Development of Moving Bed Simulation Model for Carbon Capture From Fossil Energy Systems

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CCSI™ Carbon Capture Simulation Initiative

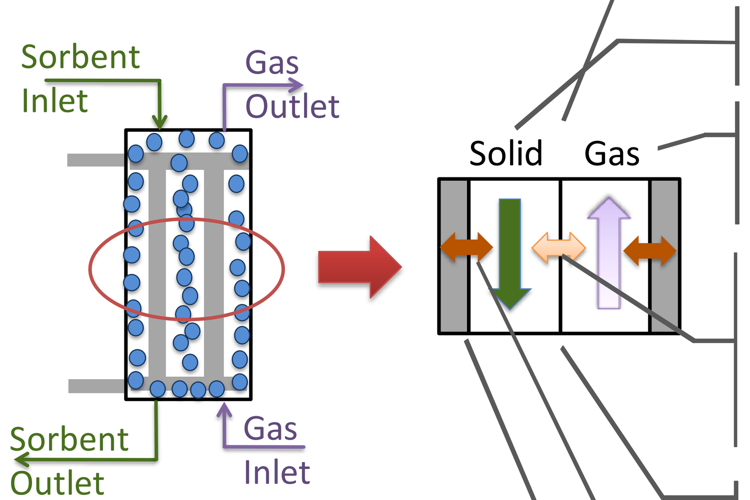
Why?

- Solid sorbents are a promising option to reduce the energy penalty associated with capturing flue gas CO_2.
- System simulations are needed to consider various process tradeoffs.
- Reactor models for these types of processes are not currently available in commercial process simulators.

Features

- Predictive computational 1 dimensional PDE process model for moving bed reactors.
- Flexible in wide range of operation conditions (unit size, gas and solid flowrates and compositions, particle properties and etc.).
- Includes reaction kinetics and correlations for heat and mass transfer between gas, solid and immersed heat exchanger tubes.

Modeling Scheme



- Shell (Gas, Solid) & Tube (Steam) Type
- Uniform Flow for Solid Phase (Const. vel.)
  Eff. Thermal Conductivity
- Plug-Flow for Gas
  Convection w/Axial Dispersion
  Pressure Drop using Ergun Eqn
- Mass Transfer
  - External Film Resistance
  - Intra-particle Diffusion
  Heat Transfer
  - Convective
- Adsorption & Desorption Isotherm
- Heat Transfer
  - Wall – Gas
  - Wall - Solid
- Heat Transfer Bet'n Wall & Steam

Major Equations

Gas Phase Balance Equation

$$-\varepsilon_b D_z \frac{\partial^2 C_i}{\partial z^2} - \frac{\partial (v_g C_i)}{\partial z} + (1-\varepsilon_b)\rho_p \frac{\partial Q_i}{\partial t} = 0$$

$$-\varepsilon_b k_g \frac{\partial^2 T_g}{\partial z^2} - C_{p,g} v_g \rho_g \frac{\partial T_g}{\partial z} - P\frac{\partial v_g}{\partial z} - (1-\varepsilon_b) h_f a_s (T_s - T_g) - h_{wg}(1-\sqrt{1-\varepsilon_b})a_w (T_w - T_g) = 0$$

Solid Phase Balance Equation

$$-J_s \frac{\partial w_i}{\partial z} - (1-\varepsilon_b)\rho_p \frac{\partial Q_i}{\partial t} = 0$$

$$-(1-\varepsilon_b) k_{sf} \frac{\partial^2 T_s}{\partial z^2} + C_{p,s} J \frac{\partial T_g}{\partial z} + (1-\varepsilon_b) h_f a_s (T_s - T_g) - h_{ws}\sqrt{1-\varepsilon_b}\, a_w (T_w - T_g) + \Delta H\left(\rho_p \frac{\partial Q_i}{\partial t}\right) = 0$$

Tube-side Balance Equation

$$-F_{st} a_{tube} \Delta H_{latent} \frac{\partial v f_{st}}{\partial z} - h_{wst} a_w (T_w - T_{st}) = 0$$

$$h_{wst} a_w (T_w - T_{st}) + h_{wg}(1-\sqrt{1-\varepsilon_b}) a_w (T_w - T_g) + h_{ws}\sqrt{1-\varepsilon_b}\, a_w (T_w - T_g) = 0$$

Pressure Drop

$$\frac{\partial P}{\partial z} = -\left(\frac{150\times 10^{-5}\mu_g (1-\varepsilon_b)^2}{(d_p \psi)^2 \varepsilon_b^{\,3}} v_g + \frac{1.75\times 10^{-5} M_w \rho_g (1-\varepsilon_b)}{(d_p\psi)\varepsilon_b^{\,3}} v_g^{\,2}\right)$$

LDF - Mass Transfer

$$\rho_p \frac{\partial Q_i}{\partial t} = k_{F,i} a (w_i^* - w_i)$$

$$\frac{1}{k_{F,i} a} = \frac{1}{k_{f,i} a_s} + \frac{r_p^{\,2}}{15 D_{e,i}}, \quad D_{e,i} = \frac{D_{0,i} e^{\frac{-E}{RT}}}{\left(1 - \frac{w_i}{w_s}\right)}$$

Z-S Equation for Effective Thermal Conductivity

$$\frac{k_{sf}}{k_g} = \frac{2}{1-\lambda B}\left[\frac{(1-\lambda)B}{(1-\lambda B)^2}\ln\frac{1}{\lambda B} - \frac{B+1}{2} - \frac{B-1}{1-\lambda B}\right]$$

$$\lambda = k_g / k_s, \ B = C\left(\frac{1-\phi}{\phi}\right)^m$$

where, ϕ is the porosity of the bed and C = 1.25, m = 10 / 9.

Wall to Fluid Heat Transfer Coefficient

$$Nu_{wg} = \frac{h_{wg} d_p}{k_g} = f(\mathrm{Re}, \mathrm{Pr})$$

$$Nu_{ws} = \frac{h_{ws} d_p}{k_{sf}} = f(\mathrm{Re}, \mathrm{Pr})$$

Dimensionless Numbers

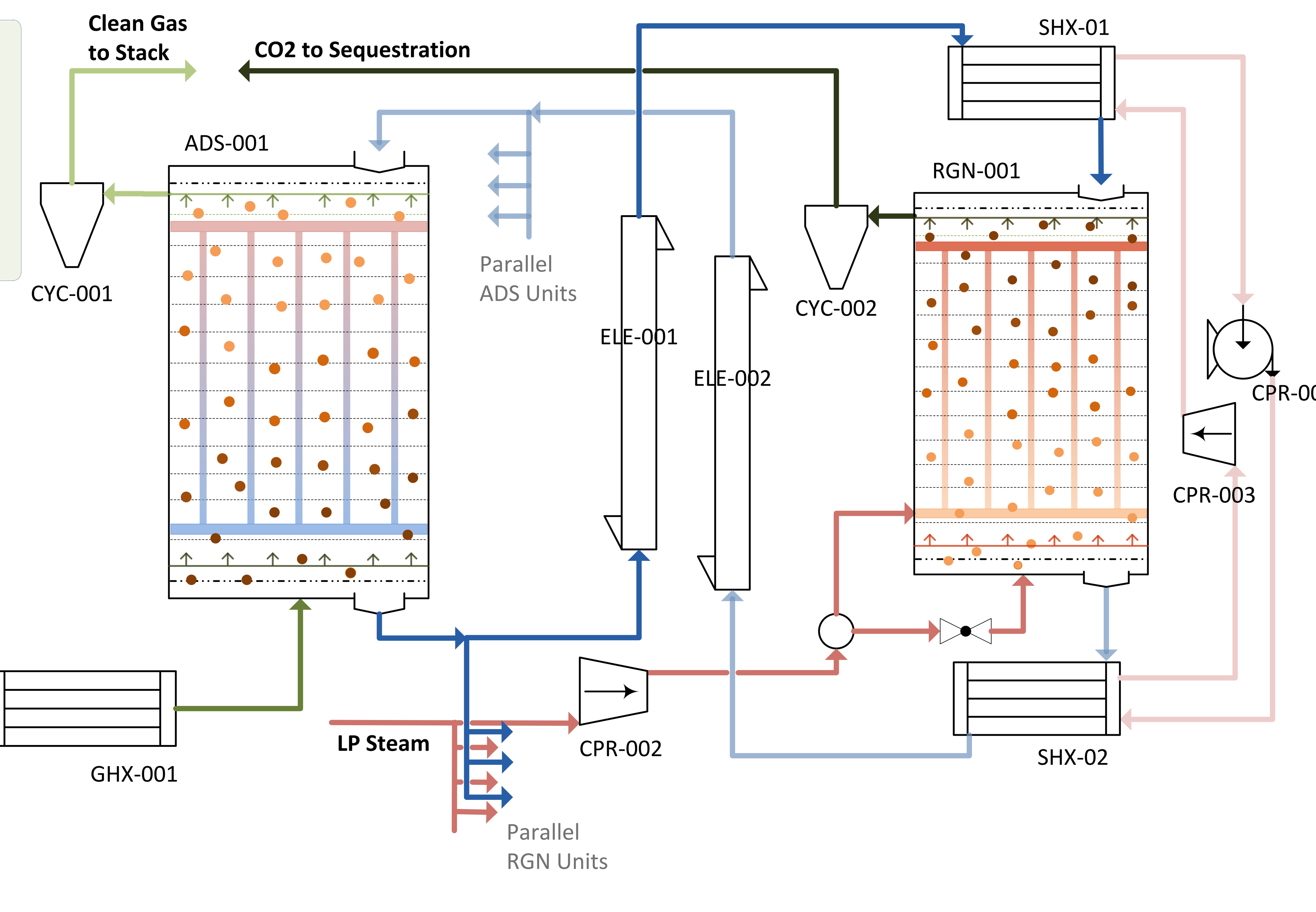
$$Pe_p = \frac{v_g d_p}{D_z} = f(\mathrm{Re}, Sc)$$

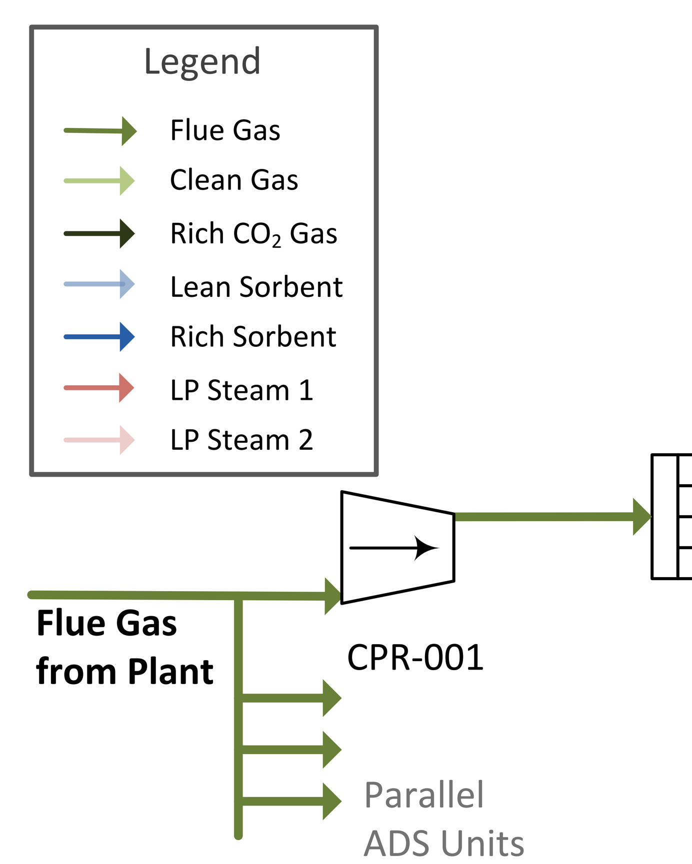
$$Sh_p = \frac{k_{f,i} d_p}{D_{m,i}} = f(\mathrm{Re}, Sc)$$

$$Nu_p = \frac{h_f d_p}{k_g} = f(\mathrm{Re}, \mathrm{Pr})$$

Overall Process System

- A process concept demonstrating how moving-bed process models for the adsorber and regenerator can be integrated to predict overall system performance.
- This detailed system model was directly used to optimize the process structure and operating parameters.

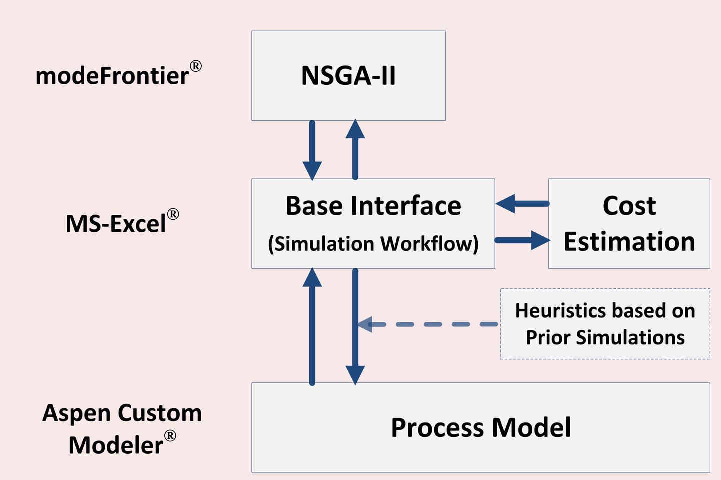




Design Variables

- 2 Integer variables
  - Number of ADS units
  - Number of RGN units
- For each reactor (ADS, RGN)
  - Diameter and height
  - Avg. voidage
  - Tube diameter
- Other operating variables for ADS
  - # of tubes
  - Gas inlet temp. in ADS
  - Sorbent inlet flowrate and temp.
- Other operating variables for RGN
  - Steam inlet flowrate
  - Circulation medium flowrate
  - Extent of regeneration

Optimization Framework



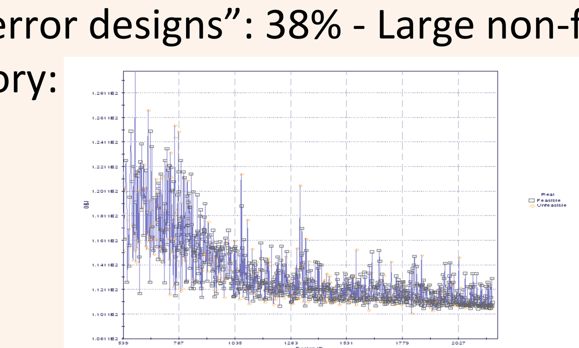
- Objective Function

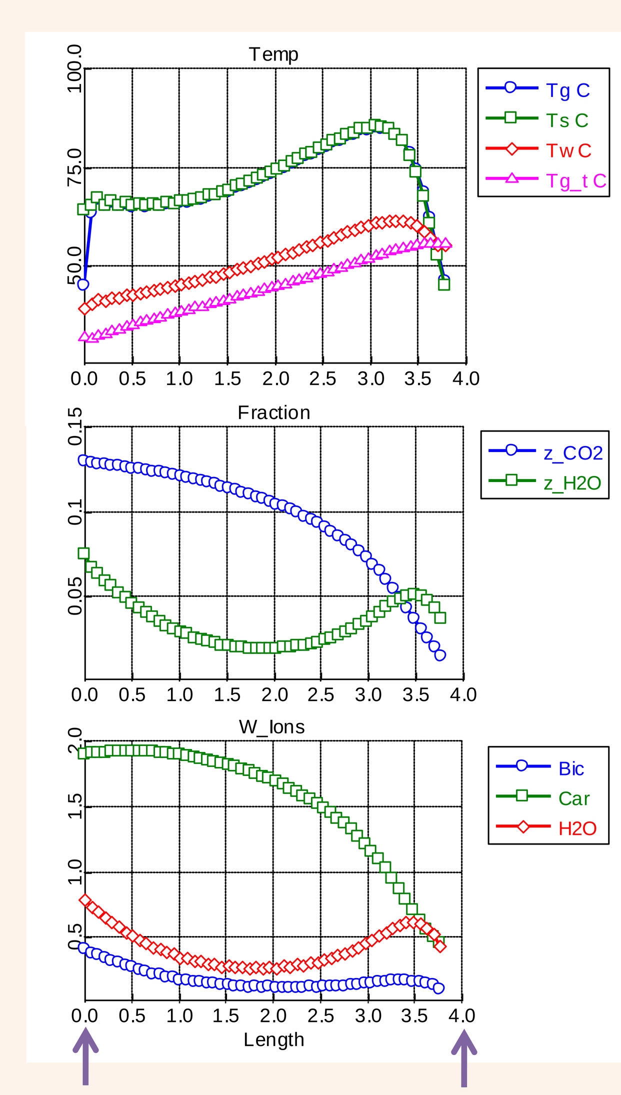
$$COE = \frac{\text{first year capital charge} + \text{first year fixed operating costs} + \text{first year variable operating costs}}{\text{annual net megawatt hours of power generated}}$$

- Process Constraints
  - Maximum gas velocity in reactors.
  - Minimum approach temp. in HXs.
  - Etc.

Optimal Design

- 15 ADS units + 12 RGN units
  - Objective value: 110.46 \$/MWh
  - After 1600 designs evaluation over 32 hours.
  - High % of "error designs": 38% - Large non-feasible area.
  - Design History:





Adsorber

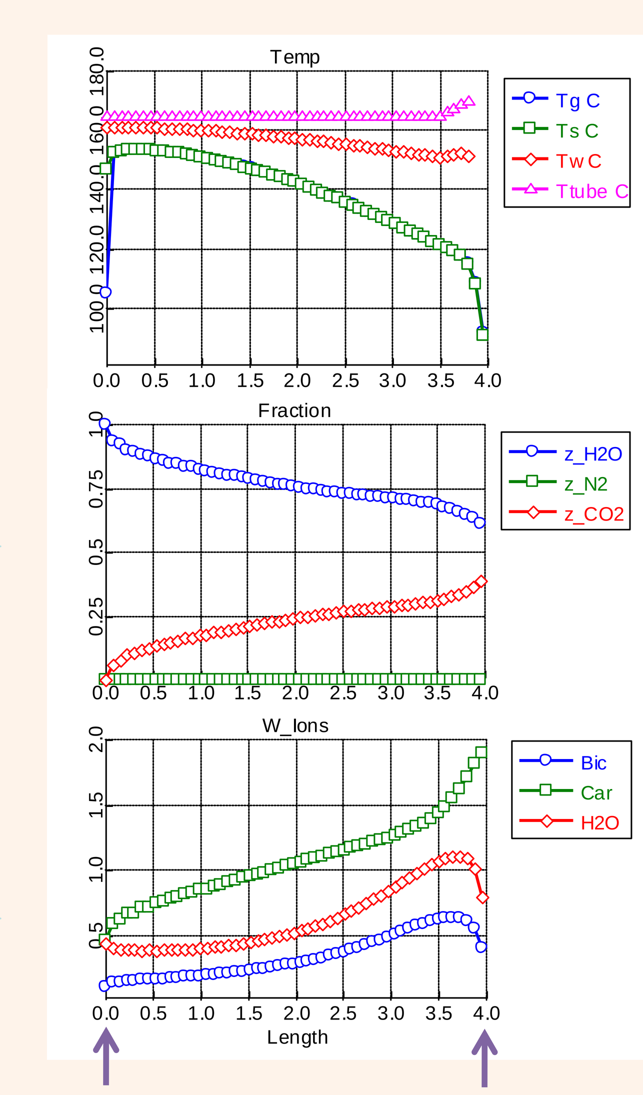
Diameter	9.909 m
Height	3.771 m
P drop (Rx / Hx)	0.12 / 0.1 bar
Flue gas, 65.5°C	5951.65 kmol/hr
Sorbent, 40°C	398.23 ton/hr
CW, 32.22°C	376.21 ton/hr

- Sorbent outlet
  Temperature: 64.11 °C
  CO2 loading: 0.565 -> 2.304 mol/kg
  H2O loading: 0.542 -> 1.194 mol/kg

Regenerator

Diameter	7.667 m
Height	3.946 m
P drop	< 0.1 bar
Injected Steam (105°C, 1.11 bar)	18.83 ton/hr
HX steam (170°C, 6.90 bar)	45.40 ton/hr

- Sorbent outlet
  Temperature: 147.07 °C
  CO2 loading: 2.304 -> 0.565 mol/kg
  H2O loading: 1.194 -> 0.542 mol/kg



Acknowledgements

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