CCSI

Carbon Capture Simulation Initiative

Dynamic Modeling and Control of an Integrated Solid Sorbent Based CO_2 Capture Process

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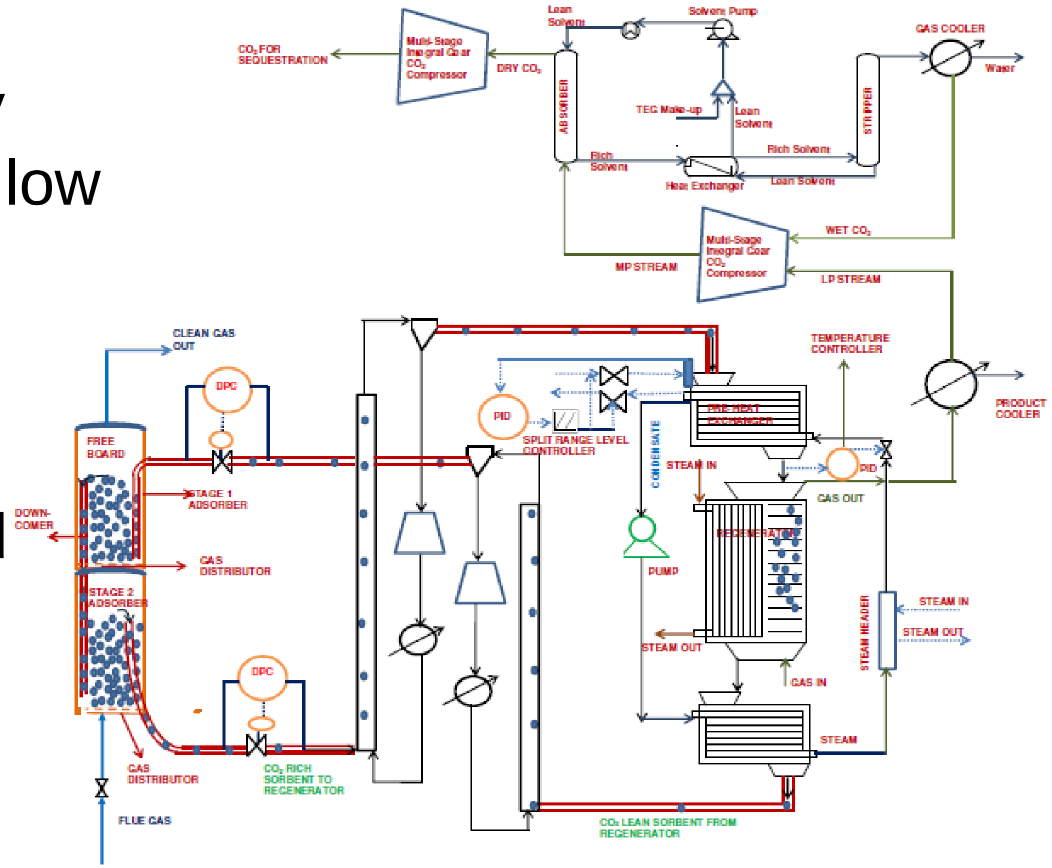
MOTIVATION

- Under the auspices of US DOE's Carbon Capture Simulation Initiative (CCSI), government and university researchers are collaborating to develop computational models and tools for various post-combustion CO2 capture technologies

- As part of this project, our current focus is on the development of dynamic models and control systems for solid-sorbent CO_2 capture processes.

Post- Combustion Solid Sorbent CO_2 Capture

- Solvent based systems typically have high energy cost for regeneration with low CO_2 carrying capacity
- Types of Beds
  - Fixed Bed
  - Bubbling Fluidized Bed (BFB)
  - Moving Bed (MB)



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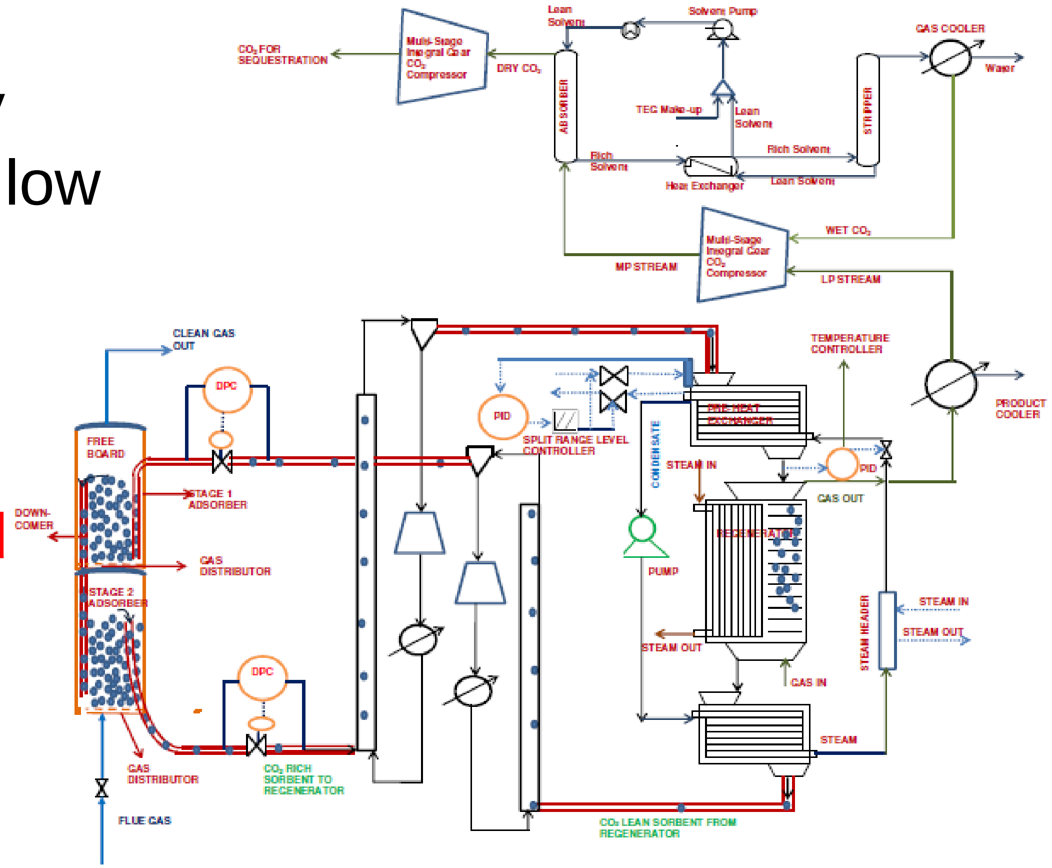
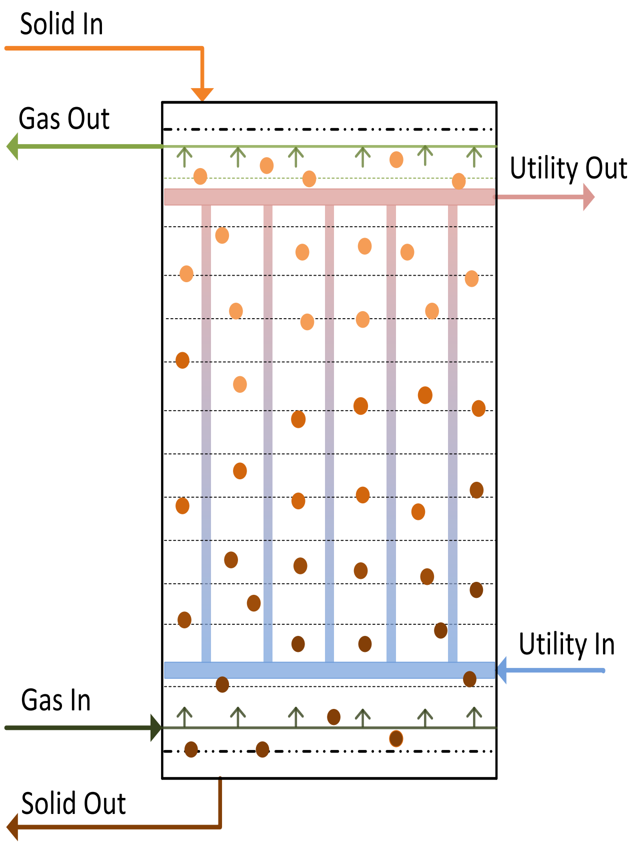


Model Development for BFB and MB

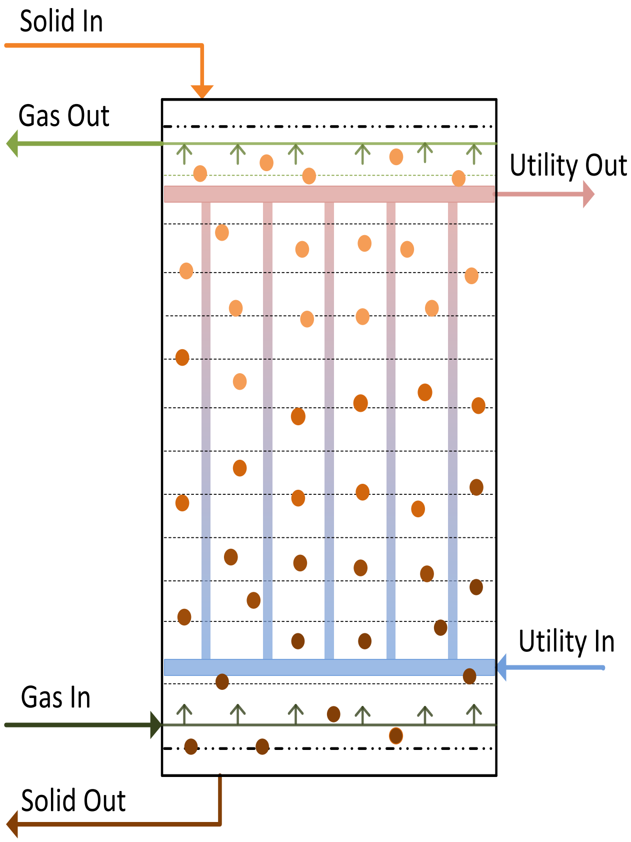
1-D, two-phase, pressure-driven and non-isothermal model developed in both ACM and gPROMS



Model Assumptions

- Vertical shell & tube type reactor
- Mass balance modeled as plug flow
- Particles are uniformly dispersed through the reactor with constant voidage
- Particle attrition ignored
- Temperature is uniform within the particles

Components in BFB and MB



- Gaseous species : CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.
- Stripping steam is used for regenerator
- Solid Sorbent: NETL 32D, a mesoporous amine-impregnated silica substrate

Kinetics

$$H_2O_{(g)} \leftrightarrow H_2O_{(phys)}$$
$$2R_2NH + CO_{2,(g)} \leftrightarrow R_2NH_2^+ + 2R_2NCO_2^-$$
$$R_2NH + CO_{2,(g)} + H_2O_{(phys)} \leftrightarrow R_2NH_2^+ + HCO_3^-$$

$$\frac{\partial Q_{H_2O}}{\partial t} = k_{H_2O}\left[RT_s c_{surf,H_2O} - \frac{1}{K_{H_2O}}\rho_s w_{H_2O}\right]$$

$$\frac{\partial Q_{Bic}}{\partial t} = k_{Bic}\left[\left(1 - \frac{2\rho_s w_{Car} + \rho_s w_{Bic}}{n_v}\right)\rho_s w_{H_2O}(RT_s c_{surf,CO_2}) - \frac{1}{K_{Bic}} w_{Bic}\rho_s{}^2\left(\frac{w_{Car} + w_{Bic}}{n_v}\right)\right]$$

$$\frac{\partial Q_{Car}}{\partial t} = k_{Car}\left[\left(1 - \frac{2\rho_s w_{Car} + \rho_s w_{Bic}}{n_v}\right)(RT_s c_{surf,CO_2})^m - \frac{1}{K_{Car}} w_{Car}\rho_s{}^2\left(\frac{w_{Car} + w_{Bic}}{n_v}\right)\right]$$

$$k_j = A_j(T_s + 273.15)exp\left(\frac{-E_j}{RT_s}\right)$$

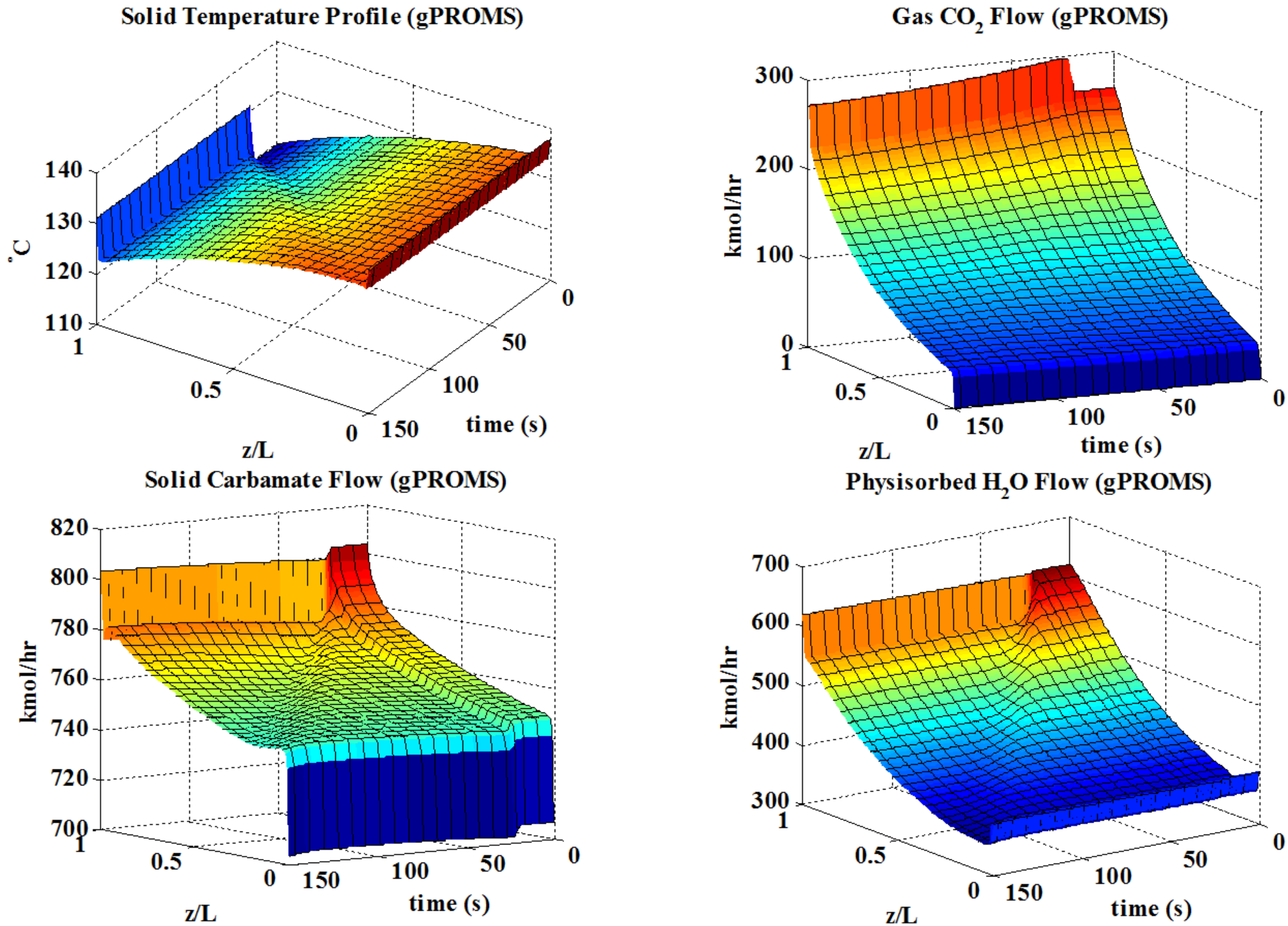
$$K_j = exp\left(\frac{-\Delta S_j}{R}\right)exp\left(\frac{-\Delta H_j}{RT_s}\right)/(P \times 10^5)$$

	ΔH_j [J/mol]	ΔS_j [J/K/mol]
H_2O	-52,100	-78.5
Bic	-36,300	-88.1
Car	-64,700	-174.6

	E_j [J/mol]	A_j
H_2O	28,200	0.0559
Bic	58,200	2.6167
Car	57,700	0.0989
m	1.17	

*Lee et al. A model for the Adsorption Kinetics of CO_2 on Amine-Impregnated Mesoporous Sorbents in the Presence of Water, 28th International Pittsburgh Coal Conference 2011, Pittsburgh, PA, USA.

MB Step Test- Sorbent Temperature



Limitations of Gas Throughput in the MB

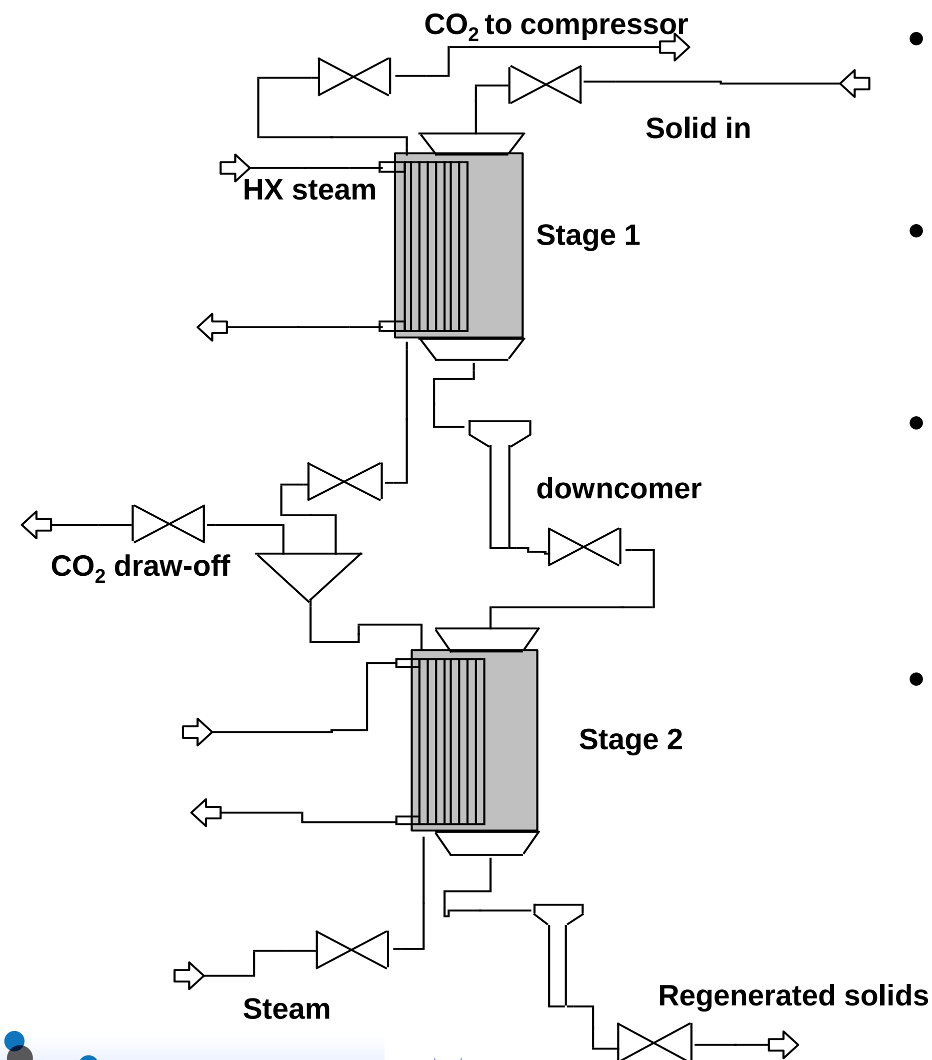
Limitation in superficial velocity of gas; need to maintain MB flow regime*

$$\frac{U_c}{\sqrt{gD_x}} = 0.463Ar^{0.145} \qquad v_g < U_c$$

- As sorbent is regenerated gas is released increasing the superficial gas velocity, maximizing at the top of the bed

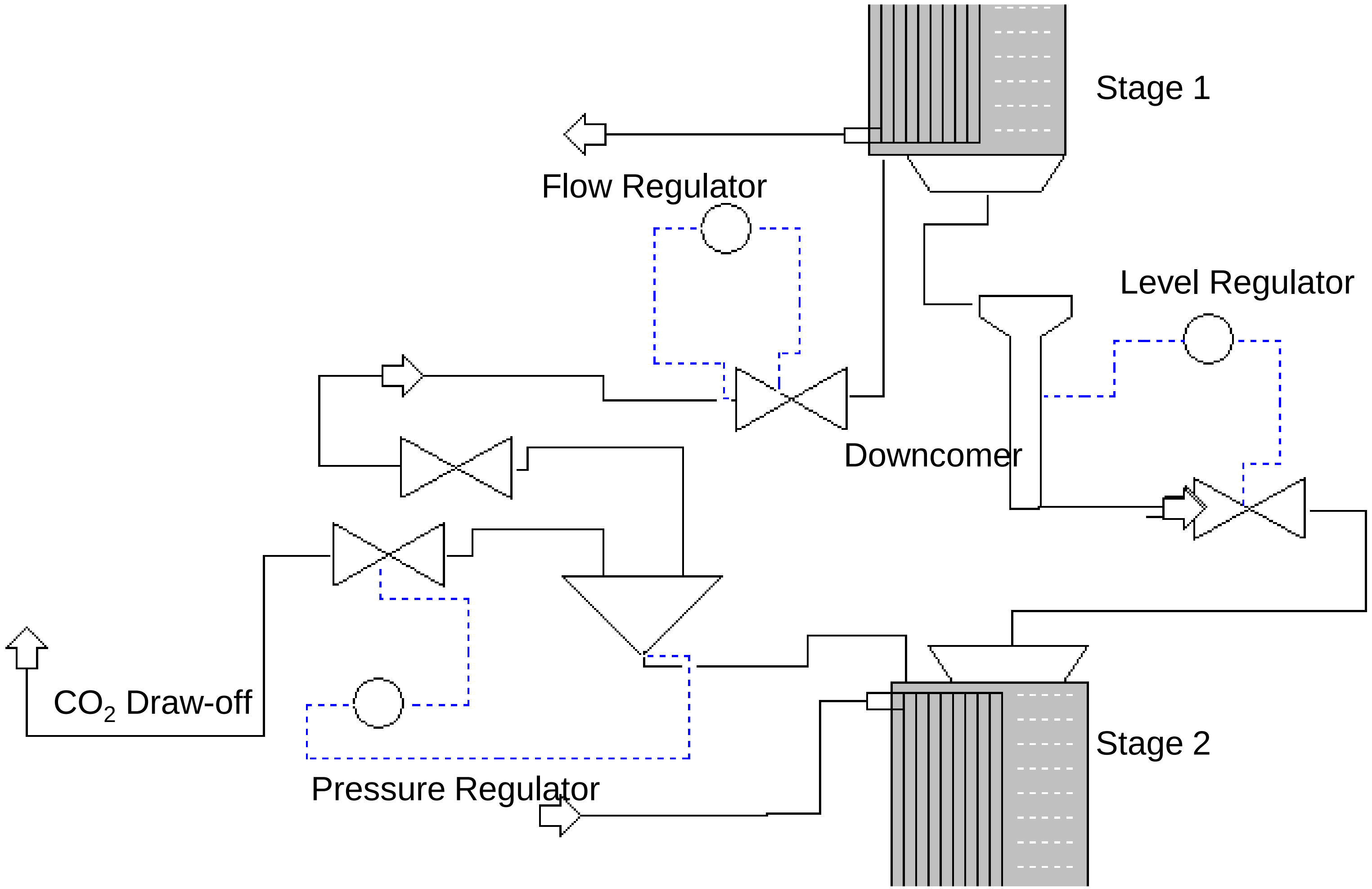
* Chehbouni, et al., *The Canadian Journal of Chemical Engineering* **1995**, 73, 41–50.

Two-Stage MB Bed



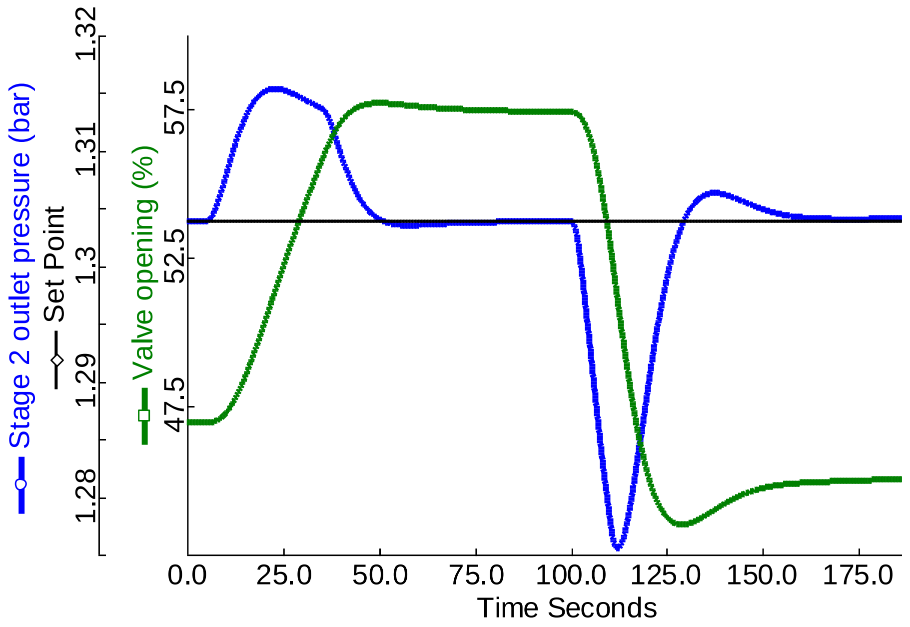
- Sorbent release of CO_2 increases gas flow and velocity at the top of reactor
- CO_2 draw-off between stages decreases velocity to stay in MB regime
- Steady-state solution is easily achieved, but creates a moving boundary problem for dynamic operation
- Control strategy required for solution

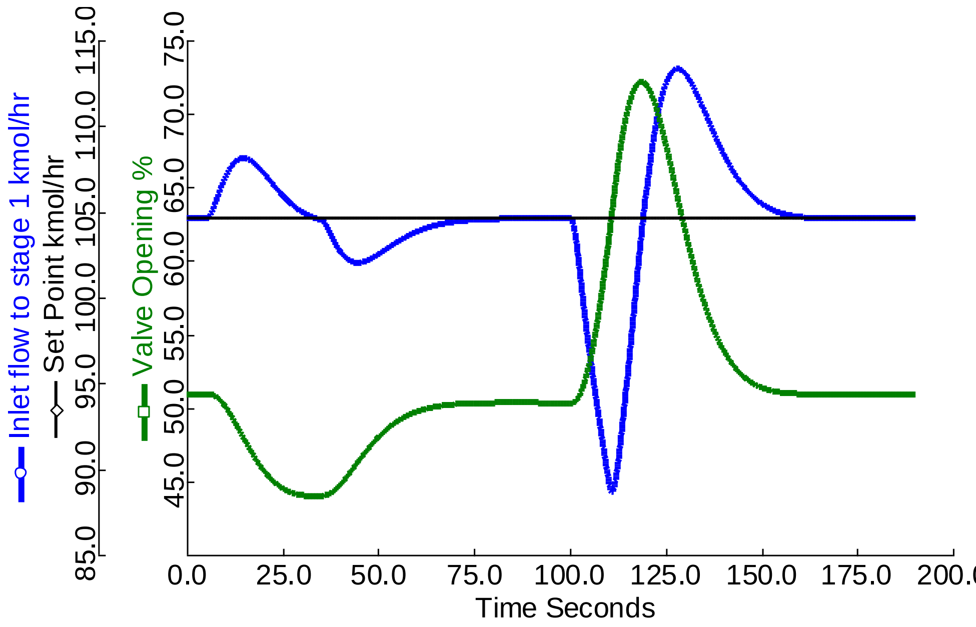
Multi-Stage MB Control Strategy



Regulation- Steam Ramp

Response to a 30 second, 22% increase ramp and 10 second, 22% decrease ramp in inlet regeneration steam





Limitations of MB for Adsorber

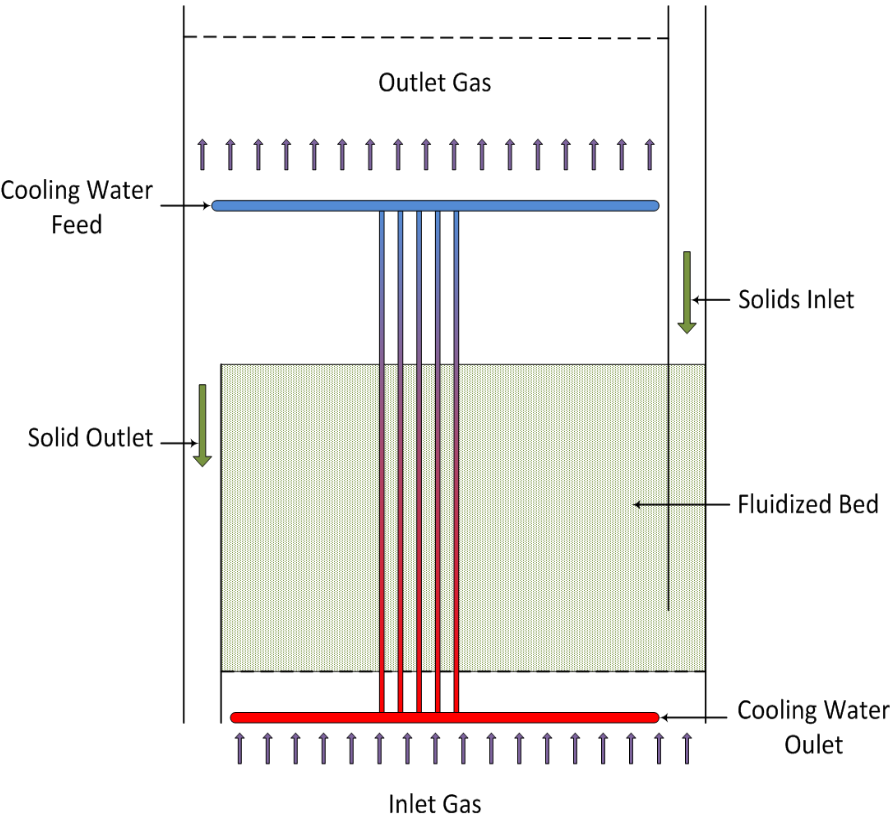
Limitation in superficial velocity of gas; need to maintain MB flow regime*

$$\frac{U_c}{\sqrt{gD_x}} = 0.463Ar^{0.145} \qquad v_g < U_c$$

- Because of the high amount of N_2 in the flue gas, a prohibitively large bed diameter or a very high number of parallel beds would be required for a MB adsorber
- Given an adsorber that is treating 2000 mol/s with 12% CO_2 and 90% capture rate, 27 MB in parallel with a diameter of 9 m each would be required.

*Chenbouni, et al., *The Canadian Journal of Chemical Engineering* **1995**, *73*, 41–50.

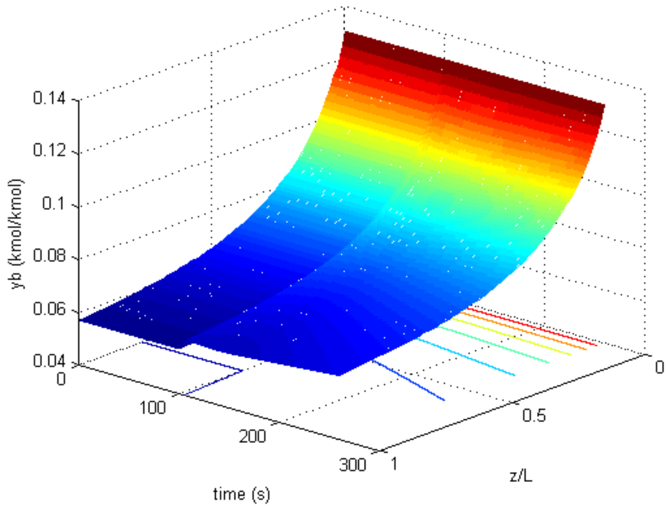
Bubbling Fluidized Bed



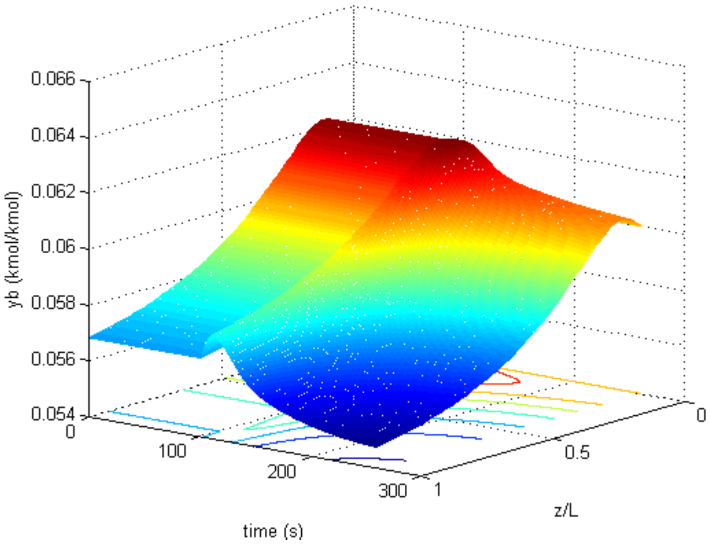
- Similar assumptions as the moving bed
- Flexible steady-state and dynamic models that can be used for both adsorber or regenerator, with underflow/overflow-type configurations

Dynamic Results – Increase Inlet Gas Flow by 20.6%

Gas CO_2 Concentration (ACM)



Gas H_2O Concentration (ACM)



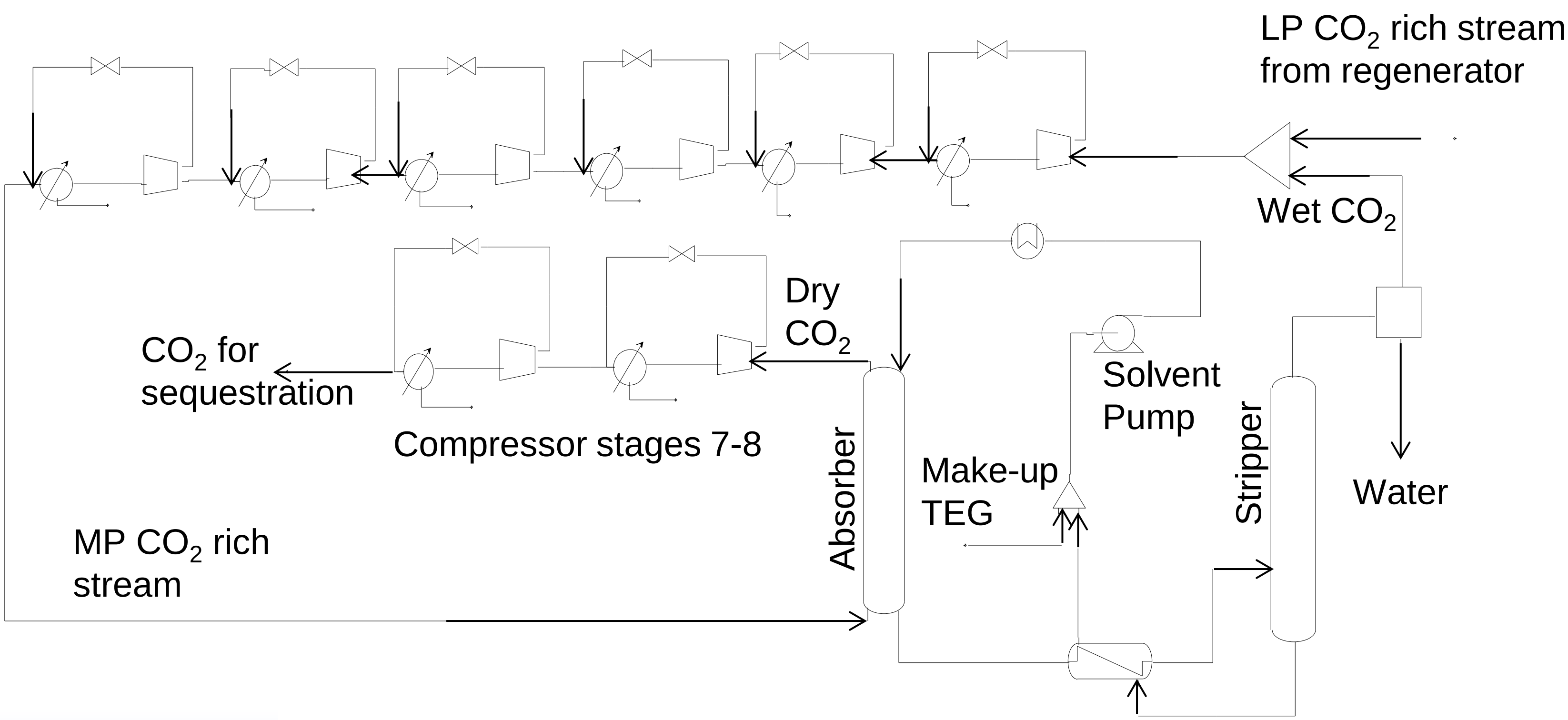
Applications of the BFB and MB Models Other than CO_2 Capture

- Any adsorption (or gas separation) process can be applied, especially for processes for heat input/removal and different flow configurations.
  - Moisture removal
  - Natural gas processing
  - Hydrogen purification
  - Novel solid sorbent processes
  - etc.

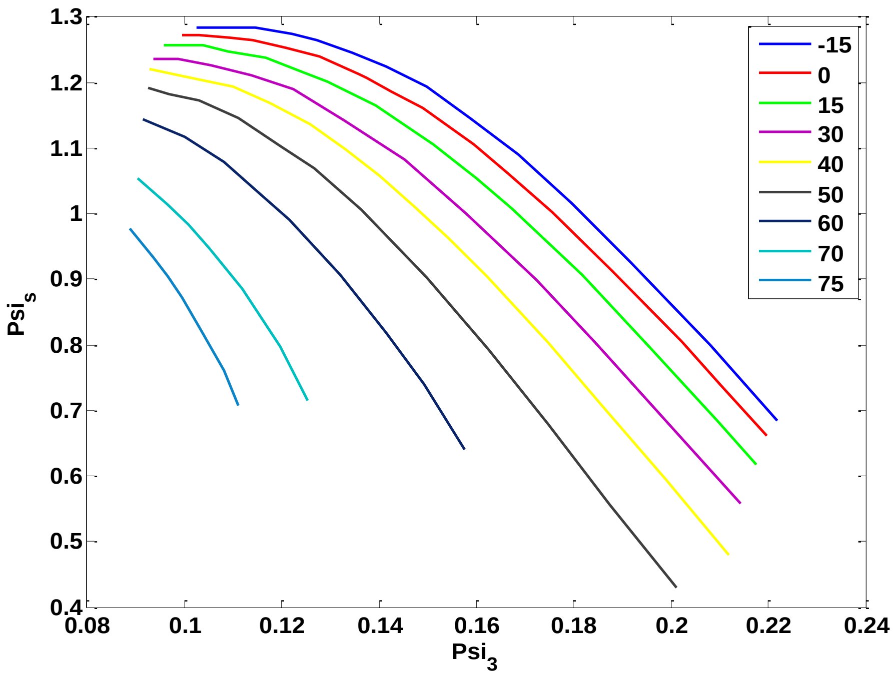
- These models can be adapted to other applications by:
  - Define new components and update physical properties
  - Input new reaction kinetic model/data

CO_2 Compression Model

Dynamic model of multi-stage integral-gear compression system with inter-stage coolers and flash vessels, recycle valves for surge control, and TEG absorber and regenerator



Performance Curves

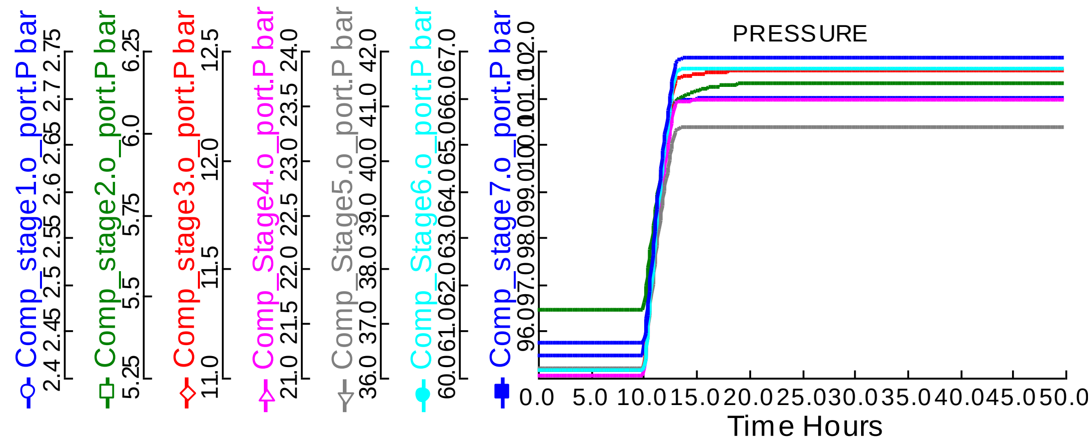


Dimensionless Performance Curves for the 1st Stage

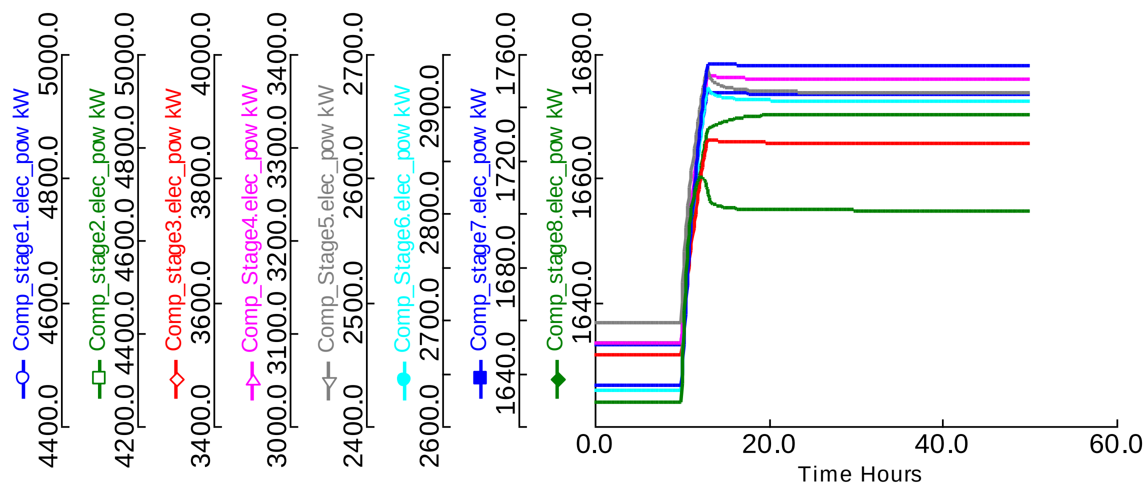
- Dimensionless exit flow coefficient and impeller isentropic head coefficient for applicability to varying Mach numbers and inlet operating conditions

Transient Step Response

Transient response in pressure as a result of 10% ramp increase in flowrate

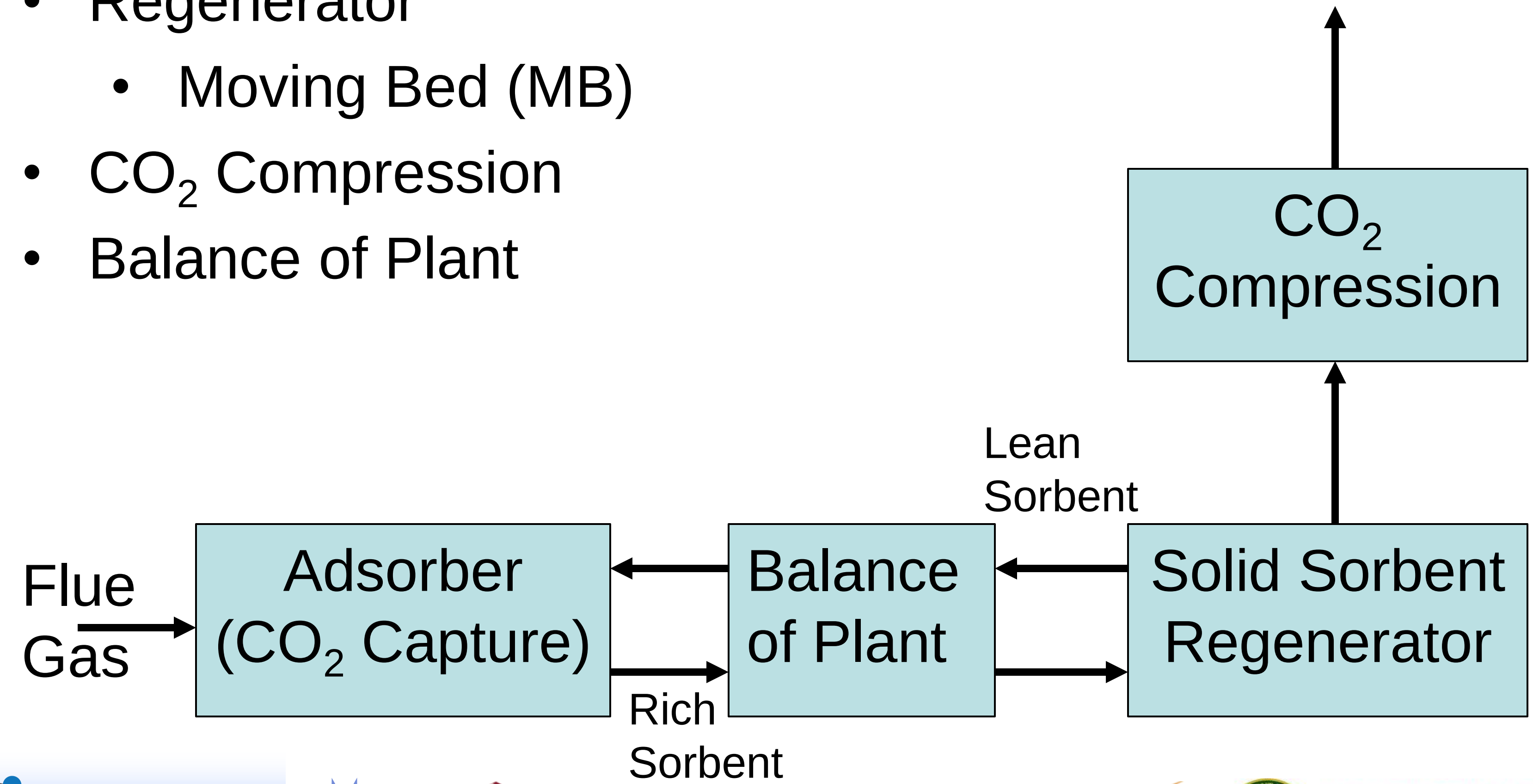


Transient response in power as a result of 10% ramp increase in flowrate



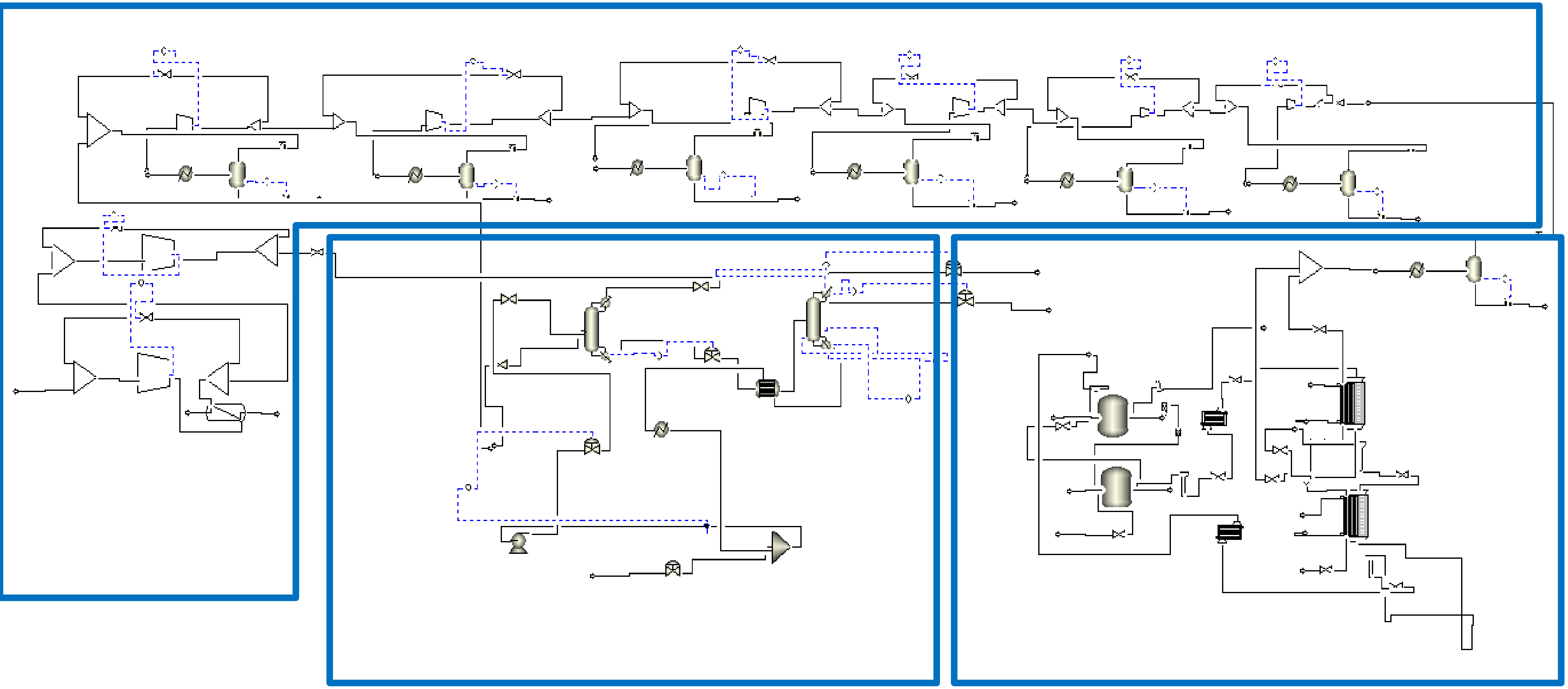
Integrated Model

- Adsorber
  - Bubbling Fluidized Bed (BFB)
- Regenerator
  - Moving Bed (MB)
- CO_2 Compression
- Balance of Plant



Integrated Process Model

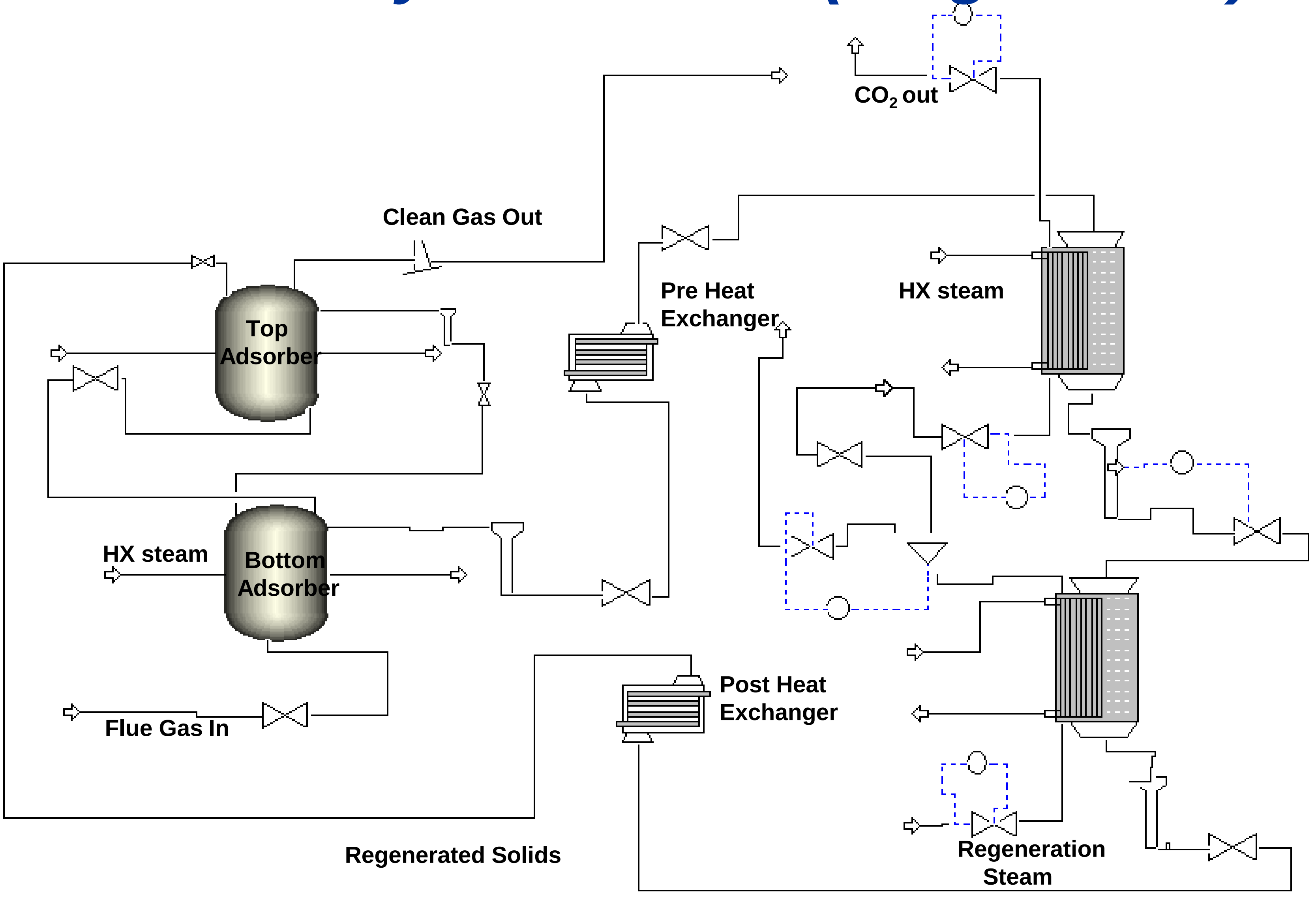
Compressor Train: 8 Stages



TEG Absorber and Stripper

Sorbent BFB Adsorber and MB Regenerator

Combined System Model (Single Train)



Inputs and Conditions

BFB Variable	Base Value	Units
Stage diameter	6	m
Stage height	2.5	m
Steam flue gas rate	400	kmol/hr
Solids inlet flow rate	658000	kg/hr
Solids inlet temperature	60	^oC
Loading of bicarbonate	0.25	mol/kg sorbent
Loading of carbamate	1.23	mol/kg sorbent
Loading of water	0.56	mol/kg sorbent

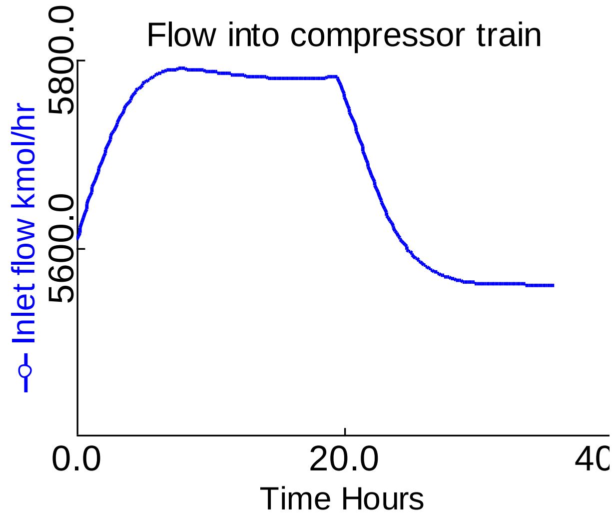
MB Variable	Base Value	Units
Stage Diameter	7	m
Stage Height	2.5	m
Steam inlet flow rate	400	kmol/hr
Solids inlet flow rate	658000	kg/hr
Solids inlet temperature	110	^oC
Loading of bicarbonate	0.62	mol/kg sorbent
Loading of carbamate	1.8	mol/kg sorbent
Loading of water	1.03	mol/kg sorbent

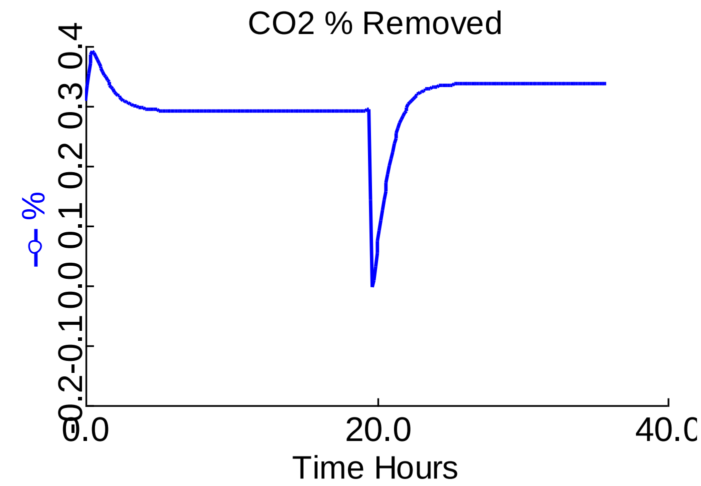
Ramp In Flue Gas Example

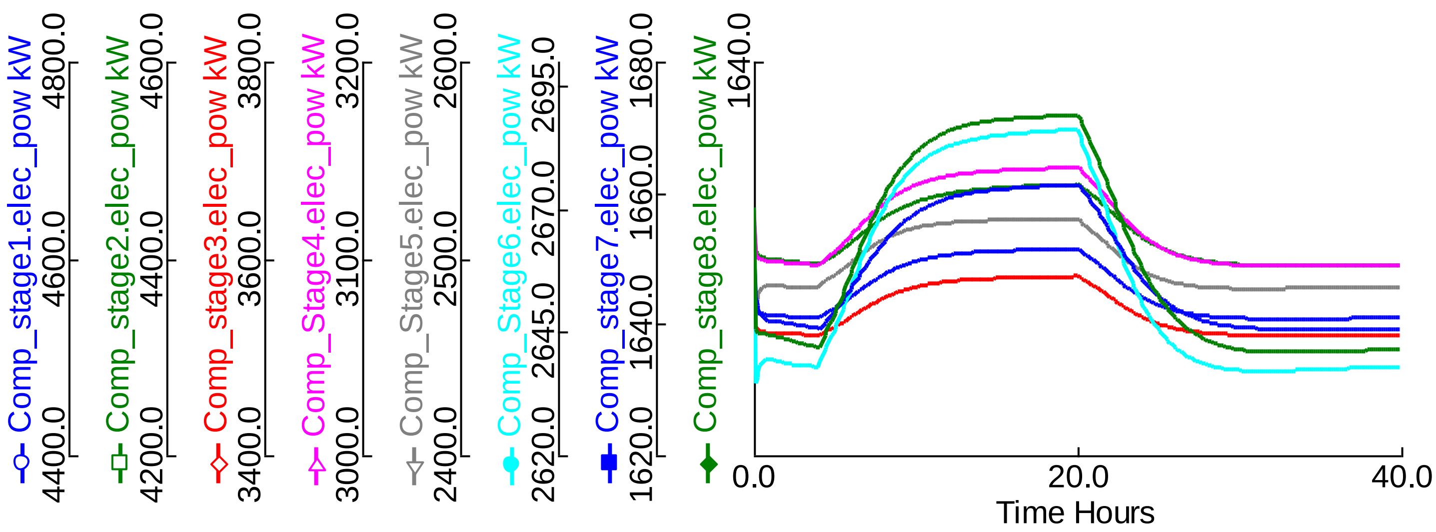
Ramp in flue gas

Time=0 : 15.8% increase

Time=20: 28.8% decrease







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NETL

Berkeley Lab

Lawrence Livermore National Laboratory

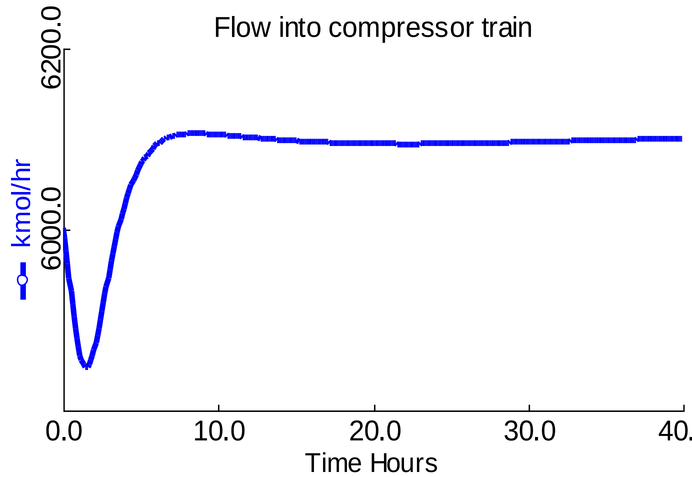
Los Alamos National Laboratory EST. 1943

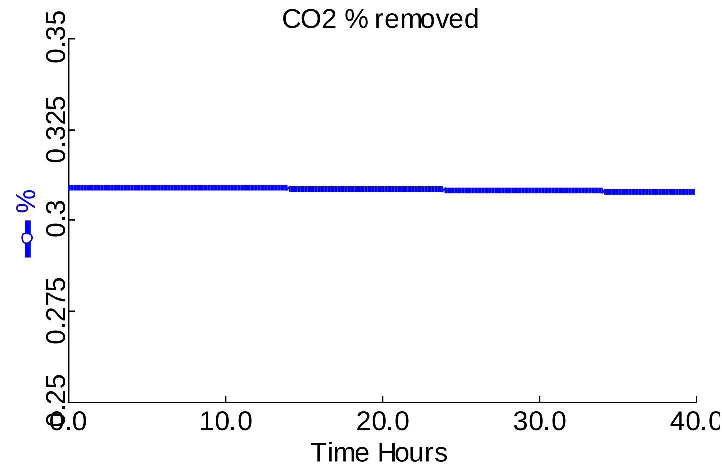
Pacific Northwest National Laboratory

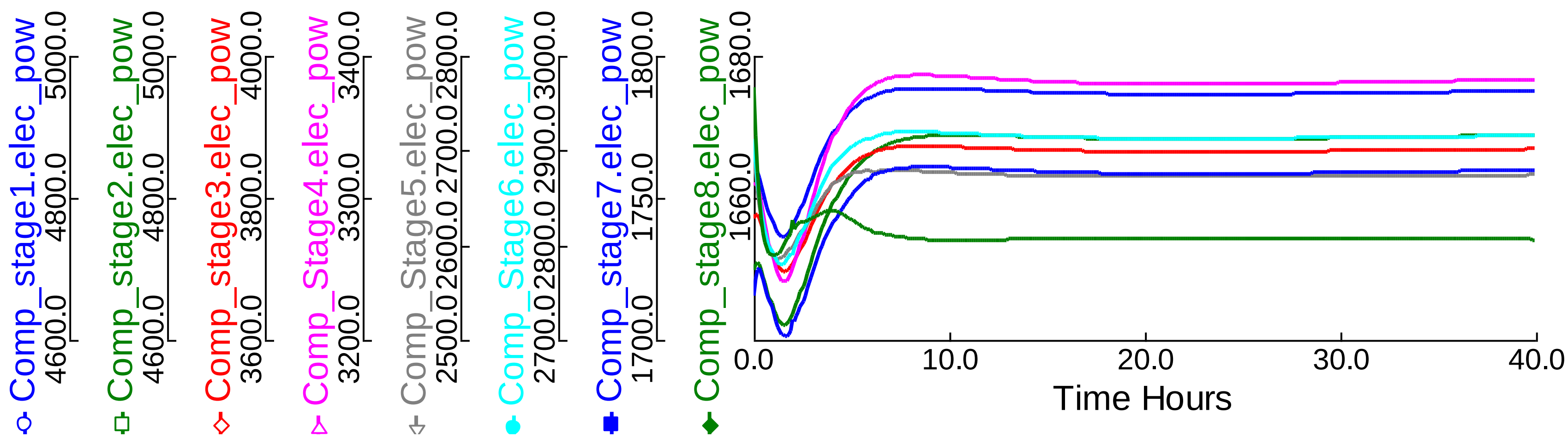
U.S. Department of Energy

Ramp in Regeneration Steam

Ramp in steam
Time=0: 27% increase







Conclusions

- Developed flexible, high-fidelity, first principle, dynamic bubbling fluidized bed and moving bed solid sorbent models for CO_2 capture and CO_2 compression
- Multi-stage moving bed model requires reduced gas velocity, resulting in a moving boundary problem
- Model can handle common disturbances
- Work still to be done
  - Process needs optimization for increase in CO_2 removal
  - Develop MB model that has several CO_2 draw-off points with advanced process controller
  - Develop Reduced order model

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