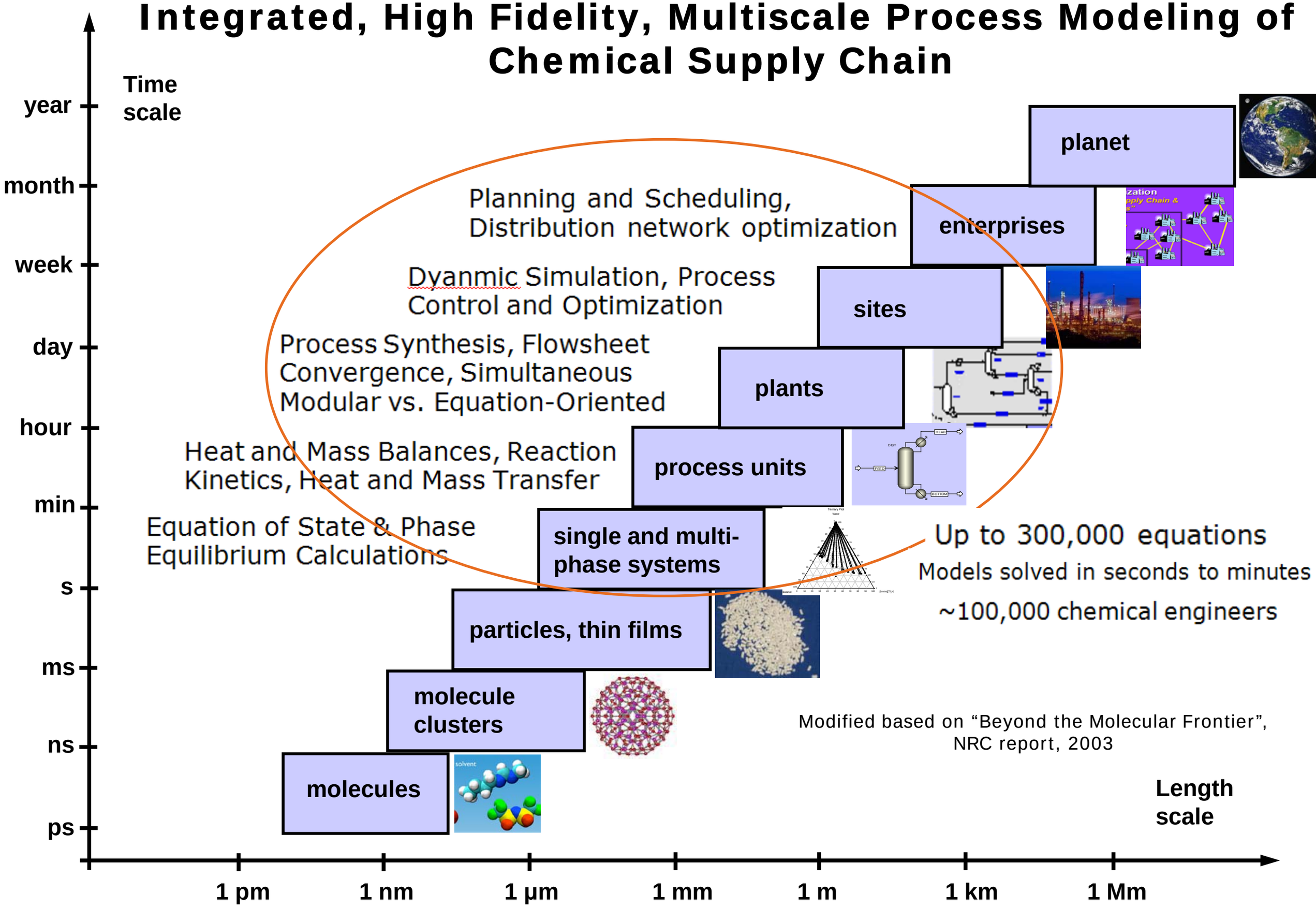
Bulk Chemicals

Polymers

Specialty Chemicals



Integrated, High Fidelity, Multiscale Process Modeling of Chemical Supply Chain



Driving Forces to Advance Process Modeling and Simulation

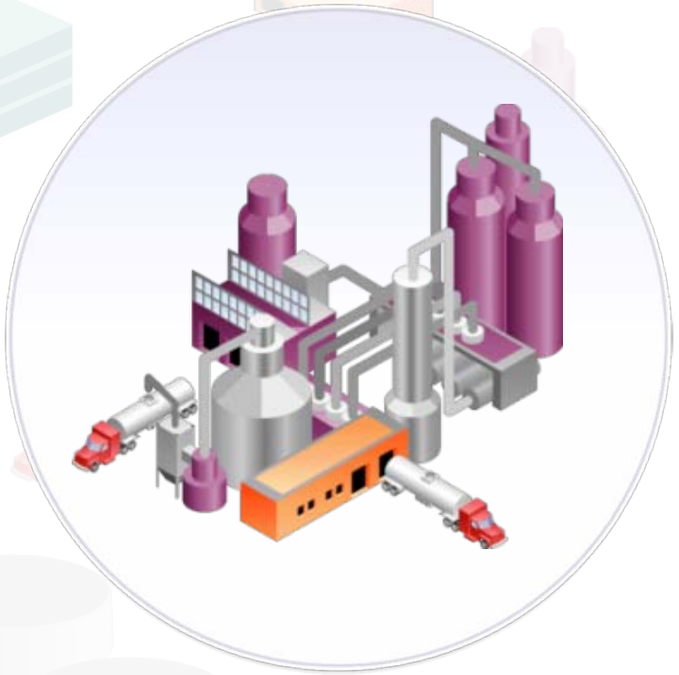
- Relentless advance in computing power and information technology
- Opportunities to bring economic value and societal impacts
- Innovations in science and engineering to model the physical and chemical world based on 1st principles

Evans, L., CACHE Trustees' meeting, 2009

IT Trends

Social Networking

Wireless Sensors



Virtualization & Cloud Computing

Smart Phones

High Performance Computing

IT Trends and Product Innovation

Best-in-class Products

Functional Enhancements

Robustness and Reliability

Problem Size and Speed

User Experience

Localization

UI Modernization

Integrated Best Practices

Collaboration

Business Processes

Common Models & Data

Common Reporting & Analysis

Service-oriented Architecture

Industry Standards

Outline

- Opportunities to Bring Economic Value and Societal Impacts
- Innovations in Science and Engineering to Model Physical & Chemical World
  - CO_2 Capture Modeling
- Summary

Modeling Key Activities

In Chemicals

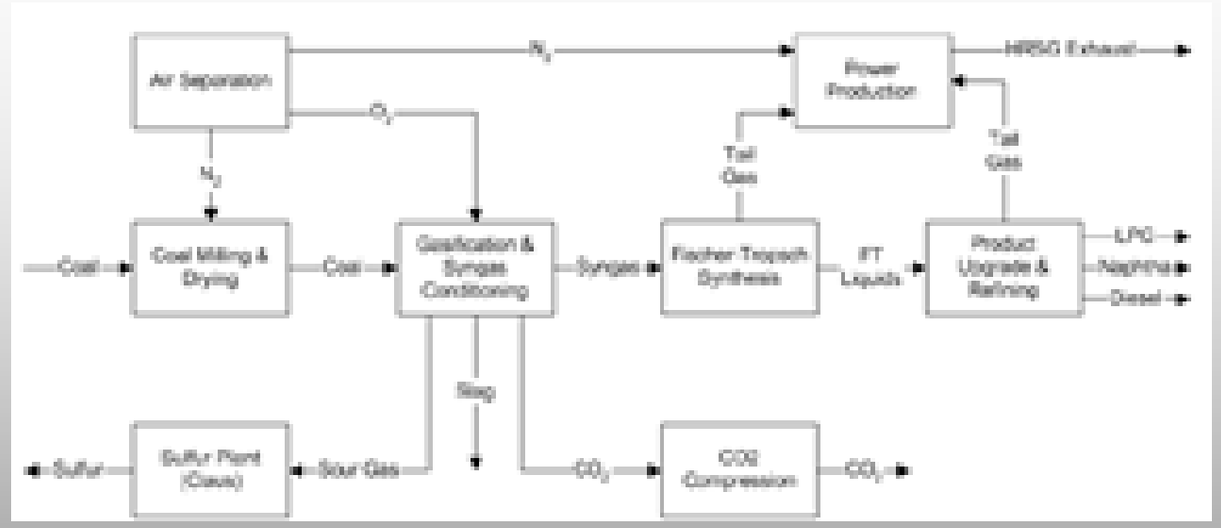
- Develop Conceptual Process Design
- Evaluate Capital and Operating Costs
- Verify Safety and Operability
- Support Plant Operations

BAARD

Develop Conceptual Process Design

Challenge | Solution | Result

- Maximize overall thermal efficiency of new coal-to-fuel (coal gasification) plants
  - Highly complex and integrated processes
  - Need to rapidly screen process alternatives



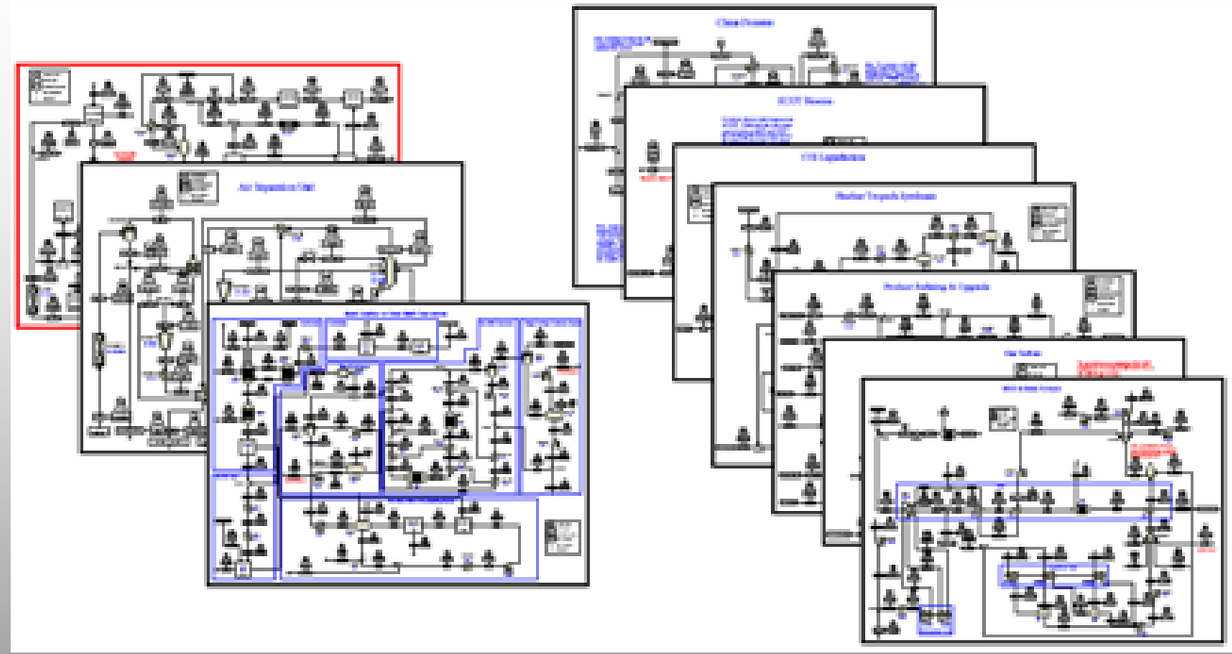
Reference: John Baardson and Steve Dopuch, Coal-to-Fuel Plant Simulation Studies for Optimal Performance and Carbon Management, Gasification Technologies Conference October 17, 2007

BAARD

Develop Conceptual Process Design

Challenge | **Solution** | Result

- Process simulation with hierarchical models representing key sections of the plant



Reference: John Baardson and Steve Dopuch, Coal-to-Fuel Plant Simulation Studies for Optimal Performance and Carbon Management, Gasification Technologies Conference October 17, 2007

BAARD

Develop Conceptual Process Design

Challenge | Solution | **Result**

- Global optimization of the whole plant
- Minimization of the parasitic energy load associated with carbon capture
- Rapid and efficient design

"Aspen Plus can be utilized for rigorous material and energy balances for CTL processes…to investigate…process efficiency improvements"

John Baardson, Baard Energy

Reference: John Baardson and Steve Dopuch, Coal-to-Fuel Plant Simulation Studies for Optimal Performance and Carbon Management, Gasification Technologies Conference October 17, 2007

BASF

Evaluate Capital and Operating Costs

Challenge | Solution | Result

BASF
The Chemical Company

- Increase capacity and reduce operating costs
- Develop better designs for new plants

Ref: Dr. Axel Polt (BASF), AspenWorld 2004, Orlando, Florida.

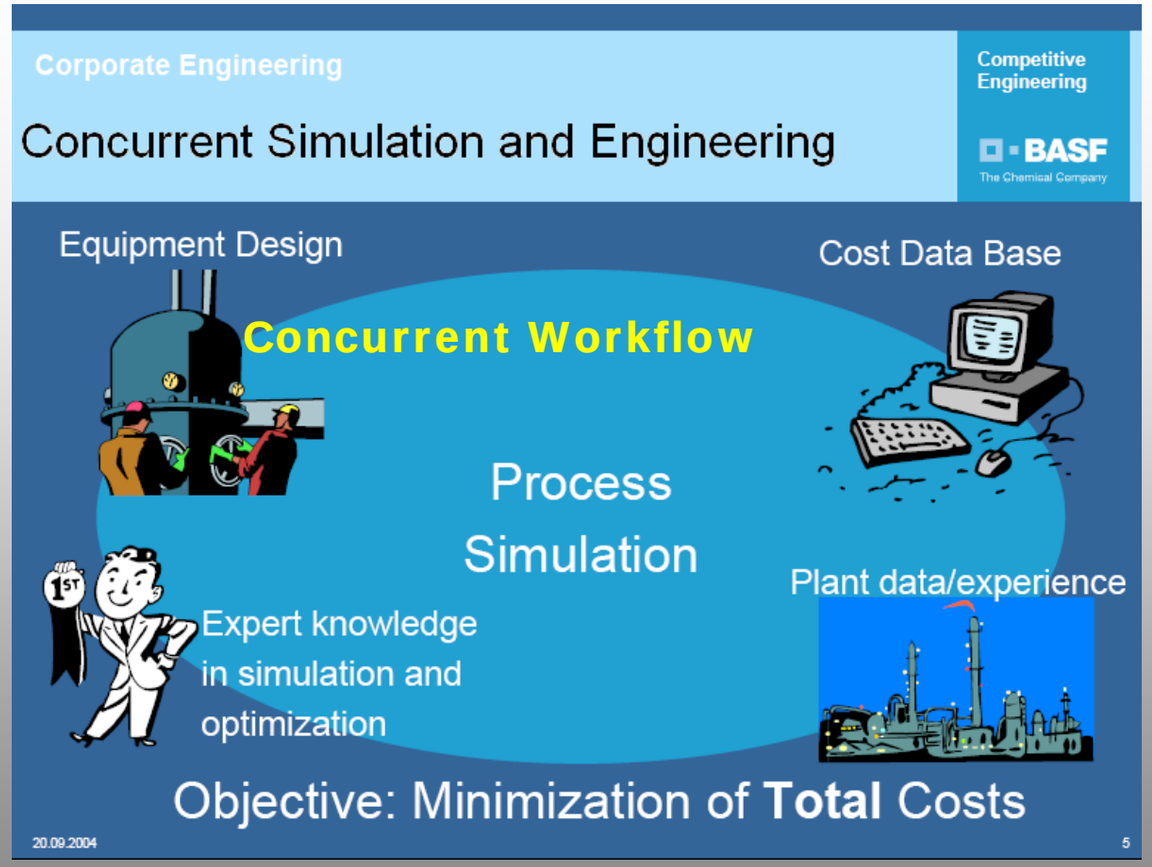
BASF

Evaluate Capital and Operating Costs

Challenge | **Solution** | Result

BASF The Chemical Company

- Cost optimization through concurrent process simulation and process engineering



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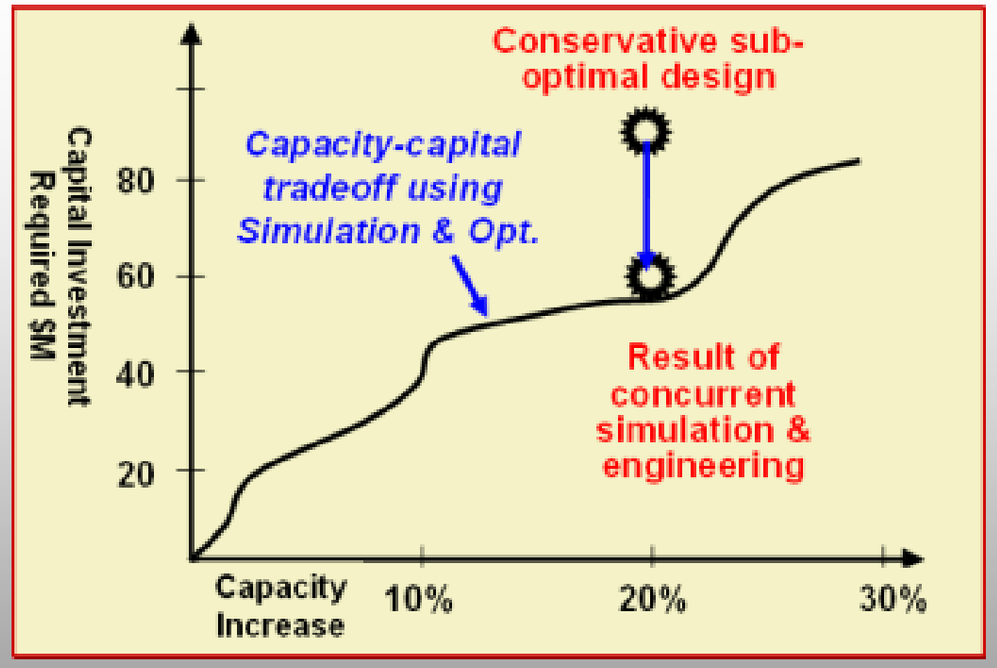
BASF

Evaluate Capital and Operating Costs

Challenge | Solution | **Result**

BASF
The Chemical Company

- Integrated approach saves 10-30% capital *
- Energy saving of $0.5 MM to $2 MM
- Smooth transition from conceptual engineering to detailed engineering



Ref: Dr. Axel Polt (BASF), AspenWorld 2004, Orlando, Florida.

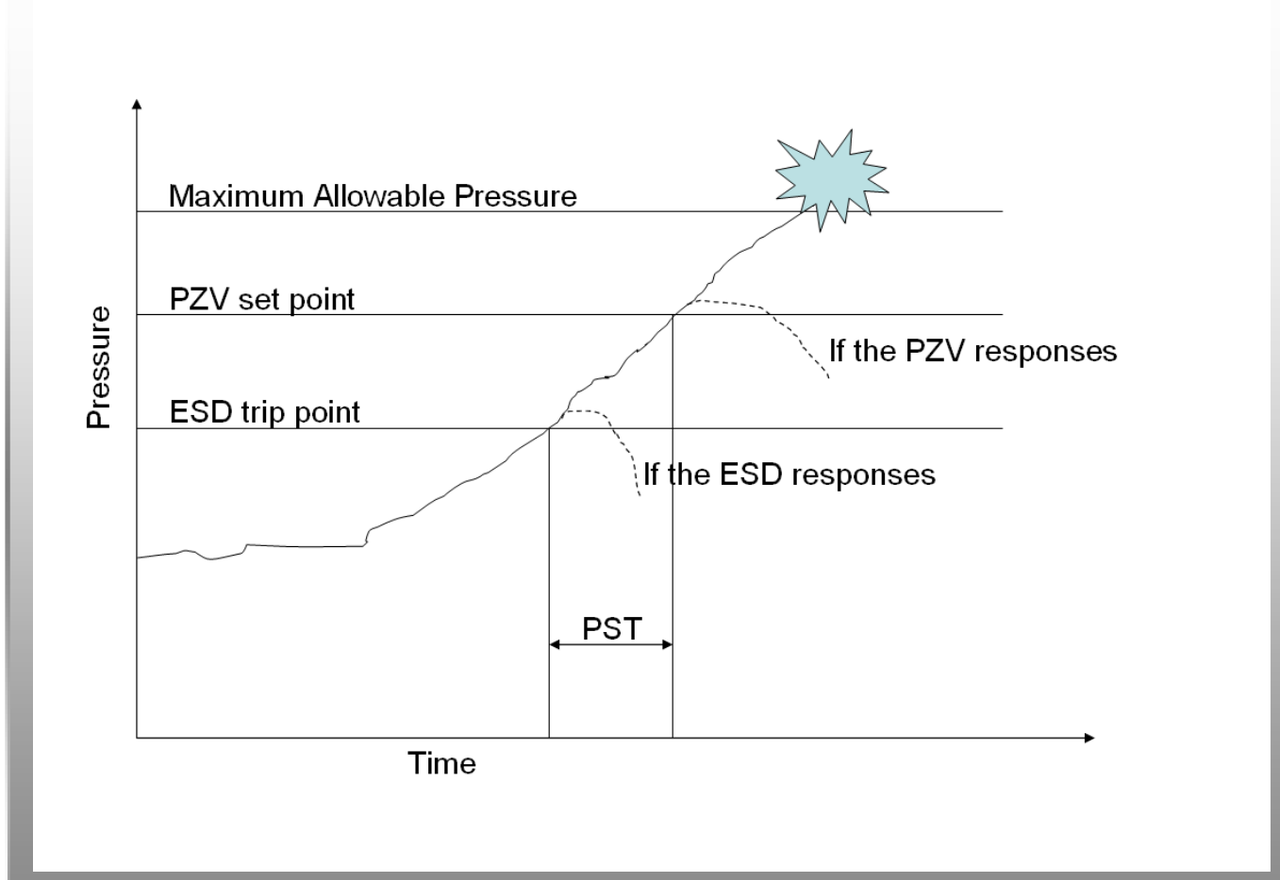
* BASF annual capital spend: $750M–$1.1B

Saudi Aramco

Verify Safety and Operability

Challenge | Solution | Result

- Design the control system for a debutanizer column
- Prevent hazardous plant events from occurring by estimating the process safety response time



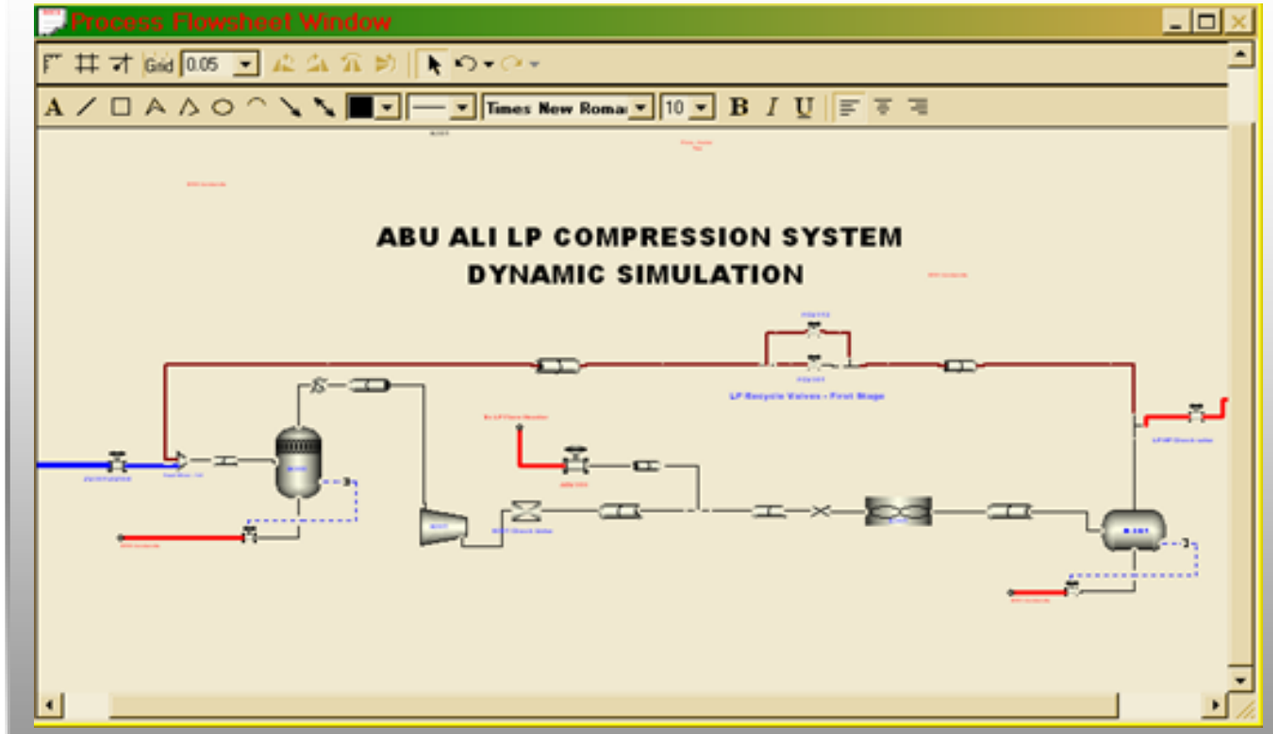
Ref: Kadhim Mohammed, Saudi Aramco, AspenTech User Conference, Berlin, April 2008

Saudi Aramco

Verify Safety and Operability

Challenge | **Solution** | Result

- Steady state process models were built and validated with design and plant data
- Models were converted to dynamic models for safety analysis



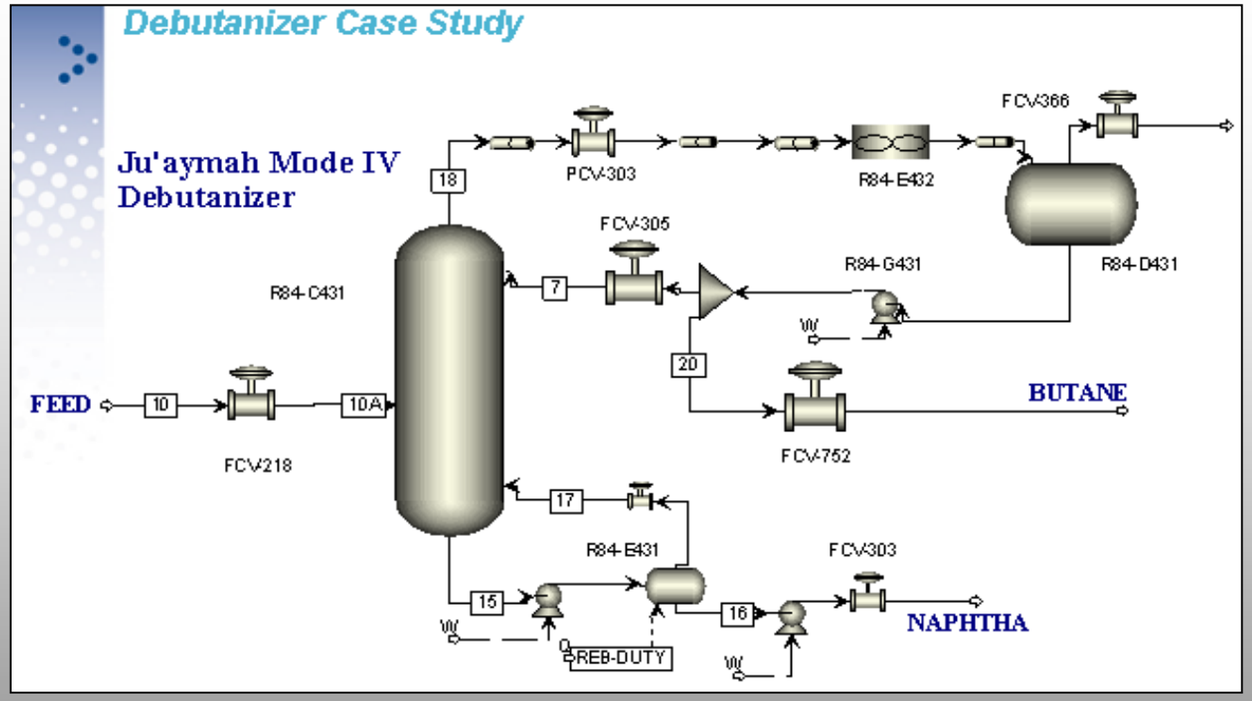
Ref: Kadhim Mohammed, Saudi Aramco, AspenTech User Conference, Berlin, April 2008

Saudi Aramco

Verify Safety and Operability

Challenge | Solution | **Result**

- The valve closure time was crucial to the safe operation of the debutanizer column
- The emergency shutdown scan time was identified, thus preventing possible plant shutdown, damage to equipment, and a halt in production



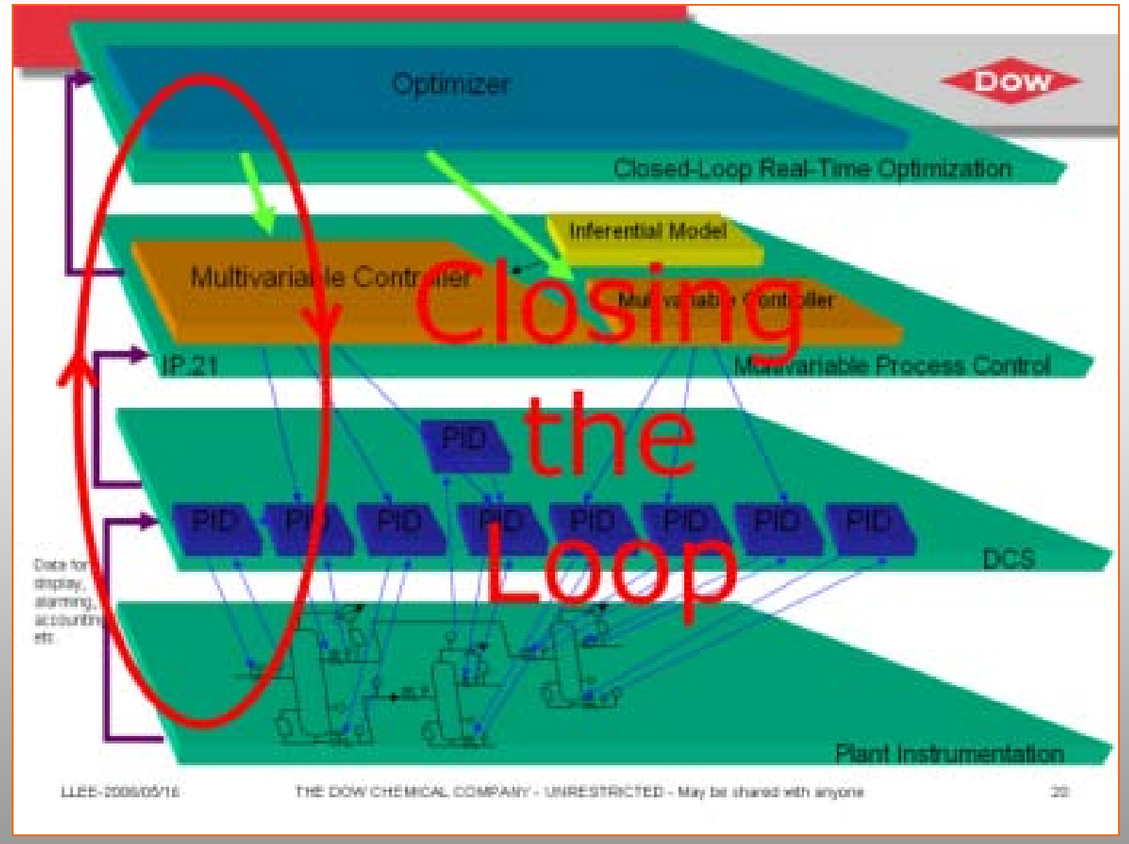
Ref: Kadhim Mohammed, Saudi Aramco, AspenTech User Conference, Berlin, April 2008

Dow

Support Plant Operations

Challenge | Solution | Result

- Optimization of ethylene production
  - Increase asset utilization year after year
  - Maximize asset capability for alternative feedstocks and off-design operations
  - Faster, on-time, flawless quality products



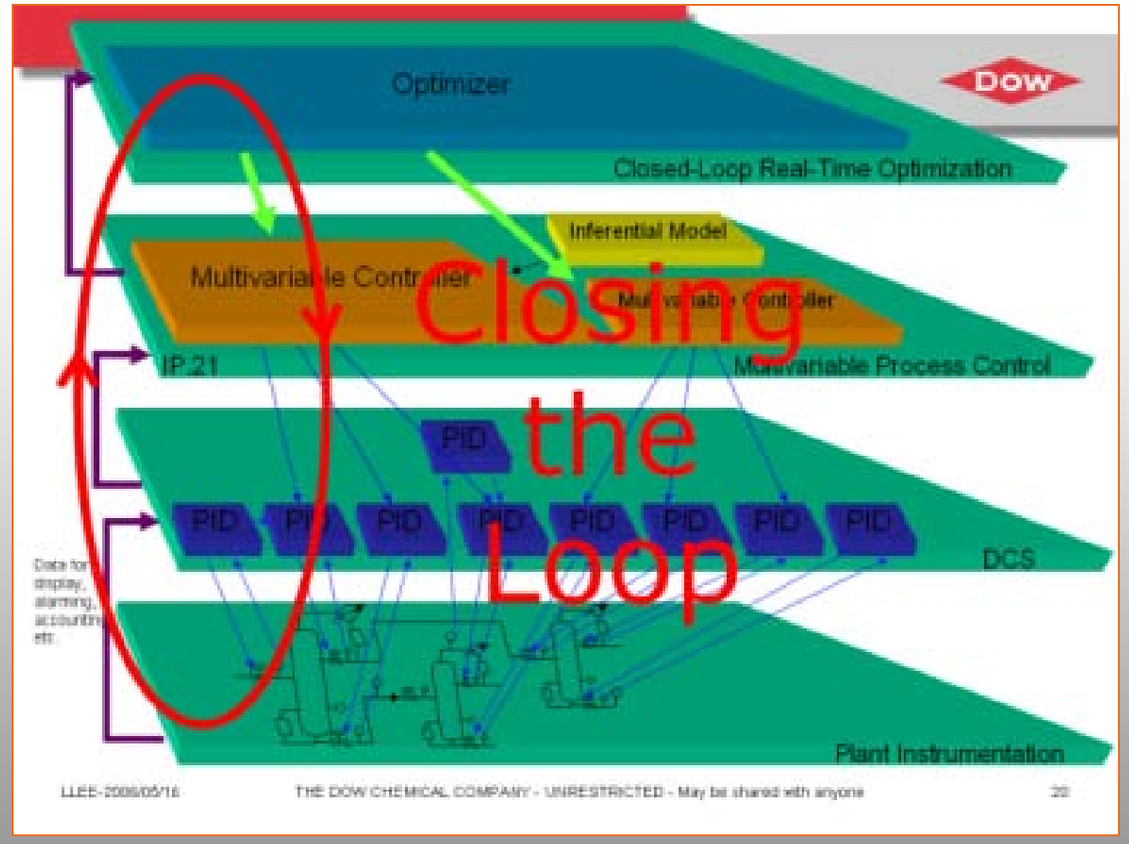
David Vickery (Dow), Process Modeling Innovation Forum, Jan 2007 and David Starks (Dow), Aspen Global User Conference, May 2009

Dow

Support Plant Operations

Challenge | **Solution** | Result

- EO process models used to support Real-Time Optimization together with Advanced Process Control to “Close the Loop”
- Apply to 15 Sites globally



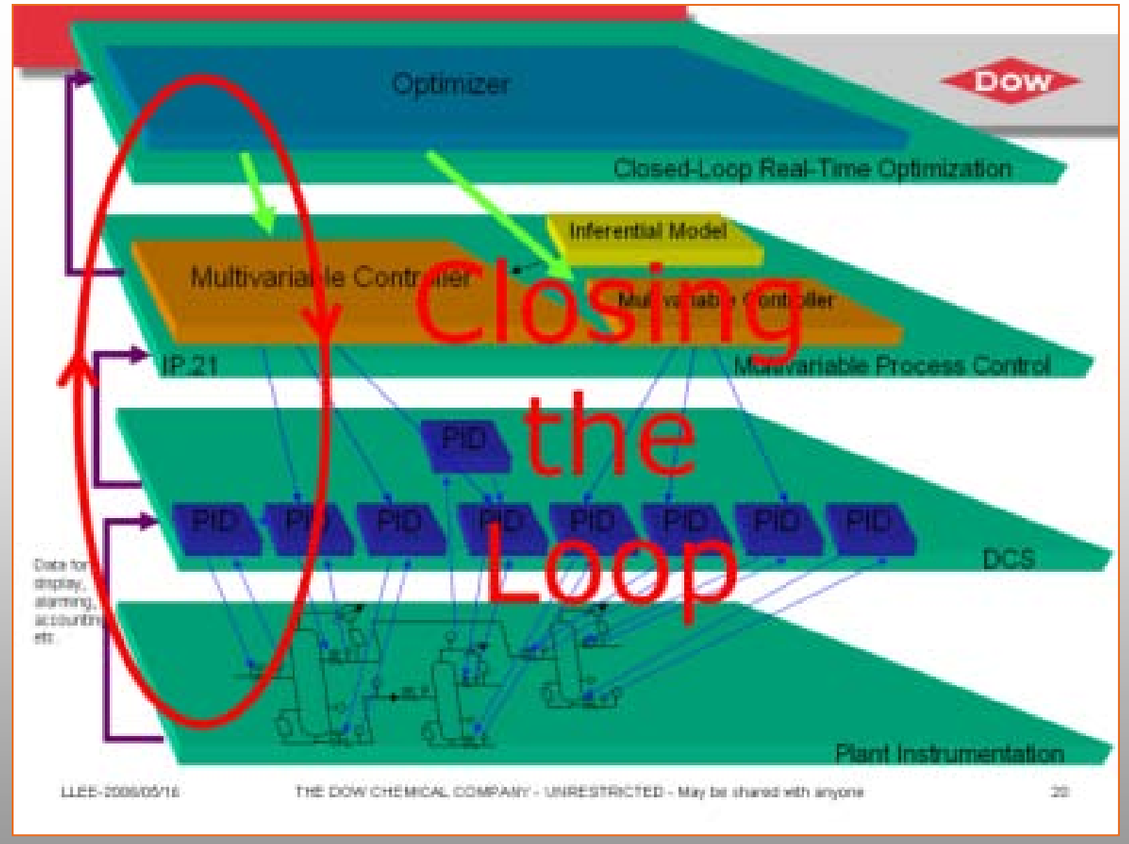
David Vickery (Dow), Process Modeling Innovation Forum, Jan 2007 and David Starks (Dow), Aspen Global User Conference, May 2009

Dow

Support Plant Operations

Challenge | Solution | **Result**

- Production capacity increased 11%
- Unit variability decreased 45%
- Off-spec decreased to zero; recycles 20% less
- Reduced start-up time by 60%
- Higher production and efficiency, including steam energy savings
- Emissions reduced by 80+%
- Feed rate increased 8%
- Nearly $700MM in cumulative benefits 2000-2009



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Process Modeling & Simulation Generates Economic Values

- Improve engineering efficiency by up to 30%
- Reduce capital costs by 10-30%
- Reduce energy consumption by over 10%
- Increase production capacity by up to 10%
- Lower other variable costs by 2-5%

Improve
design and operation
of chemical plants

Outline

- Opportunities to Bring Economic Value and Societal Impacts
- Innovations in Science and Engineering to Model Physical & Chemical World
  - CO_2 Capture Modeling
- Summary

Transformational Technology Innovation

Engineering Software
- Distillation Algorithm
- Electrolyte Properties
- Heat Exchanger Design
- Cost Estimation
- Dynamic Simulation
- Production Planning

PC / Desktop Revolution
- Economic Evaluation
- Heat Exchanger Design and Energy Analysis
- Basic Engineering Collaborative Environment
- Polymer Process Modeling
- Model Predictive Control (APC)
- Real Time Optimization
- Planning Tool
- Retail Gasoline Distribution

Enterprise Integration
- Integrated Engineering, Manufacturing & Supply Chain
- Integrated Simulation, Economics, Heat Exchanger Design and Energy Analysis
- Integrated Basic Engineering
- Integrated Manufacturing
- Integrated Supply Chain
- Enterprise Master Data Model
- Solvent Screening
- **CO_2 Capture**

1970s 1980s 1990s 2000s 2010

Chemical Engineering Science

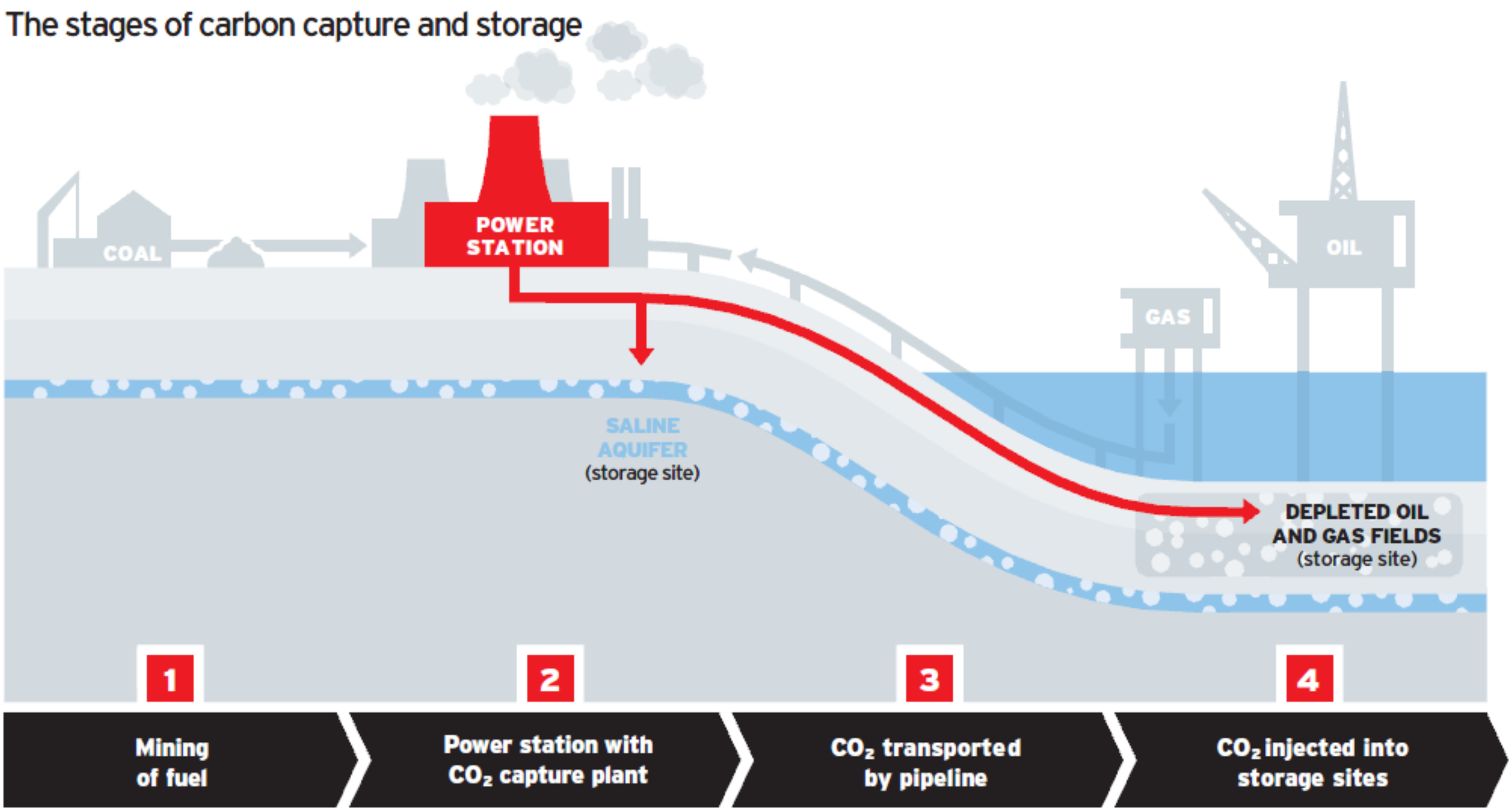
Simulation Methodology

Mathematical Algorithms

Software Engineering

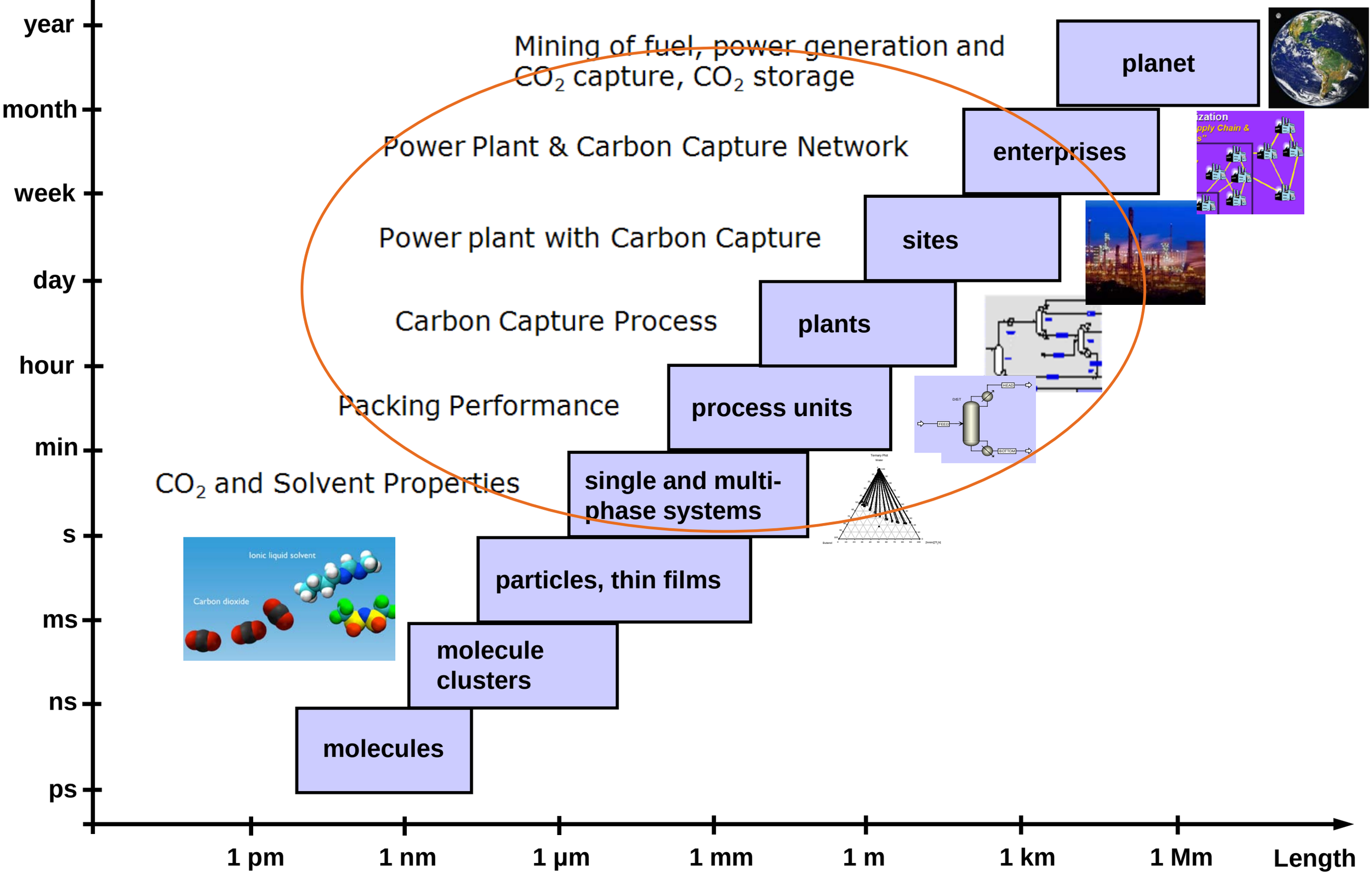
Industry Best Practice

Carbon Capture and Storage



The Daily Telegraph, June 10, 2010

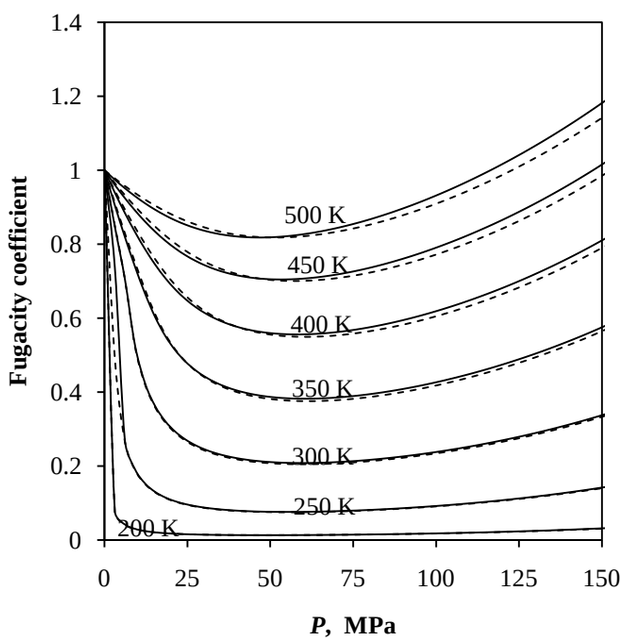
Integrated, High Fidelity, Multiscale Process Modeling of CO_2 Capture & Storage

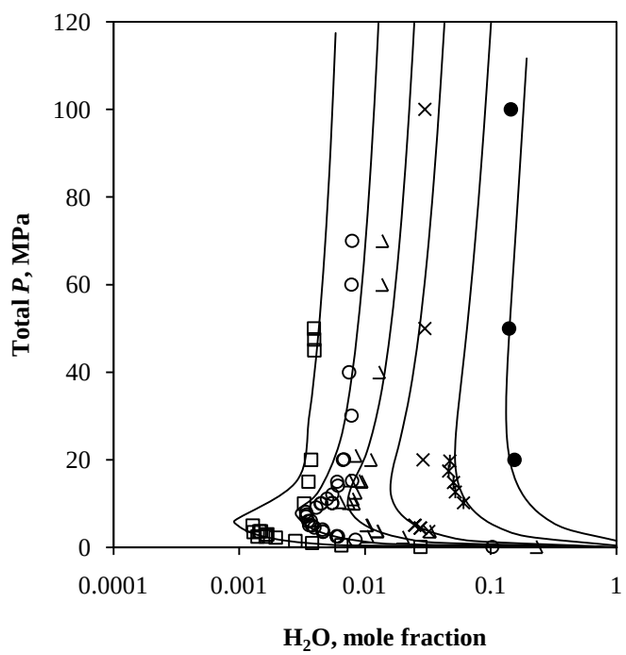


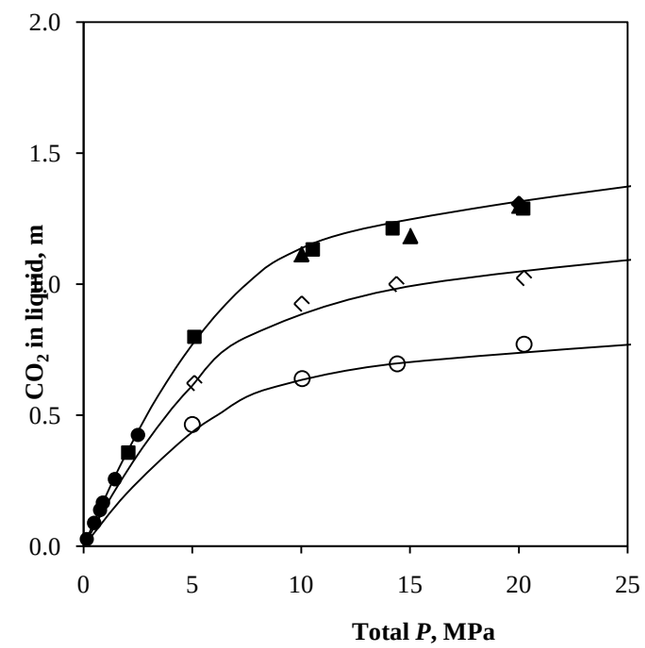
Modified based on "Beyond the Molecular Frontier", NRC report, 2003

CO_2 Properties

- Compression, Transportation and Storage of Supercritical CO_2
  - Phase Behavior at high pressure
  - Hydrate Formation, Scaling, Corrosion
  - Salting-Out by concentrated brine in aquifer







Solvents Used in CO_2 Capture

- Chemical solvents:

  MEA, DEA, TEA, MDEA, DGA, DIPA, AMP, PZ, NH3, NaOH, Na_2CO_3, K_2CO_3

- Physical solvents:

  Methanol, DEPG, NMP, Sulfolane, Propylene carbonate

- Mixed Amines

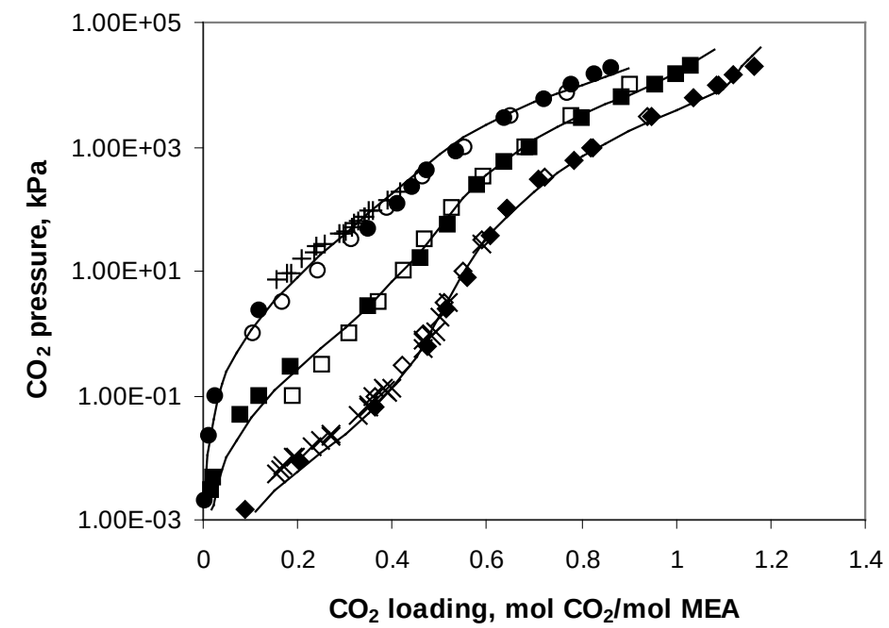
  MEA-MDEA, MEA-AMP, MDEA-PZ, PZ-K2CO3, etc.

- Proprietary solvents

  Cansolv, CORAL, RITE, KS-1/2/3, CASTOR-1/2, etc.

Solvent Properties

- Phase Equilibrium and Thermophysical Properties
  - Operating pressure
  - CO_2 loading capacity
  - Solvent volatility
  - Heat of absorption
  - Solid precipitation
- Reaction Kinetics
  - CO_2 capture mechanism and rate
  - Thermal and oxidative decomposition
- Transport Properties
  - Viscosity
  - Surface Tension
  - Density



$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

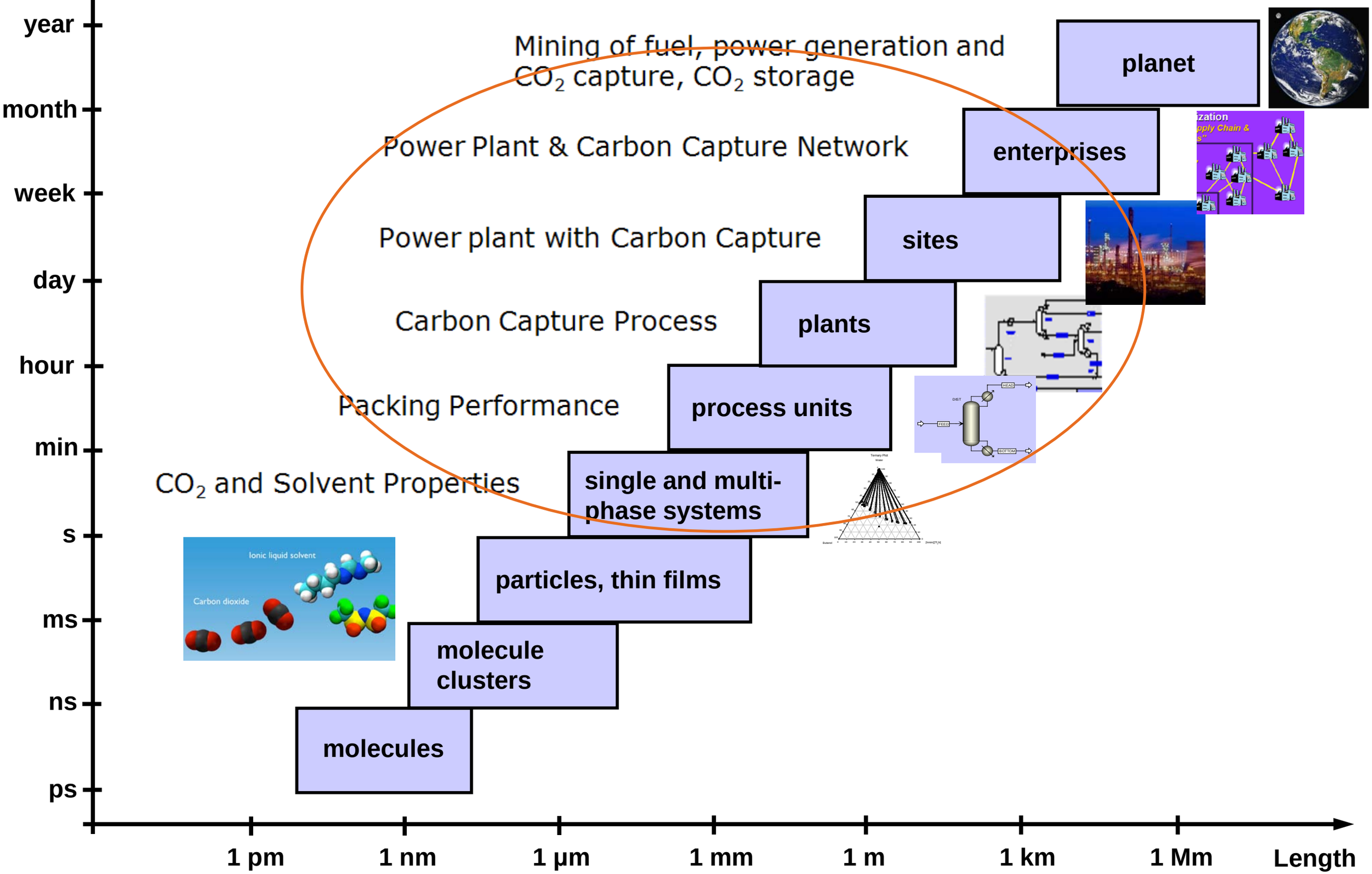
$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+$$

$$MEACOO^- + H_2O \leftrightarrow^+ +MEA + HCO_3^-$$

Integrated, High Fidelity, Multiscale Process Modeling of CO_2 Capture & Storage



Modified based on "Beyond the Molecular Frontier", NRC report, 2003

Modeling Tray/Packing Performance

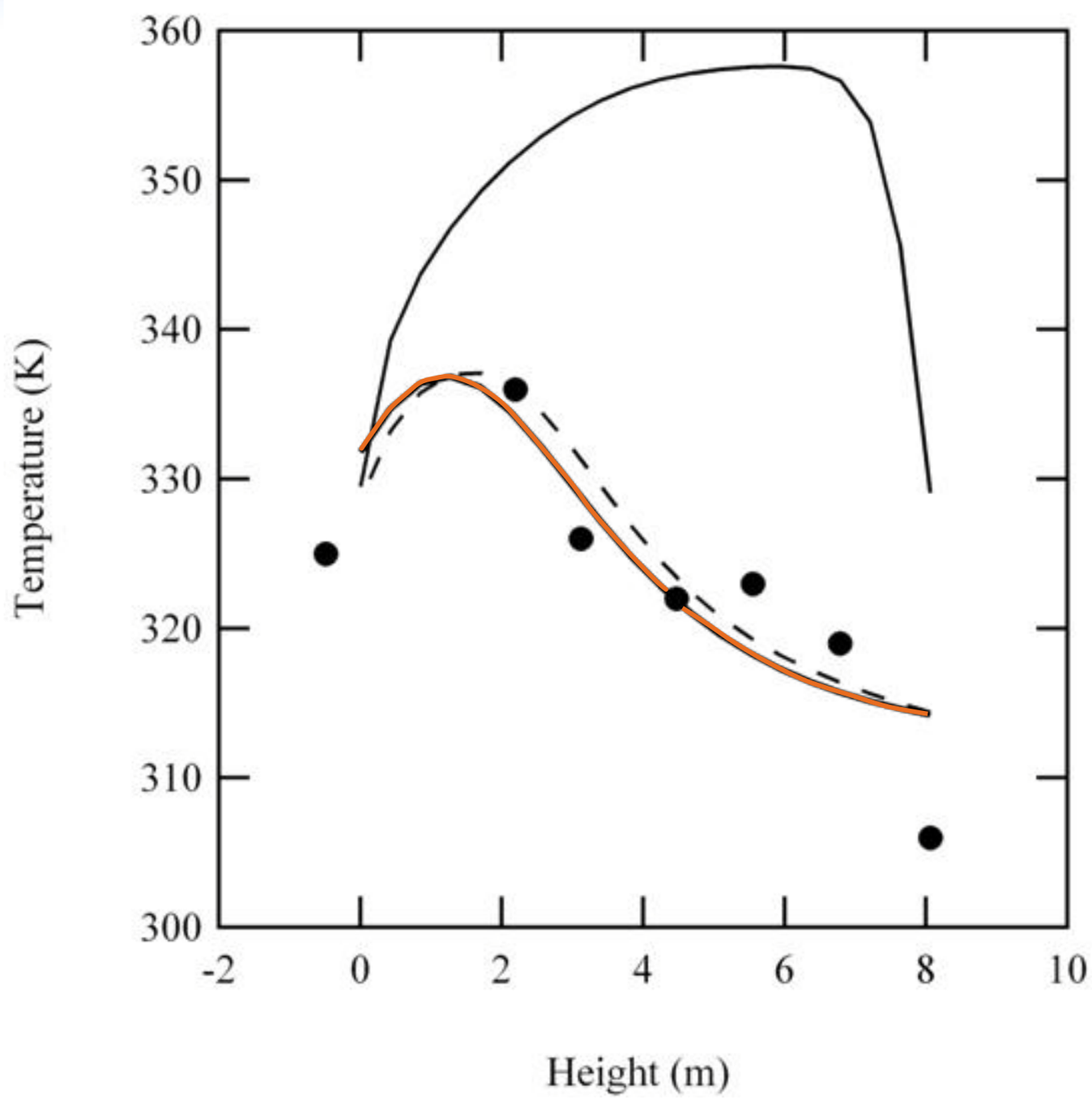
Mass Transfer Correlations

Bubble-Cap Trays	Sieve Trays	Valve Trays	Random Packing	Structured Packing
AIChE	AIChE	AIChE	Onda	Bravo-Rocha-Fair 1985
Hughmark	Chan-Fair (1984 & RF)	Scheffe-Weiland	Bravo-Fair	Bravo-Rocha-Fair 1992
Gerster (RF)	Zuiderweg		Billet & Schultes	Billet & Schultes
	Chen-Chuang			

Correlations also required for interfacial area, heat transfer, liquid holdup and pressure drop

CO_2 Absorption Into Aqueous MEA

Comparison of three random packing correlations



CO_2/MEA/H_2O
IMTP 40 - case 32
30.48 wt % MEA inlet
25.20 mol % CO_2 inlet

Bravo & Fair
Onda
This Work
Experiment

BF82 Amine Load: 0.45 mol/mol
BF82 CO_2 Removal : 95%
Onda Amine Load: 0.42 mol/mol
Onda CO_2 Removal : 79%
Amine Load This Work: 0.447 mol/mol
CO_2 Removal This Work: 94.4%

Measured Amine Loading: 0.428 mol/mol
Measured CO_2 Removal: 95%

Developing Mass Transfer Correlations

Data analysis approach

- Assume that the defining expressions are given by power laws

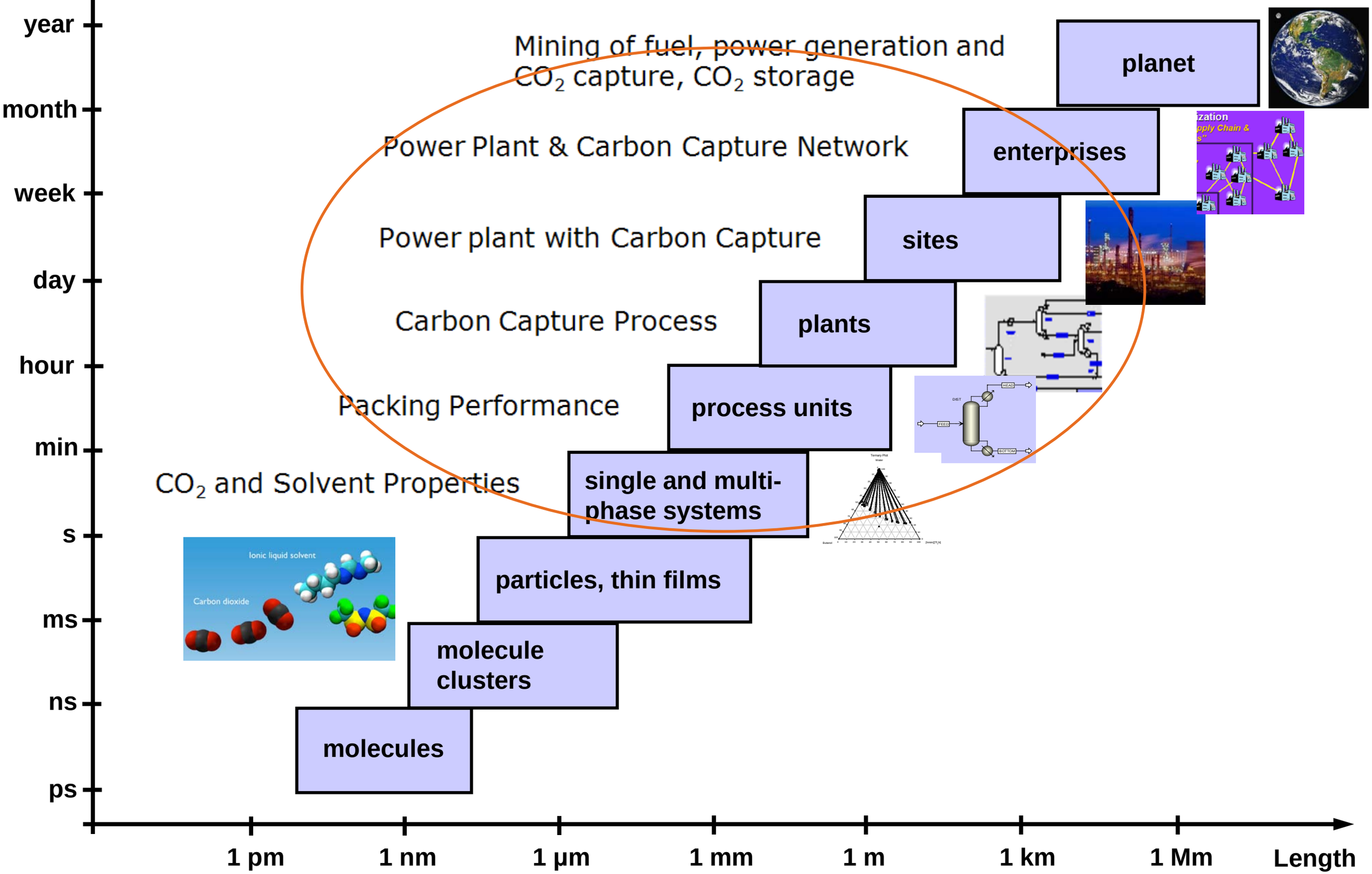
$$k_x = K_x \, Re_L^a \, Sc_L^b \left(\frac{c_L D_L}{d_e} \right)$$

$$k_y = K_y \, Re_V^m \, Sc_V^n \left(\frac{c_V D_V}{d_e} \right)$$

$$a_m = A_m a_d \, Re_L^\alpha \, We_L^\beta \, Fr_L^\chi \, Re_V^\delta \left(\frac{\rho_V}{\rho_L} \right)^\varepsilon \left(\frac{\mu_V}{\mu_L} \right)^\phi$$

- Limit data included in the fit to regions that are amenable to a description by pure power laws

Integrated, High Fidelity, Multiscale Process Modeling of CO_2 Capture & Storage



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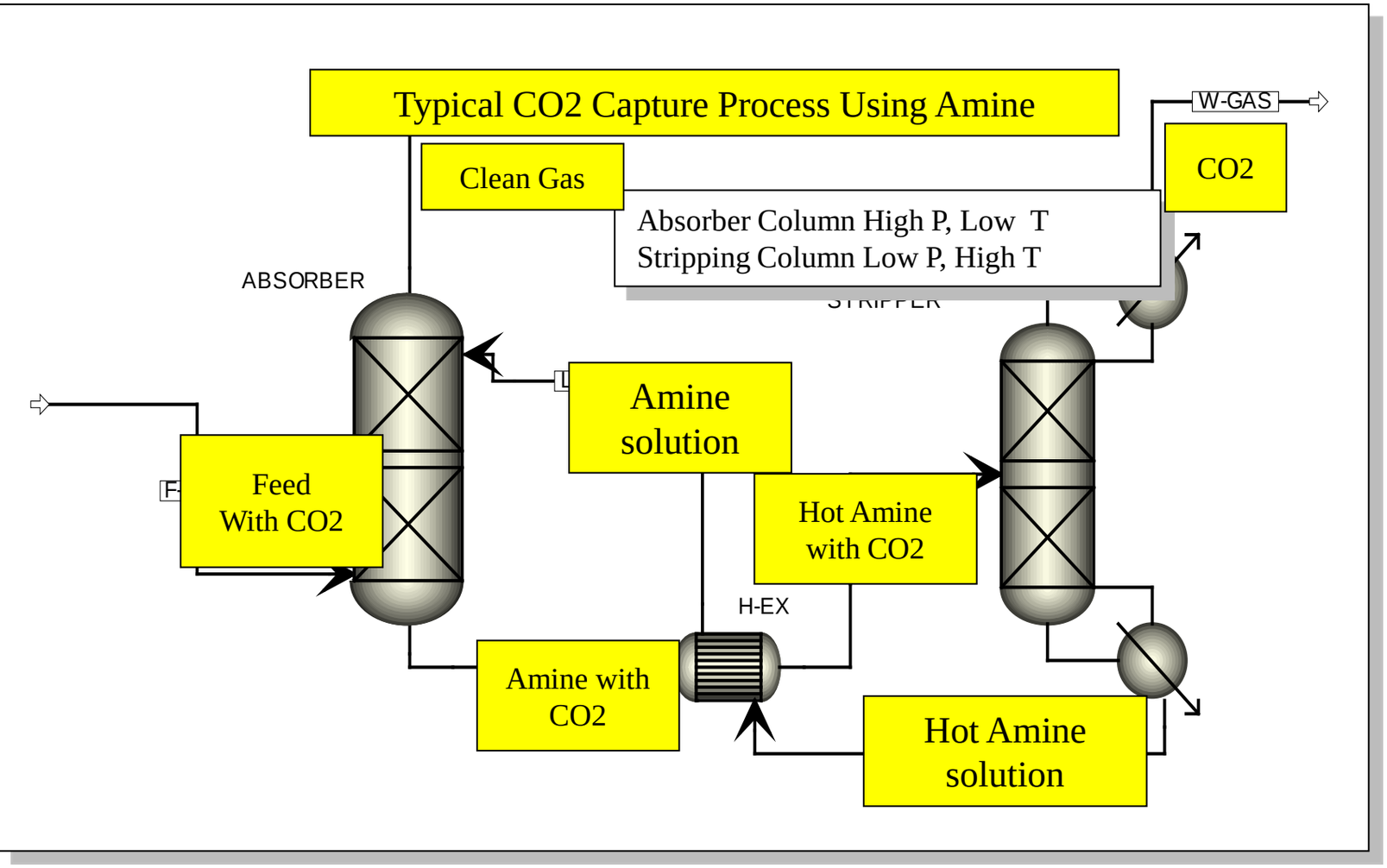
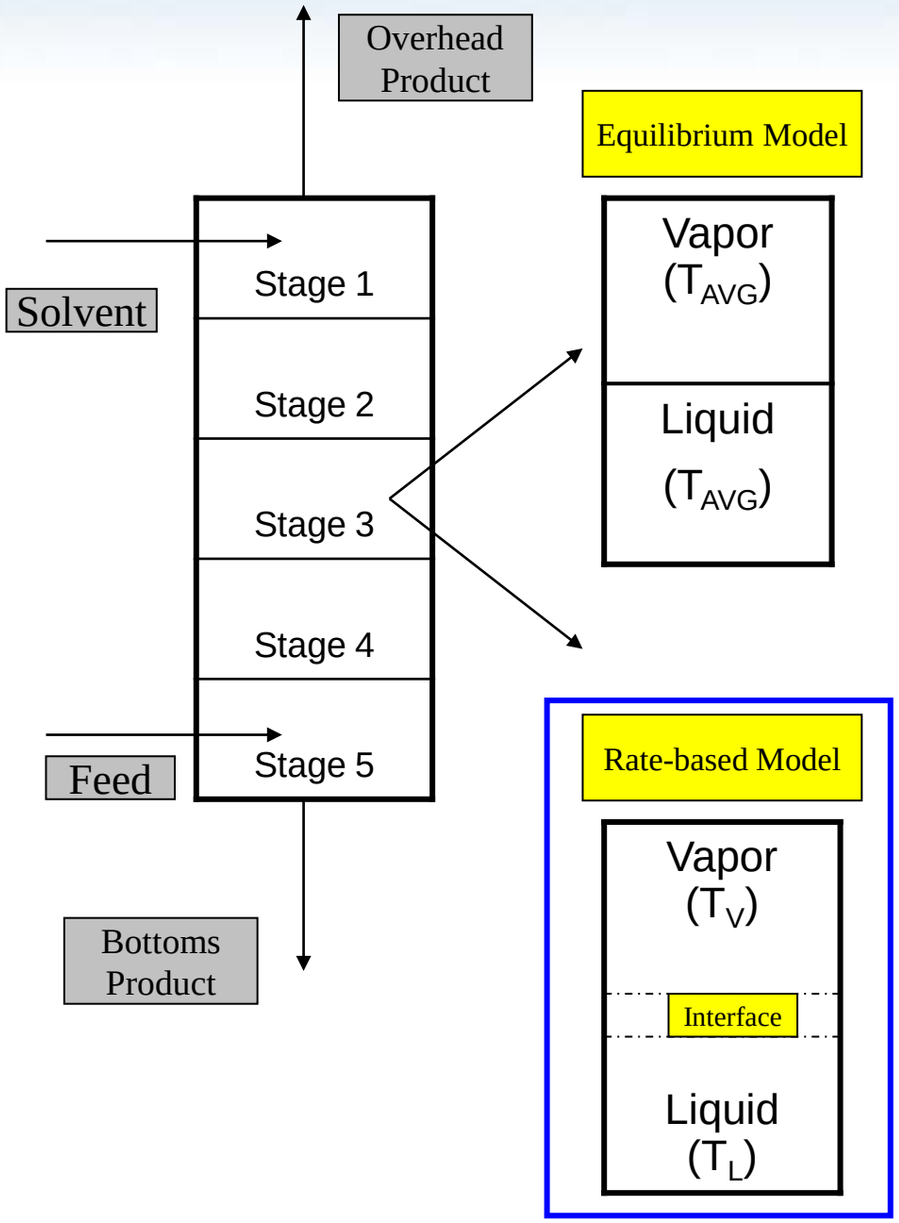
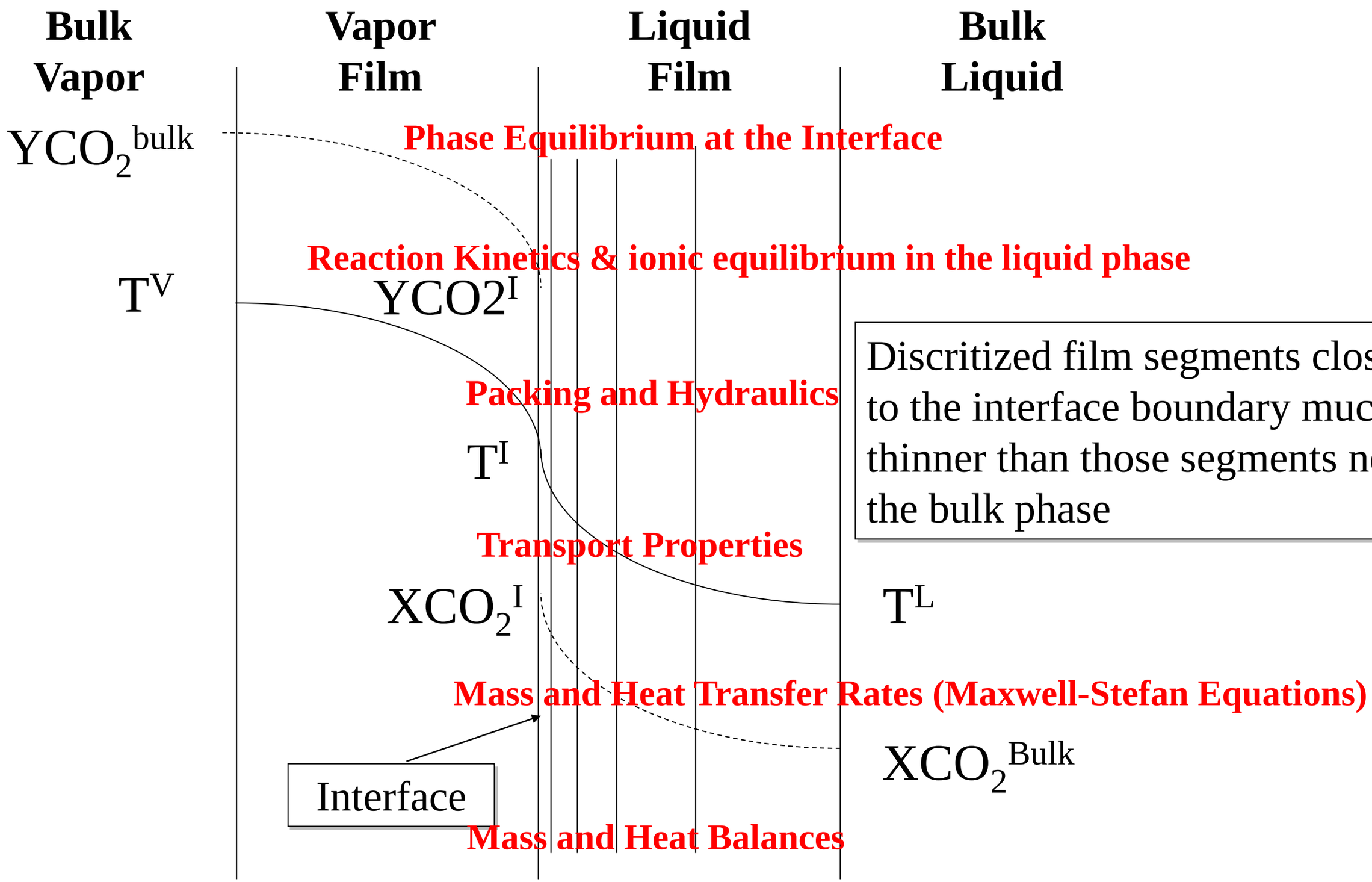
Modeling CO_2 Capture Processes: Equilibrium Stage Modeling vs. Rate-Based Modeling



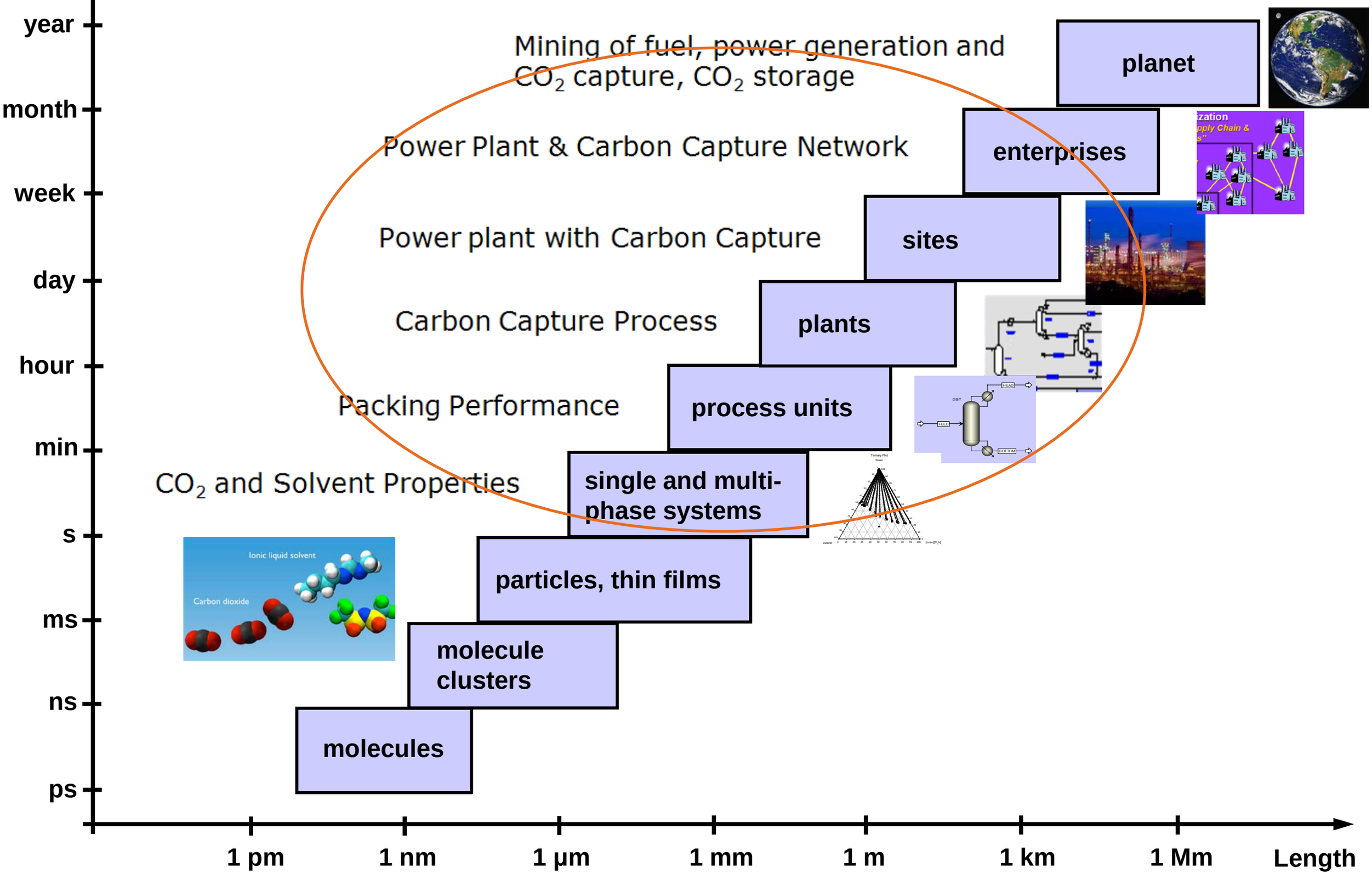


Modeling Heat and Mass Transfer for CO_2 Absorption with Amines



Discritized film segments closer to the interface boundary much thinner than those segments near the bulk phase

Integrated, High Fidelity, Multiscale Process Modeling of CO_2 Capture & Storage



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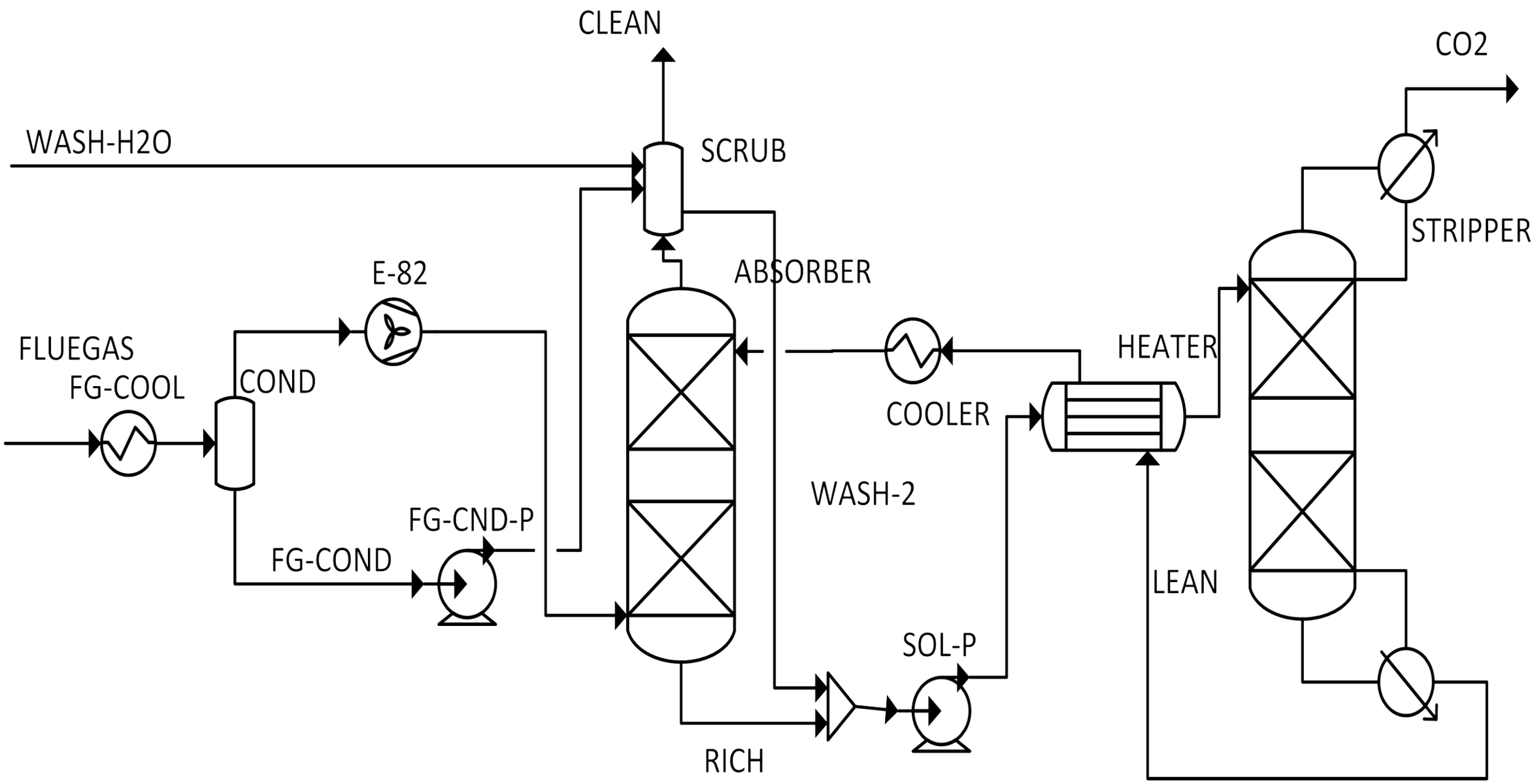
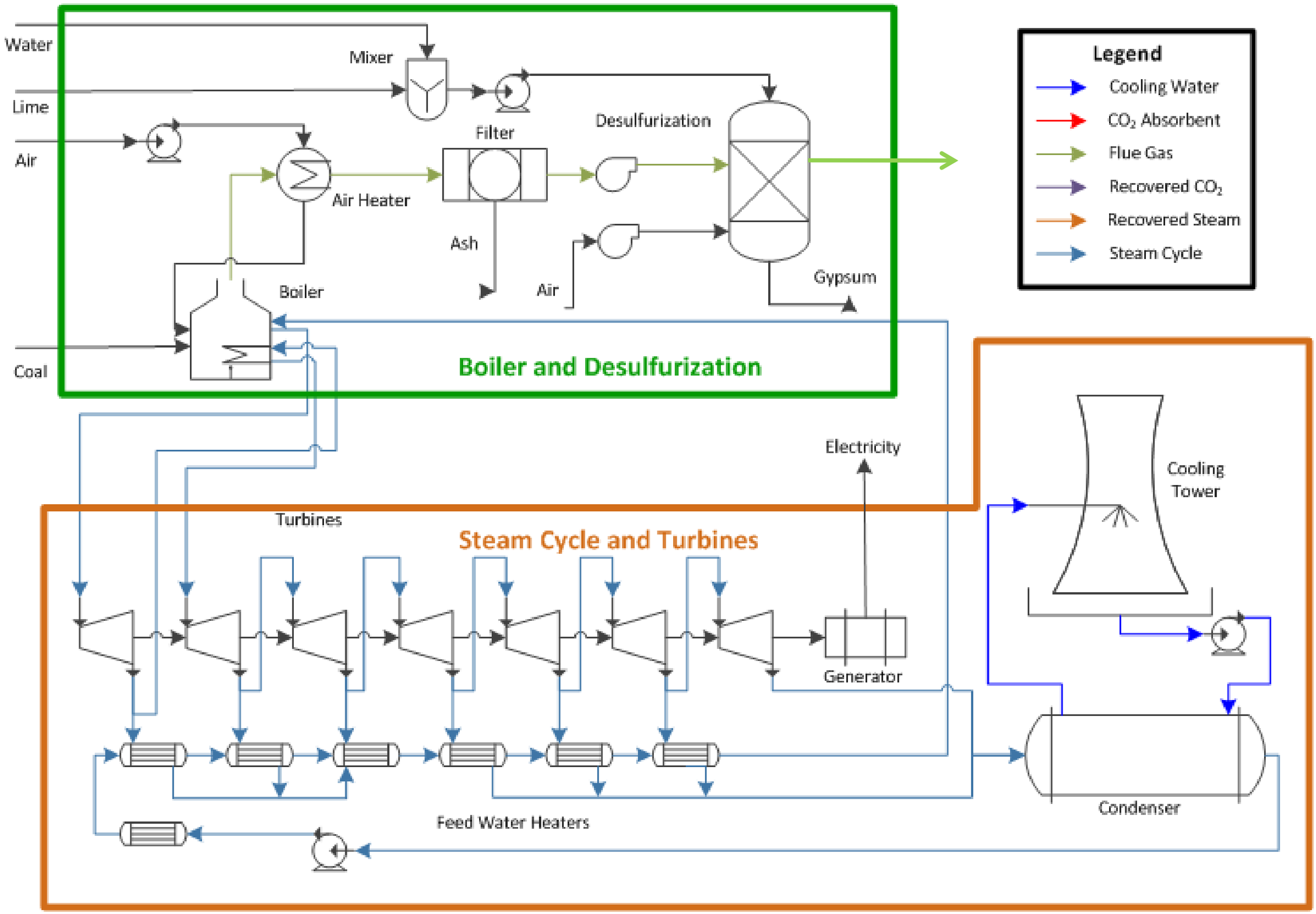
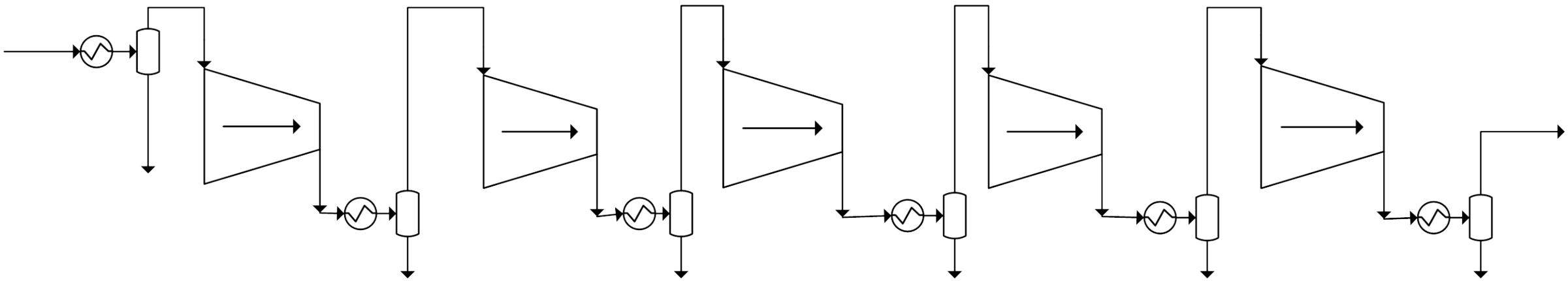
MEA Module


CLEAN
CO2
WASH-H2O
SCRUB
STRIPPER
E-82
ABSORBER
FLUEGAS
FG-COOL
COND
HEATER
COOLER
WASH-2
FG-CND-P
FG-COND
LEAN
SOL-P
RICH

Subcritical PC Plant

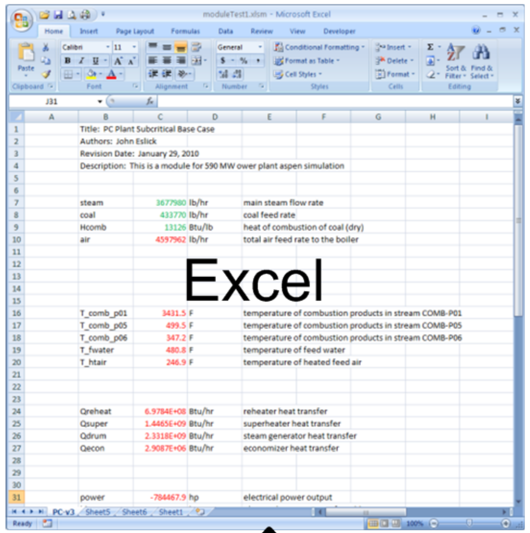


Compression



- Multi-stage compression
- Intercoolers 265 F to variable T
- Water returned to process
- Final pressure 2200 psia

NETL Modular Framework for Design and Optimization

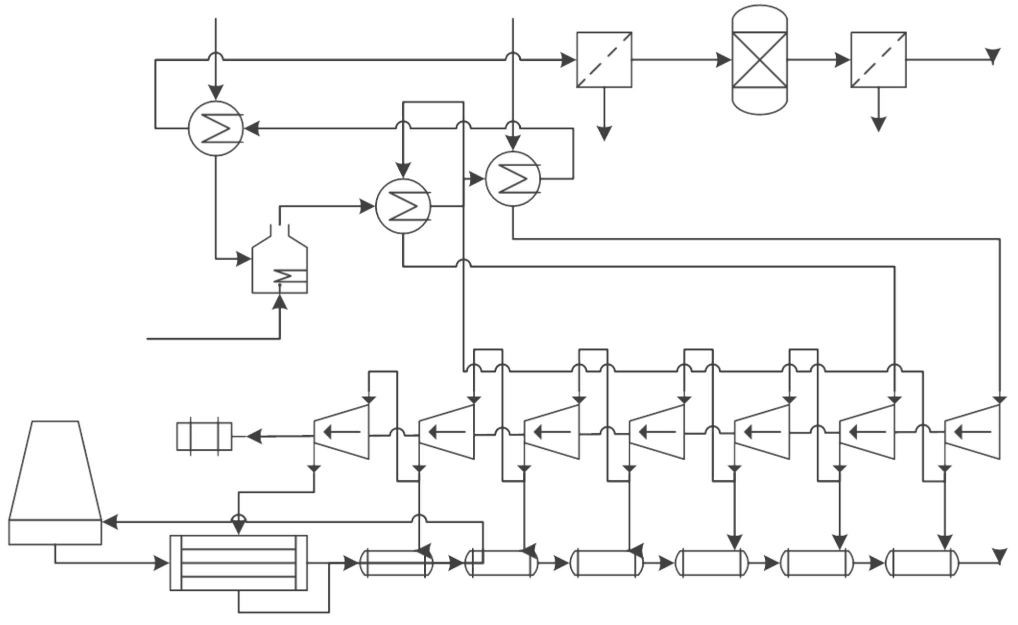


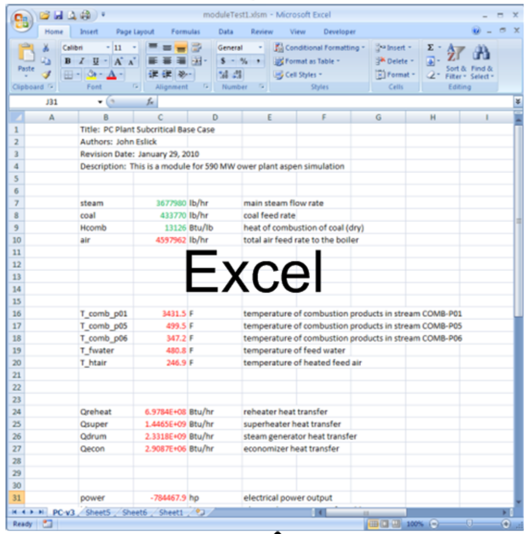
Title: PC Plant Subcritical Base Case
Authors: John Eslick
Revision Date: January 29, 2010
Description: This is a module for 590 MW ower plant aspen simulation

steam	3677980	lb/hr	main steam flow rate
coal	433770	lb/hr	coal feed rate
Hcomb	13126	Btu/lb	heat of combustion of coal (dry)
air	4597962	lb/hr	total air feed rate to the boiler
T_comb_p01	3431.5	F	temperature of combustion products in stream COMB-P01
T_comb_p05	499.5	F	temperature of combustion products in stream COMB-P05
T_comb_p06	347.2	F	temperature of combustion products in stream COMB-P06
T_fwater	480.8	F	temperature of feed water
T_htair	246.9	F	temperature of heated feed air
Qreheat	6.9784E+08	Btu/hr	reheater heat transfer
Qsuper	1.4465E+09	Btu/hr	superheater heat transfer
Qdrum	2.3318E+09	Btu/hr	steam generator heat transfer
Qecon	2.9087E+06	Btu/hr	economizer heat transfer
power	-784467.9	hp	electrical power output

Excel

Power Plant Module





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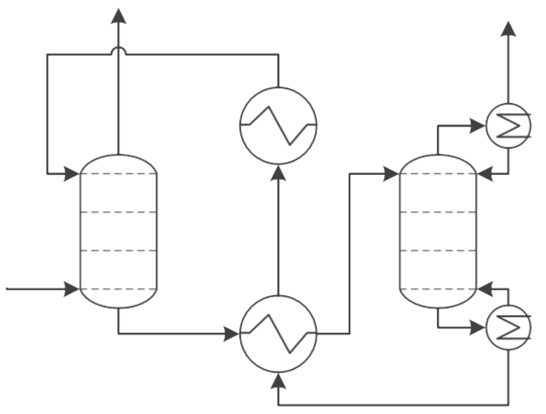
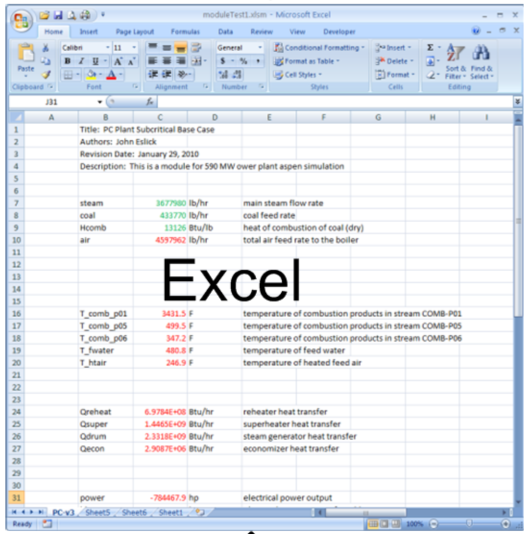
T_comb_p05	499.5	F	temperature of combustion products in stream COMB-P05
T_comb_p06	347.2	F	temperature of combustion products in stream COMB-P06
T_fwater	480.8	F	temperature of feed water
T_htair	246.9	F	temperature of heated feed air
Qreheat	6.9784E+08	Btu/hr	reheater heat transfer
Qsuper	1.4465E+09	Btu/hr	superheater heat transfer
Qdrum	2.3318E+09	Btu/hr	steam generator heat transfer
Qecon	2.9087E+06	Btu/hr	economizer heat transfer
power	-784467.9	hp	electrical power output

Excel

CO_2 Capture Module



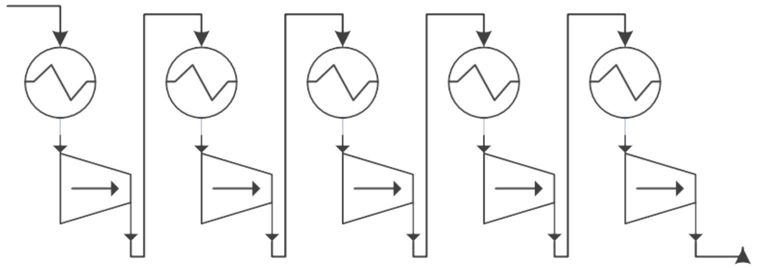


Title: PC Plant Subcritical Base Case
Authors: John Eslick
Revision Date: January 29, 2010
Description: This is a module for 590 MW ower plant aspen simulation

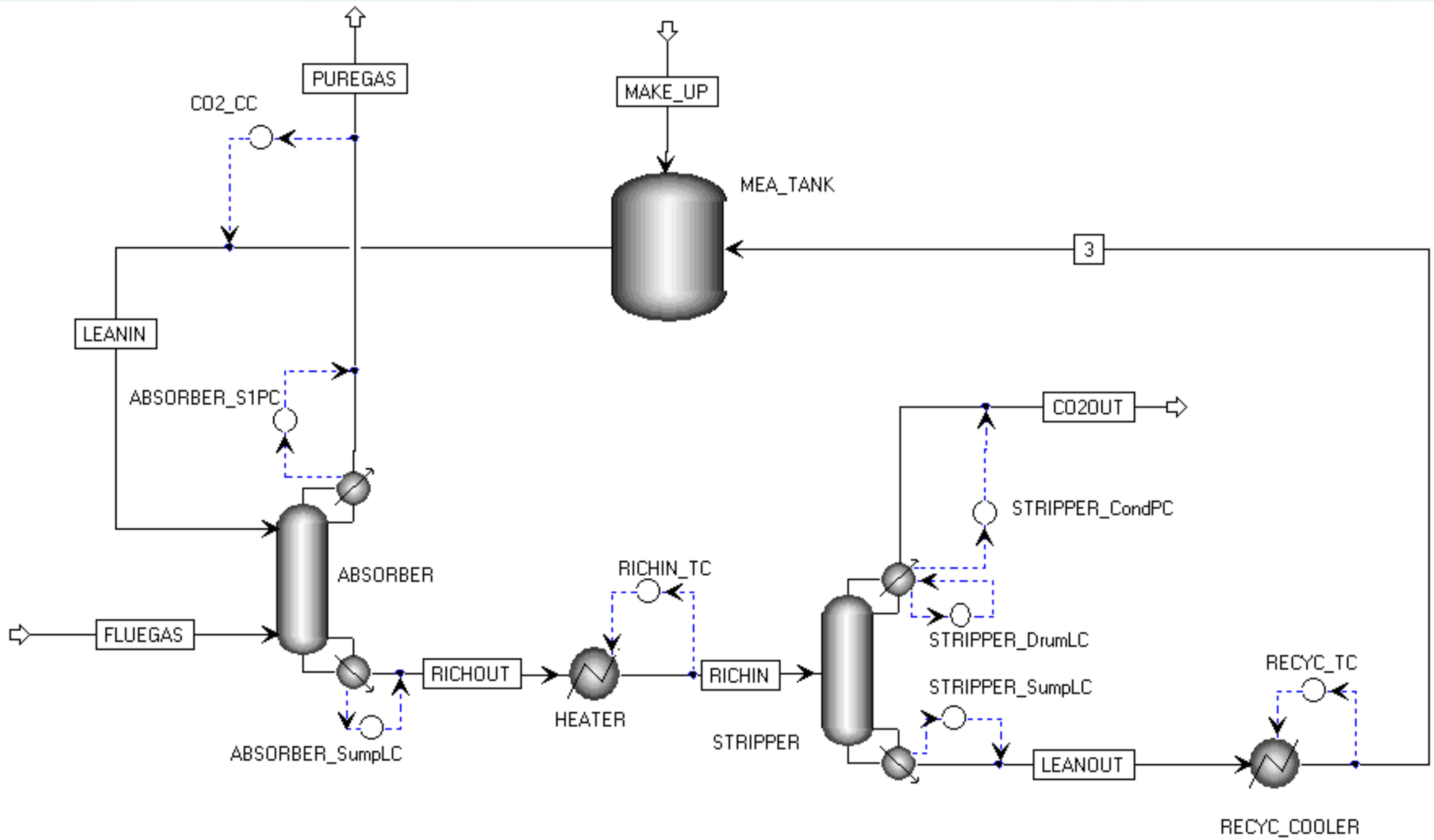
steam	3677980	lb/hr	main steam flow rate
coal	433770	lb/hr	coal feed rate
Hcomb	13126	Btu/lb	heat of combustion of coal (dry)
air	4597962	lb/hr	total air feed rate to the boiler
T_comb_p01	3431.5	F	temperature of combustion products in stream COMB-P01
T_comb_p05	499.5	F	temperature of combustion products in stream COMB-P05
T_comb_p06	347.2	F	temperature of combustion products in stream COMB-P06
T_fwater	480.8	F	temperature of feed water
T_htair	246.9	F	temperature of heated feed air
Qreheat	6.9784E+08	Btu/hr	reheater heat transfer
Qsuper	1.4465E+09	Btu/hr	superheater heat transfer
Qdrum	2.3318E+09	Btu/hr	steam generator heat transfer
Qecon	2.9087E+06	Btu/hr	economizer heat transfer
power	-784467.9	hp	electrical power output

Excel

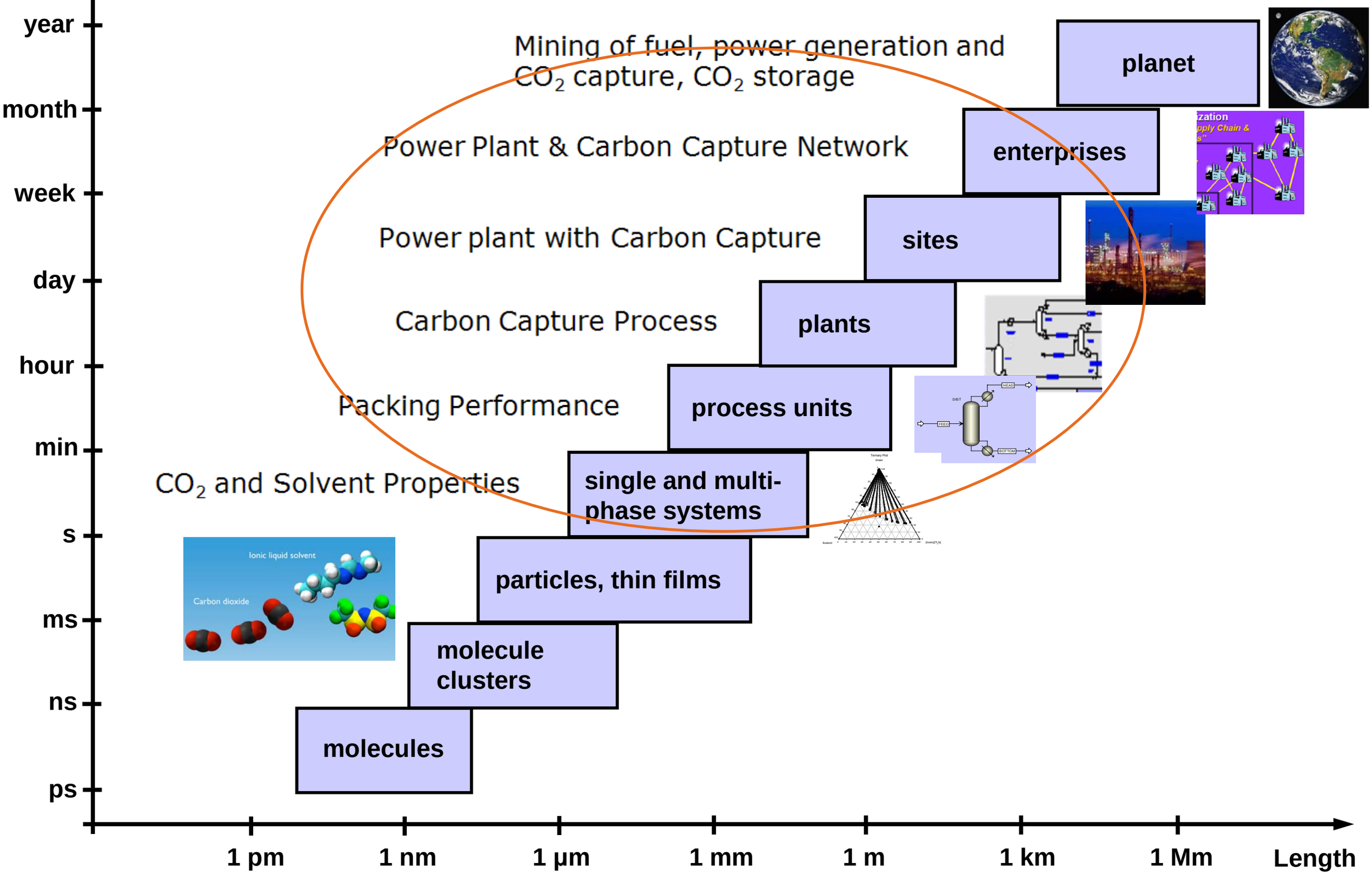
Compression Module



Dynamic Simulation of Carbon Capture Process and Integration with Power Plant



Integrated, High Fidelity, Multiscale Process Modeling of CO_2 Capture & Storage



Modified based on "Beyond the Molecular Frontier", NRC report, 2003

Summary

- Integrated, high fidelity, multiscale process models have generated tremendous economic values over the decades
- Process modeling and simulation technology will continue to thrive and advance as chemical engineers make contributions to capture economic opportunities and to address societal challenges
- Chemical engineers must be well trained in process simulation and continue to innovate in science and engineering to better enable modeling of the physical and chemical world based on 1st principles

Acknowledgement

- David Miller of National Energy Technology Laboratory kindly provided four carbon capture modeling slides