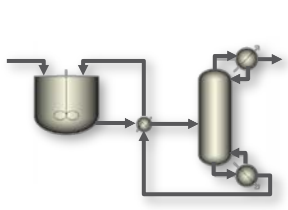

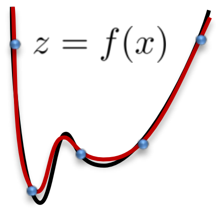

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

Surrogate Model based Optimal Design of Carbon Capture Process

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CAPD CENTER

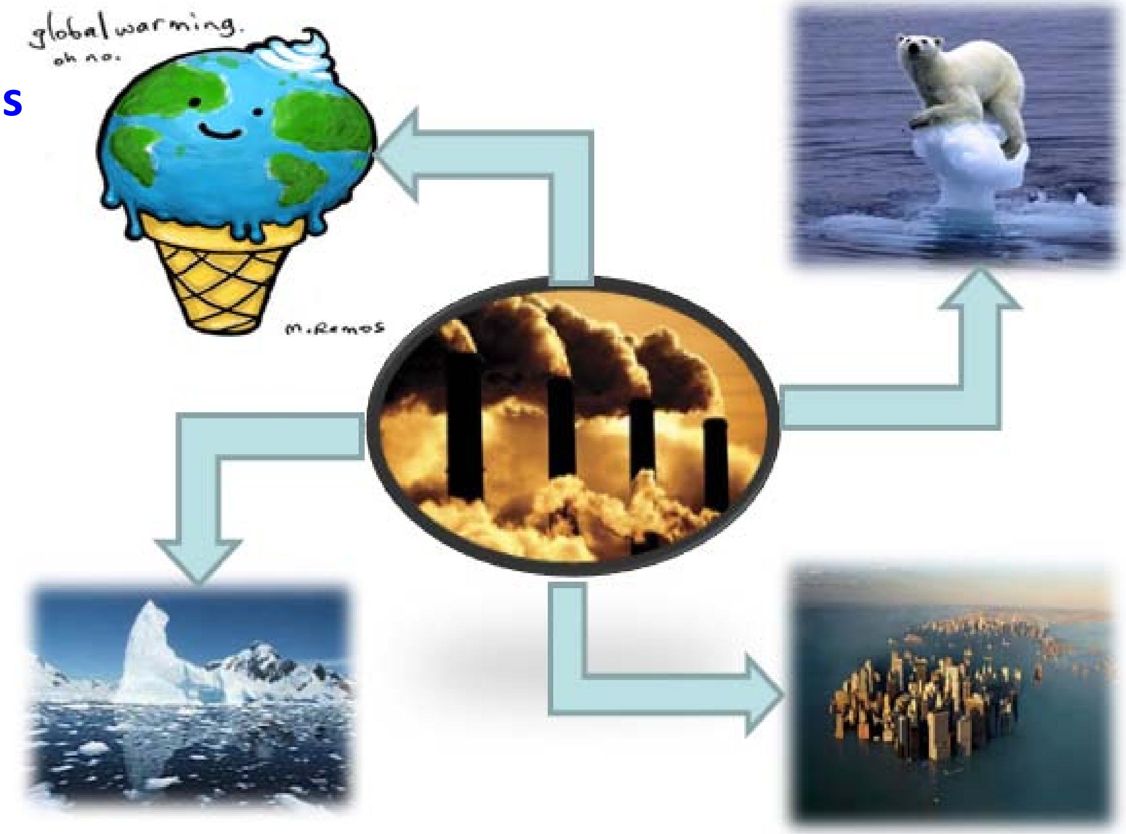
Carnegie Mellon University

NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

CCSI™

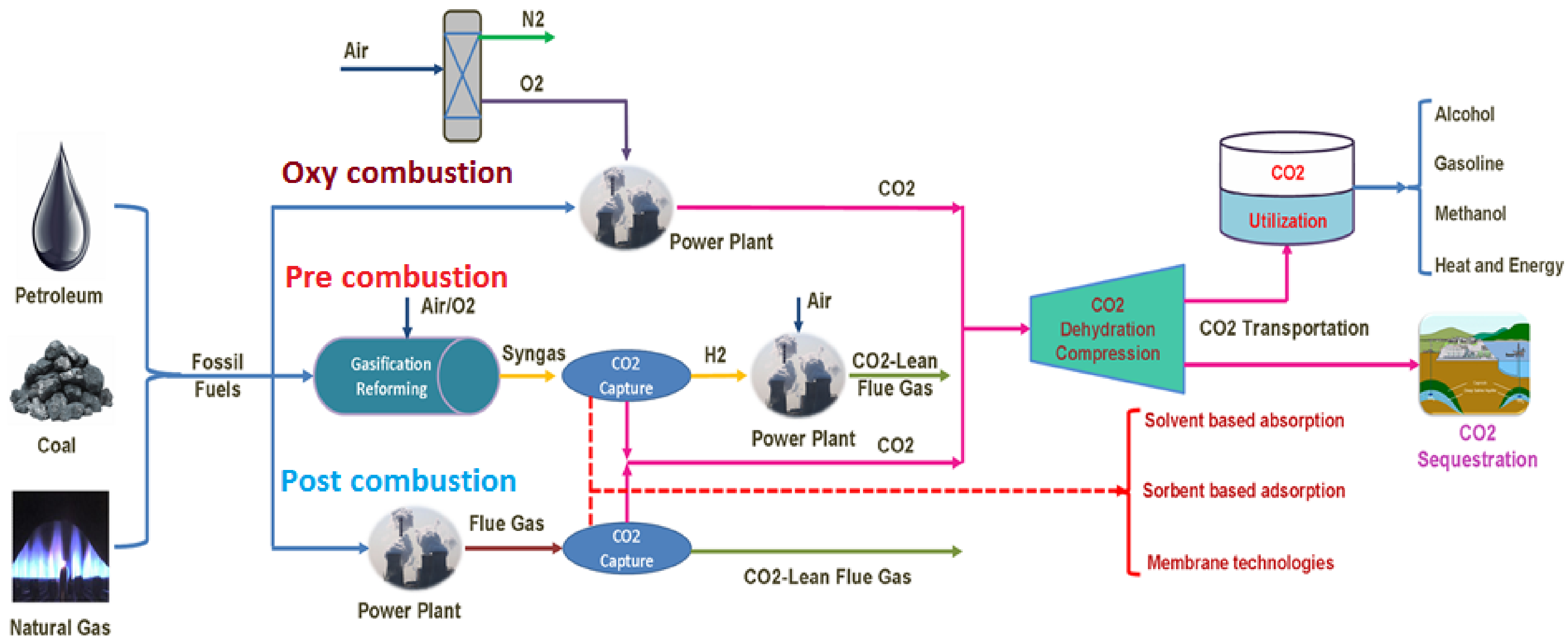
MOTIVATION

- **Backbone of the energy supply: Fossil fuels**
  petroleum, coal, natural gas
- **One-third of U.S. CO_2 emissions come from power plant**
- **Global warming issues**
  —Ice melting at poles
  —Rising of ocean levels
- **Available carbon capture technologies would increase electricity costs**



CO2 CAPTURE TECHNOLOGIES

Summary of the current CO2 carbon capture technologies



Most widely investigated CO2 capture technology: Post combustion

CO2 CAPTURE TECHNOLOGIES

MEA solvent based post-combustion capture technology

- **Highly energy intensive**
- **Large solvent makeup due to their thermal and oxidative degradation**
- **High cost**

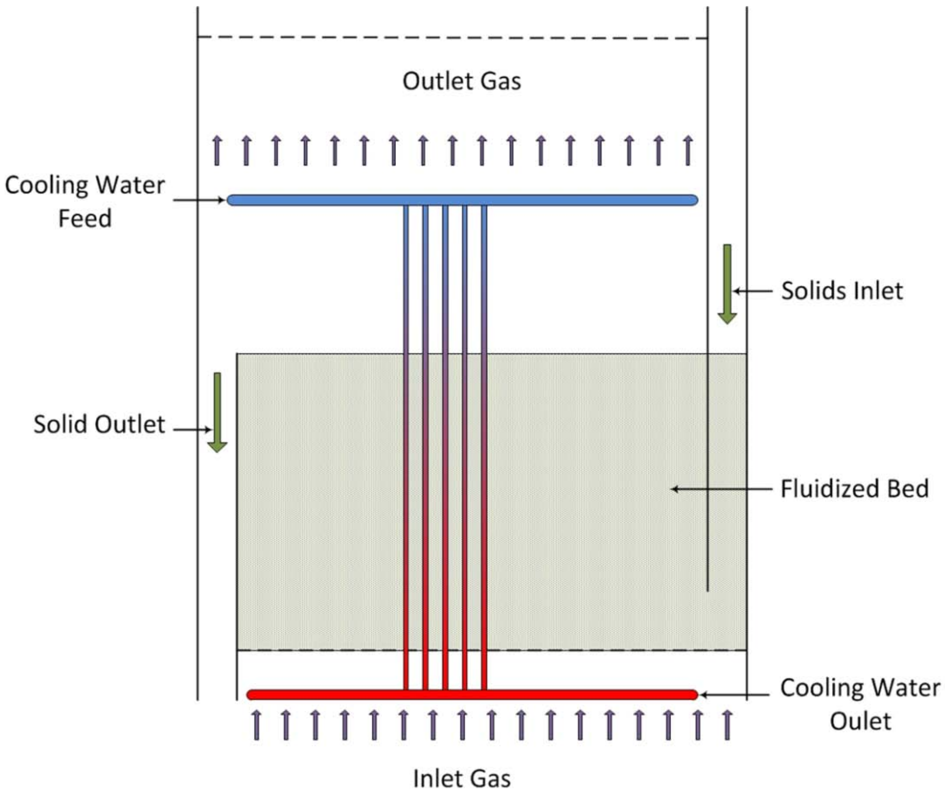
(*Samanta, I&EC Research, 2012*)

Cost-effective capture technology is extremely needed to reduce the CO2 emission

- **Growing interest: solid sorbent based adsorption process**
  - **—Reduced energy for regeneration**
  - **—Greater capacity and selectivity**
- **DOE: Carbon Capture Simulation Initiative (CCSI)**
  - **—Bubbling fluidized bed adsorber/regenerator**
  - **—Moving bed adsorber/regenerator**

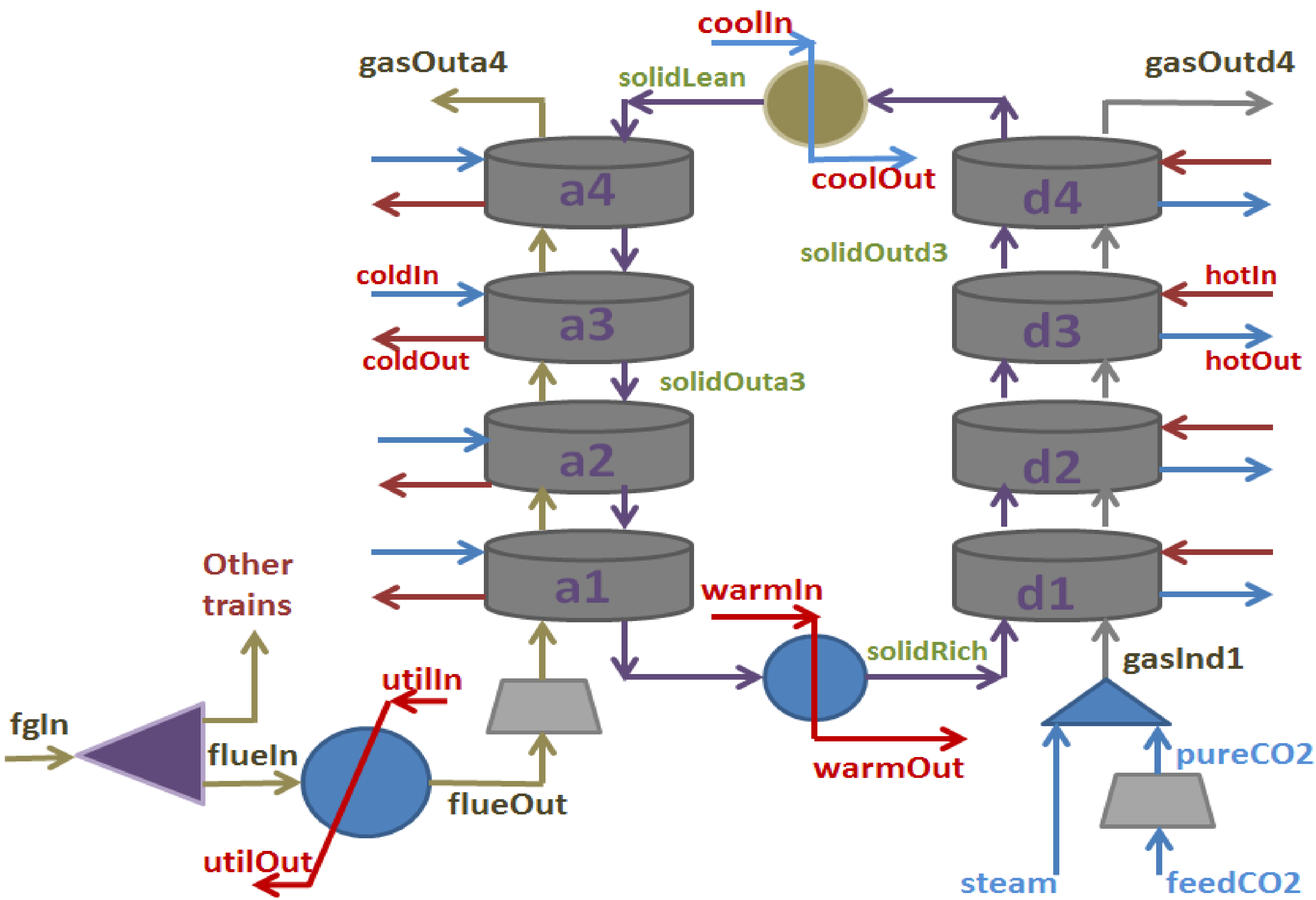
BUBBLING FLUIDIZED BED REACTOR

- **Bubbling fluidized bed**
  - **1D model**
  - **Modeled in Aspen Custom modeler**
  - **Differential model**
  - **Uses Aspen Properties package**



Andrew Lee, US DOE-National Energy Technology laboratory, Morgantown, WV

CO2 CAPTURE PROCESS FLOWSHEET



General flow sheet for carbon capture process

OBJECTIVES AND HURDLES

- **Objectives**

  Achieve the set carbon capture rate

  Minimizing the cost of electricity (COE)

  Identify & develop the optimized bubbling fluidized bed process designs

  —Optimal configuration

  —Optimal design conditions

  —Optimal operating conditions

- **Hurdles**

  Computationally intractable for large scale nonlinear optimization because of the detailed first principle models

- **Handles**

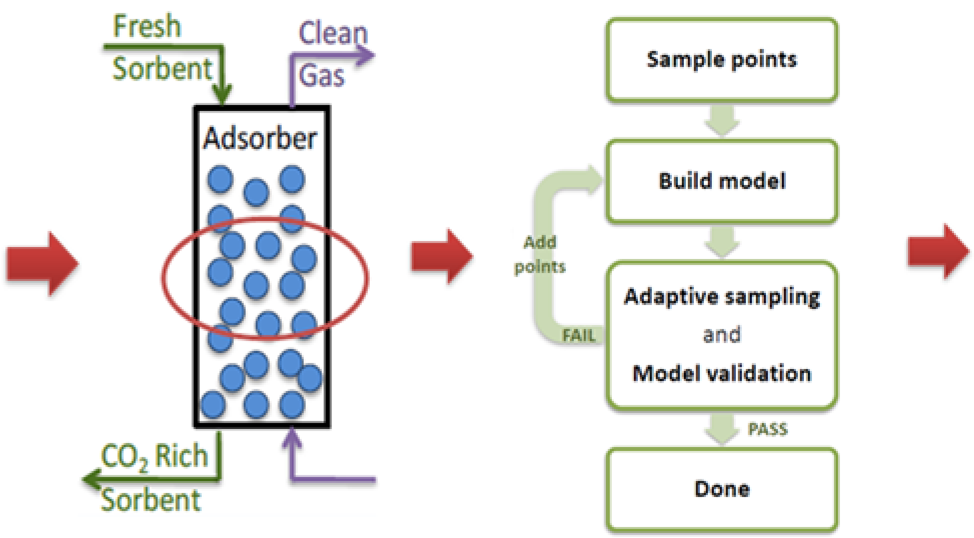
  Generate the set of low complexity algebraic surrogate models

  —Automated Learning of Algebraic Models for Optimization(ALAMO)

(*http://archimedes.cheme.cmu.edu/?q=alamo*)

SURROGATE MODEL GENERATION

$$x \in \mathbb{R}^D \qquad x^l \leq x \leq x^u \qquad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \\ \vdots \\ x_D \end{pmatrix}$$

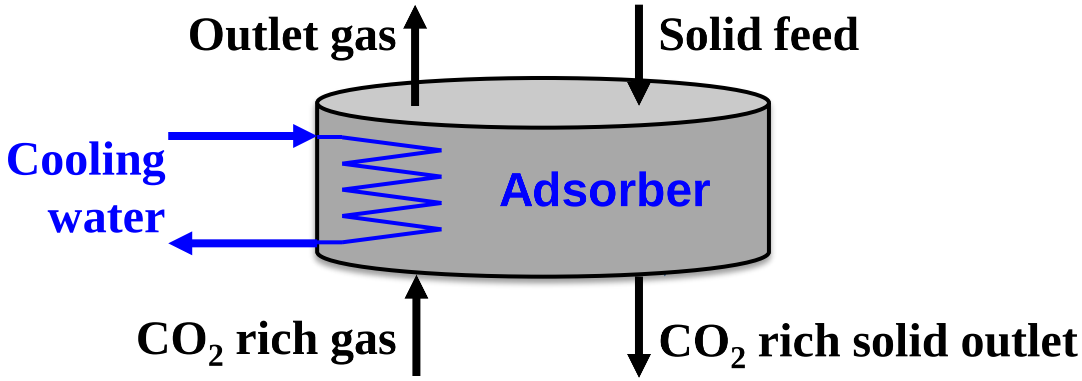


$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix} \qquad z \in \mathbb{R}^K \qquad z = f(x)$$

- **Independent variables** x
  - **Geometry**
  - **Operating conditions**
  - **Inlet flow conditions**
- **Dependent variables** z
  - **Geometry required**
  - **Operating condition required**
  - **Outlet flow conditions**
  - **Design constraints**

BUBBLING FLUIDIZED BED

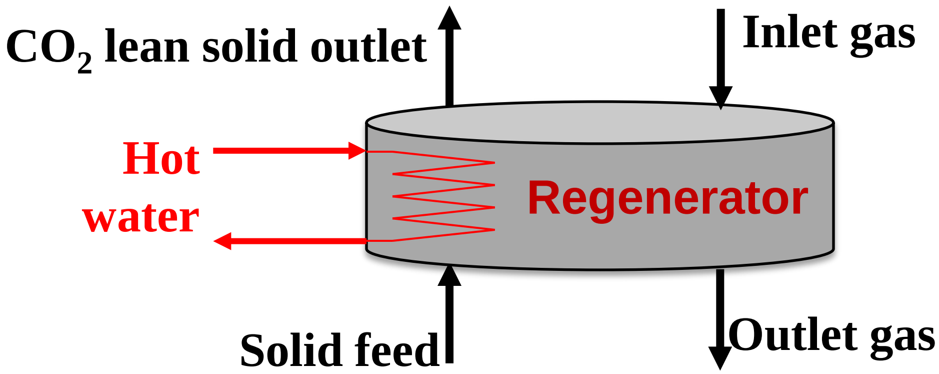
Bubbling fluidized bed adsorber diagram



- **Model inputs (16 total)**
  - **Geometry (3)**
  - **Operating conditions (5)**
  - **Gas mole fractions (2)**
  - **Solid compositions (2)**
  - **Flow rates (4)**
- **Model outputs (14 total)**
  - **Geometry required (2)**
  - **Outlet pressure (1)**
  - **Gas mole fractions (3)**
  - **Solid compositions (3)**
  - **Flow rates (2)**
  - **Outlet temperatures (3)**

BUBBLING FLUIDIZED BED

Bubbling fluidized bed regenerator diagram

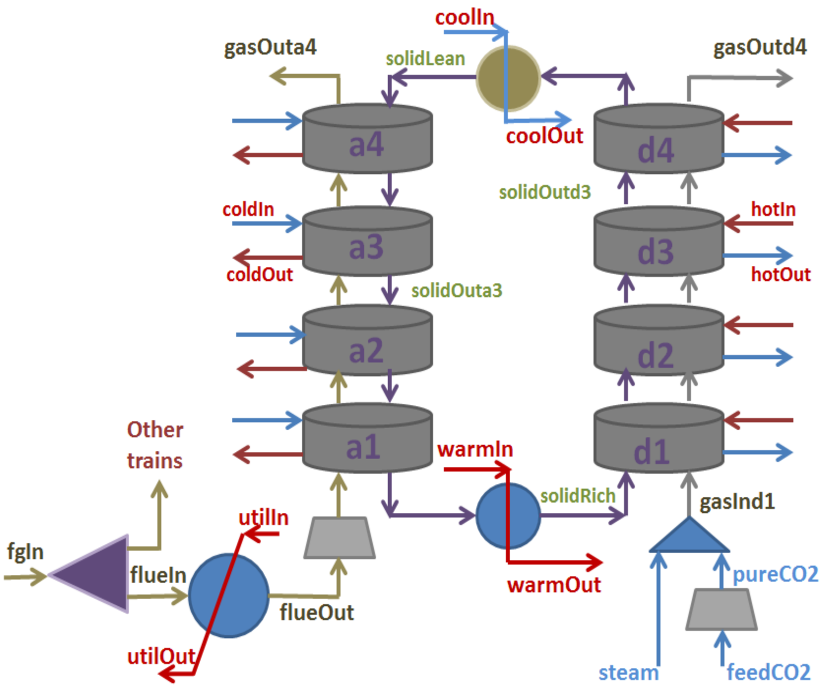


- **Model inputs (14 total)**
  - Geometry (3)
  - Operating conditions (5)
  - Gas mole fractions (1)
  - Solid compositions (2)
  - Flow rates (3)
- **Model outputs (14 total)**
  - Geometry required (2)
  - Inlet pressure (1)
  - Gas mole fractions (3)
  - Solid compositions (3)
  - Flow rates (2)
  - Outlet temperatures (3)

NONLINEAR OPTIMIZATION FORMULATION

Assumptions for nonlinear programming formulation

- Each stage is a single stage operation
- Utility cost for sorbent HX is negligible
- No pressure change for liquid and solid flow
- Each stage of adsorber/regenerator operation requires attached heat exchanger
- Surrogate models for fluidized bed adsorber and regenerator
- First principle models for SolidRich/SolidLean heat exchanger, blower, mixer



NONLINEAR OPTIMIZATION FORMULATION

Nonlinear Optimization Model

- Parameters
- Variables
- Equations
  - Economic modules
  - Process modules
    - Material balances
    - Hydrodynamic/Energy balances
    - Reactor surrogate models
  - Link between economic modules and process modules
  - Bounds for variables

f_1 **First principle models**

f_2 **Surrogate models**

f_3 **Economic modules**

F_1 **Constraints on geometry**

F_2 **Constraints on cost**

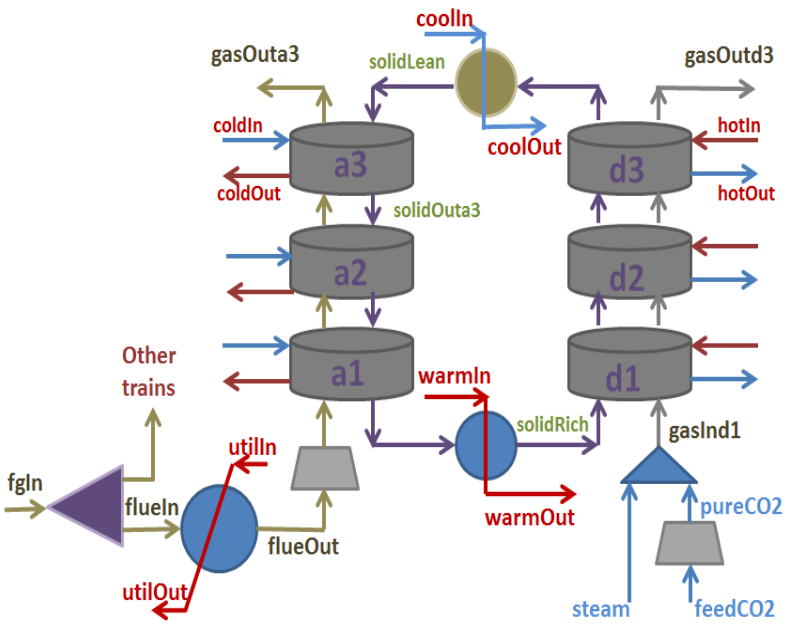
F_3 **Constraints on capture rate**

$$
\begin{aligned}
\min \quad & COE \\
s.t. \quad & f_1(x_1, x_2, \ldots, x_n) = 0 \\
& f_2(X_1, X_2, \ldots, X_n) = 0 \\
& f_3(x, X) = 0 \\
& F_1(x_1, x_2, \ldots, x_n) \geq 0 \\
& F_2(x_1, x_2, \ldots, x_n) \geq 0 \\
& F_3(x, X) \geq 0 \\
& x_i^{lo} \leq x_i \leq x_i^{up}; \ \forall i \in N \\
& X_i^{lo} \leq X_i \leq X_i^{up}; \ \forall i \in N
\end{aligned}
$$

Nonlinear programming to seek the optimal design/operation levels

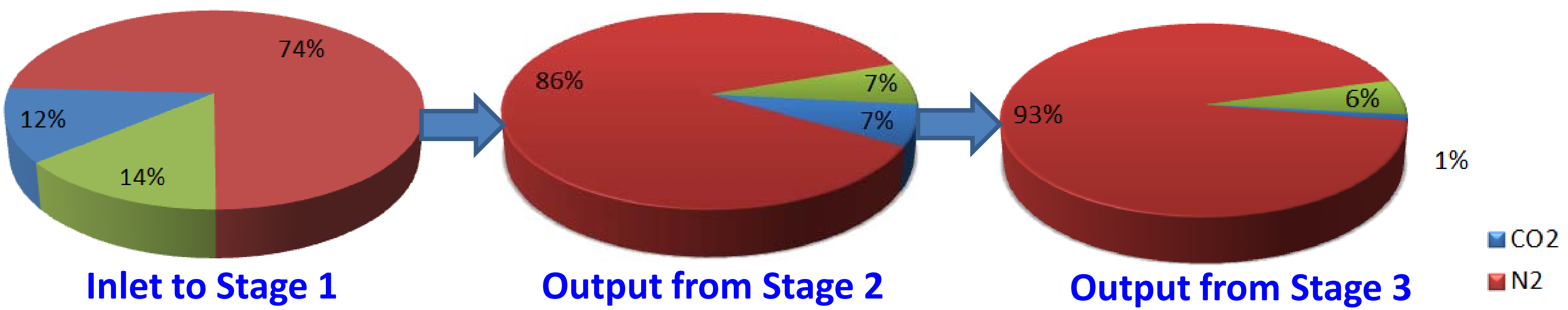
Using GAMS/BARON Software

CASE STUDY



Variables	Lower bound	Value	Upper bound
COE($/MWh)	-	108.5	1000
CapEX($)	1.0E+8	1.9E+8	1.0E+10
steamF(kgmol/s)	0.3	0.3	1
steamFlow(kg/s)	-	216	-
feedCO2F(kgmol/s)	0.1	0.1366	0.4
Derate(MW)	-	213.98	650
utilInF(kgmol/s)	5	9.26	10

CapEx: Capital overnight cost
derate: derating of the plant due to steam Take-off
steamFlow: Steam Take-off amount from power plant



Molar composition of flue gas

CONCLUSIONS

- **We developed a surrogate model based framework to seek the optimal design/operating levels for a fixed arrangement of pieces of equipment**

- **ALAMO provides surrogate models of adsorbers and regenerators and thus the whole nonlinear programming has a lower complexity**

- **Next steps:**
  - **—Formulate MINLP to optimize simultaneously the topology of the plant and the corresponding design/operating levels**
  - **—Select reactor type for each stage**
  - **—More complex superstructures…**