Steady-State and Dynamic Modeling of a Moving Bed Reactor for Solid-Sorbent CO_2 Capture

Srinivasarao Modekurti, **Debangsu Bhattacharyya**
West Virginia University, Morgantown, WV

Stephen E. Zitney
National Energy Technology Laboratory, Morgantown, WV

David C. Miller
National Energy Technology Laboratory, Pittsburgh, WV

AIChE 2013 Annual Meeting
San Francisco, CA, USA, November 3-8, 2013

OUTLINE

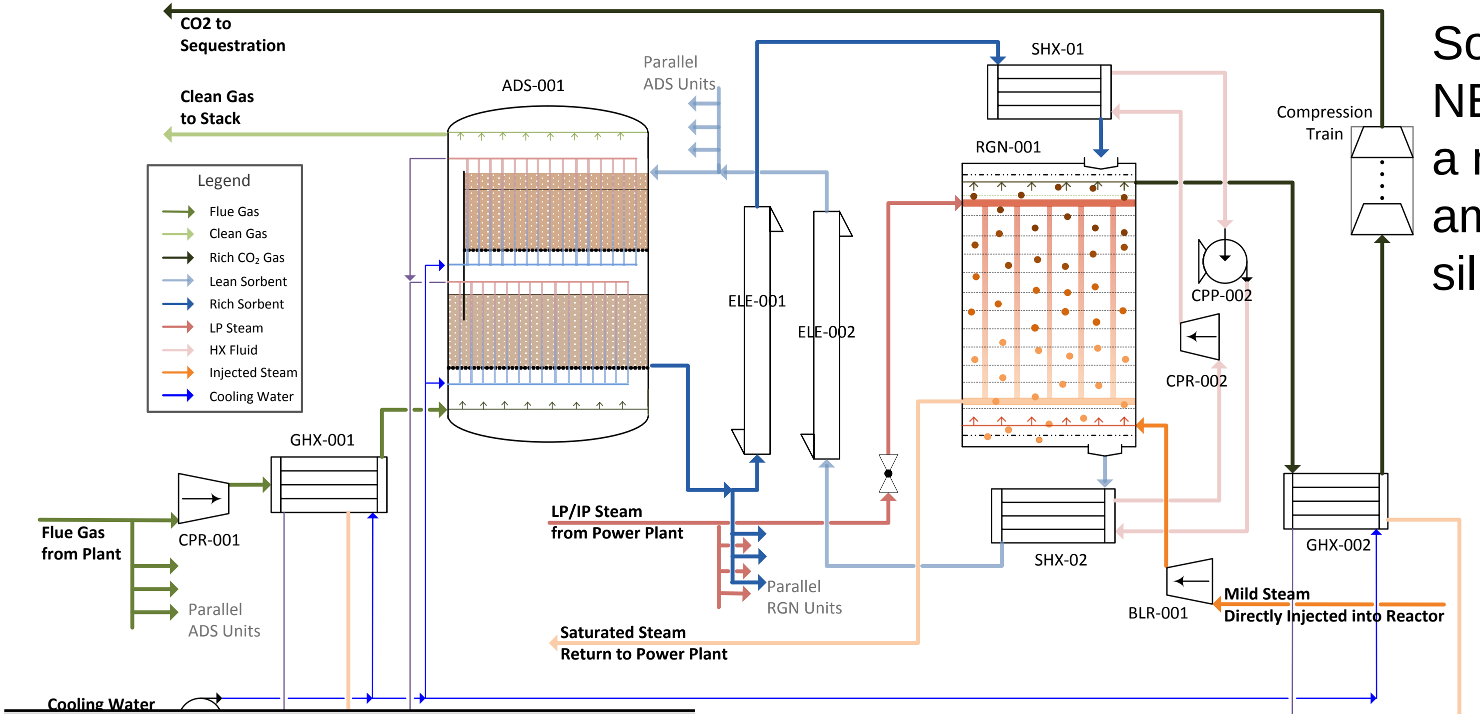
- Motivation
- Dynamic Model Development
- Results and Discussions
- Conclusions

MOTIVATION

- Under the auspices of US DOE’s *Carbon Capture Simulation Initiative (CCSI),* we are developing computational models of various post-combustion CO_2 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.

Optimized Process Developed using CCSI Toolset



Solid Sorbent: NETL 32D, a mesoporous amine-impregnated silica substrate

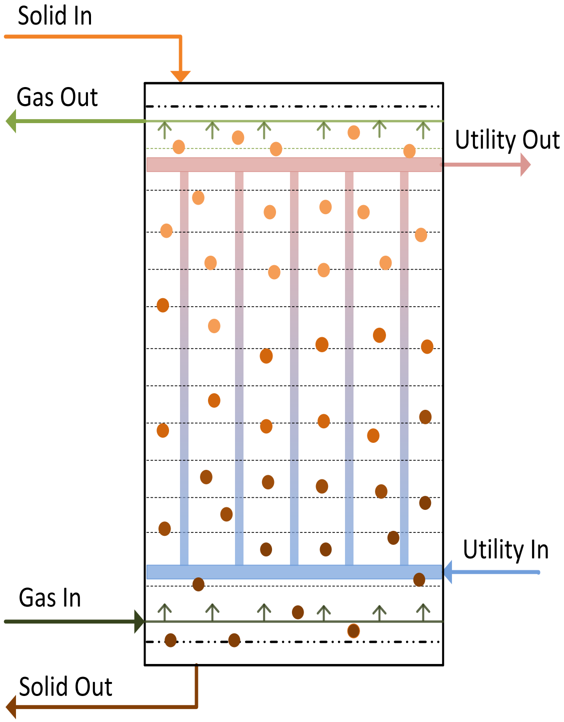
	ADS-001A	ADS-001B
Diameter (m)	9.748	
Bed Depth (m)	7.232	4.854
Total HX Area (m^2)	1733.7	941.3

	RGN-001
Diameter (m)	7.147
Height (m)	4.592
Total HX Area (m^2)	1573.1

	Solid Sorbent	MEA[27] (Δ10°C HX)	MEA[27] (Δ5°C HX)
Q_Rxn (GJ/tonne CO2)	1.82	1.48	1.48
Q_Vap (GJ/tonne CO2)	0	0.61	0.74
Q_Sen (GJ/tonne CO2)	0.97	1.35	0.68
Total Q	2.79	3.44	2.90

MOVING BED DYNAMIC MODEL DEVELOPMENT

- 1-D two-phase pressure-driven non-isothermal dynamic model of a moving bed reactor as part of a solid-sorbent CO_2 capture process

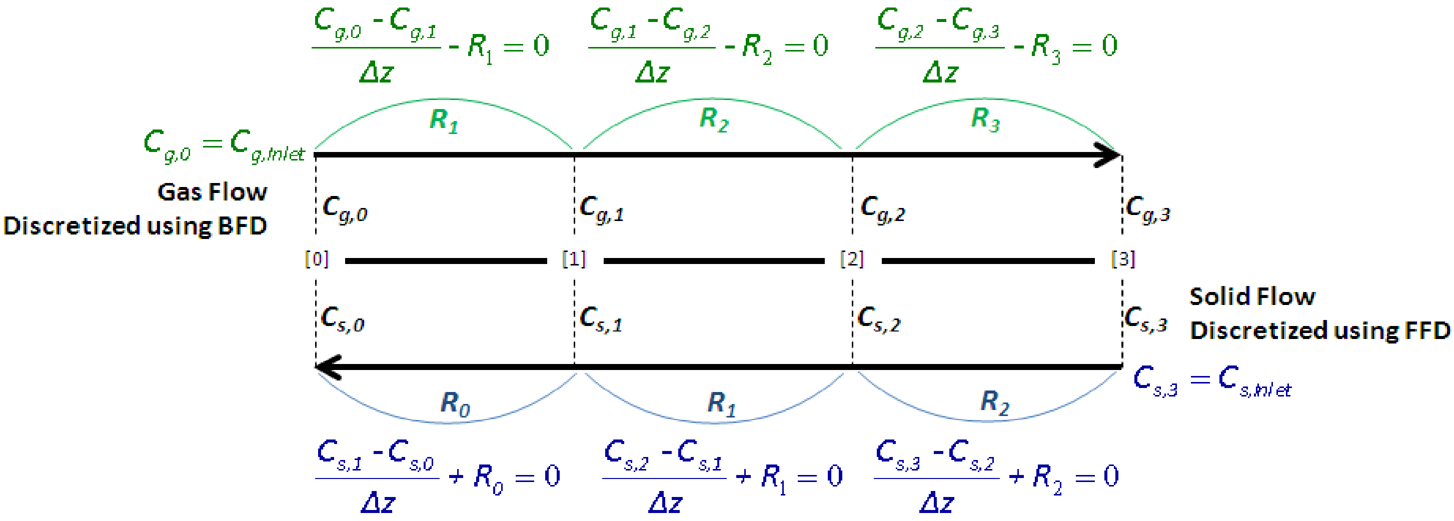


Model Assumptions

- Vertical shell & tube type reactor
- Gas and solids flows are modeled by plug flow model with axial dispersion.
- Particles are uniformly dispersed through the reactor with constant voidage
- Particle attrition ignored
- Temperature is uniform within the particles

- Gaseous species : CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.

MODEL DEVELOPMENT



$$\frac{C_{g,0} - C_{g,1}}{\Delta z} - R_1 = 0 \qquad \frac{C_{g,1} - C_{g,2}}{\Delta z} - R_2 = 0 \qquad \frac{C_{g,2} - C_{g,3}}{\Delta z} - R_3 = 0$$

$C_{g,0} = C_{g,Inlet}$

Gas Flow
Discretized using BFD

Solid Flow
Discretized using FFD

$C_{s,3} = C_{s,Inlet}$

$$\frac{C_{s,1} - C_{s,0}}{\Delta z} + R_0 = 0 \qquad \frac{C_{s,2} - C_{s,1}}{\Delta z} + R_1 = 0 \qquad \frac{C_{s,3} - C_{s,2}}{\Delta z} + R_2 = 0$$

- Radial variation neglected
- Perforated trays are used to distribute the solids uniformly
- Stripping steam is used
- The solids enter the bed from a preheater at about 95ºC

CONSERVATION EQUATIONS

Gas Phase

$$\varepsilon_b D_z \frac{\partial^2 C_i}{\partial z^2} - \frac{\partial (v_g C_i)}{\partial z} + (1 - \varepsilon_b) \sum_j \nu_{i,j} \frac{\partial Q_j}{\partial t} = 0$$

Effective Axial Dispersion Coefficient*

$$\frac{1}{Pe'} = \frac{D_z}{v d_p} = \frac{20}{ReSc} + \frac{1}{2}$$

Solid Phase

$$J_s \frac{\partial w_j}{\partial z} - (1 - \varepsilon_b) \frac{\partial Q_j}{\partial t} = 0$$

*Ruthven, D. M. *Principles of adsorption and adsorption processes*; Wiley-Interscience, 1984

CONSERVATION EQUATIONS CONTD.

Energy Balance

Gas Phase

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

Solid Phase

$$C_{p,s} J_s \frac{\partial T_s}{\partial z} - (1-\varepsilon_b) h_{gs} a_s \left(T_s - T_g\right) + \sqrt{1-\varepsilon_b}\, h_{ws} a_w (T_w - T_s) + \sum_j \Delta H_{rxn,j} \rho_s \frac{\partial Q_j}{\partial t} = 0$$

Tube wall

$$h_t a_w (T_t - T_w) - \left(1 - \sqrt{1-\varepsilon_b}\right) h_{wg} a_w \left(T_w - T_g\right) - \sqrt{1-\varepsilon_b}\, h_{ws} a_w (T_w - T_s) = 0$$

$$v_t \Delta H_{vap} \frac{\partial vf}{\partial z} - h_t a_w (T_t - T_w) = 0$$

Immersed Heat Exchanger Model

Heat Transfer Coefficient calculated by modified Packet Renewal theory[1]

$$Nu = \frac{h_{gs} d_p}{k_g} = 2 + 1.1 \mathrm{Pr}^{1/3} \mathrm{Re}_p^{0.6}$$

$$\tau_i = 0.44 \left[\frac{d_p g}{{v_{mf}}^2 \left(f_{n,i} - a_h \right)^2} \right]^{0.14} \left(\frac{d_p}{d_x} \right)^{0.225}$$

$$f_{b,i} = 0.33 \left[\frac{{v_{mf}}^2 \left(f_{n,i} - a_h \right)^2}{d_p g} \right]^{0.14}$$

Between Solids and Heat Exchanger Tube[2]

$$h_{d,i} = 2 \sqrt{ \frac{k_{p,a,i} \rho_s c_{p,s,e,i} \left(1 - \varepsilon_{d,i} \right)}{\pi \tau_i} }$$

Between Gas and Heat Exchanger Tube[1]

$$Nu_{h,i} = 0.009 Ar_i^{0.5} \mathrm{Pr}_i^{0.33}$$

$$Nu_{h,i} = \frac{h_{l,i} d_p}{k_{g,i}}$$

Overall Heat Transfer Coefficient

$$h_{t,i} = f_{b,i} h_{d,i} + \left(1 - f_{b,i} \right) h_{l,i}$$

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[1] Baskakov, et al., *Heat Transfer to Objects Immersed in Fluidized Beds.* Powder Technology, 1973. **8**, pg. 273-282.

[2] Mickley and Fairbanks., *Heat Transfer to Objects Immersed in Fluidized Beds.* Powder Technology, 1973. **8**, pg. 273-282.

Pressure drop

Modified Ergun Equation is used by using the slip velocity between the interstitial fluid velocity and particle velocity instead of the superficial velocity

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

HYDRODYNAMIC MODEL

Maximum Gas Velocity for Maintaining the Bed in the Moving Bed Regime*

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

Constraint

$$v_g < U_c$$

$$Ar_i = \frac{d_p{}^3 \rho_{g,i} \left(\rho_s - \rho_{g,i} \right) g}{\mu_{g,i}{}^2}$$

External mass transfer resistance is considered by using Frössling correlation

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

REACTION KINETICS

$$H_2O_{(g)} \leftrightarrow H_2O_{(phys)}$$

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

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

$$\frac{\partial Q_{Car}}{\partial t} = k_{Car}\left[\left(1 - \frac{2\rho_s w_{Car} + \rho_s w_{Bic}}{n_v}\right)\left(P \times 10^5 y_{CO_2}\right)^m - \frac{1}{K_{Car}} w_{Car}{\rho_s}^2\left(\frac{w_{Car} + w_{Bic}}{n_v}\right)\right]$$

$$\frac{\partial Q_{Bic}}{\partial t} = k_{Bic}\left[\left(1 - \frac{2\rho_s w_{Car} + \rho_s w_{Bic}}{n_v}\right)\rho_s w_{H_2O}\left(P \times 10^5 y_{CO_2}\right) - \frac{1}{K_{Bic}} w_{Bic}{\rho_s}^2\left(\frac{w_{Car} + w_{Bic}}{n_v}\right)\right]$$

$$\frac{\partial Q_{H_2O}}{\partial t} = k_{H_2O}\left[P \times 10^5 y_{H_2O} - \frac{1}{K_{H_2O}} \rho_s w_{H_2O}\right]$$

*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.

REACTION KINETICS

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

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

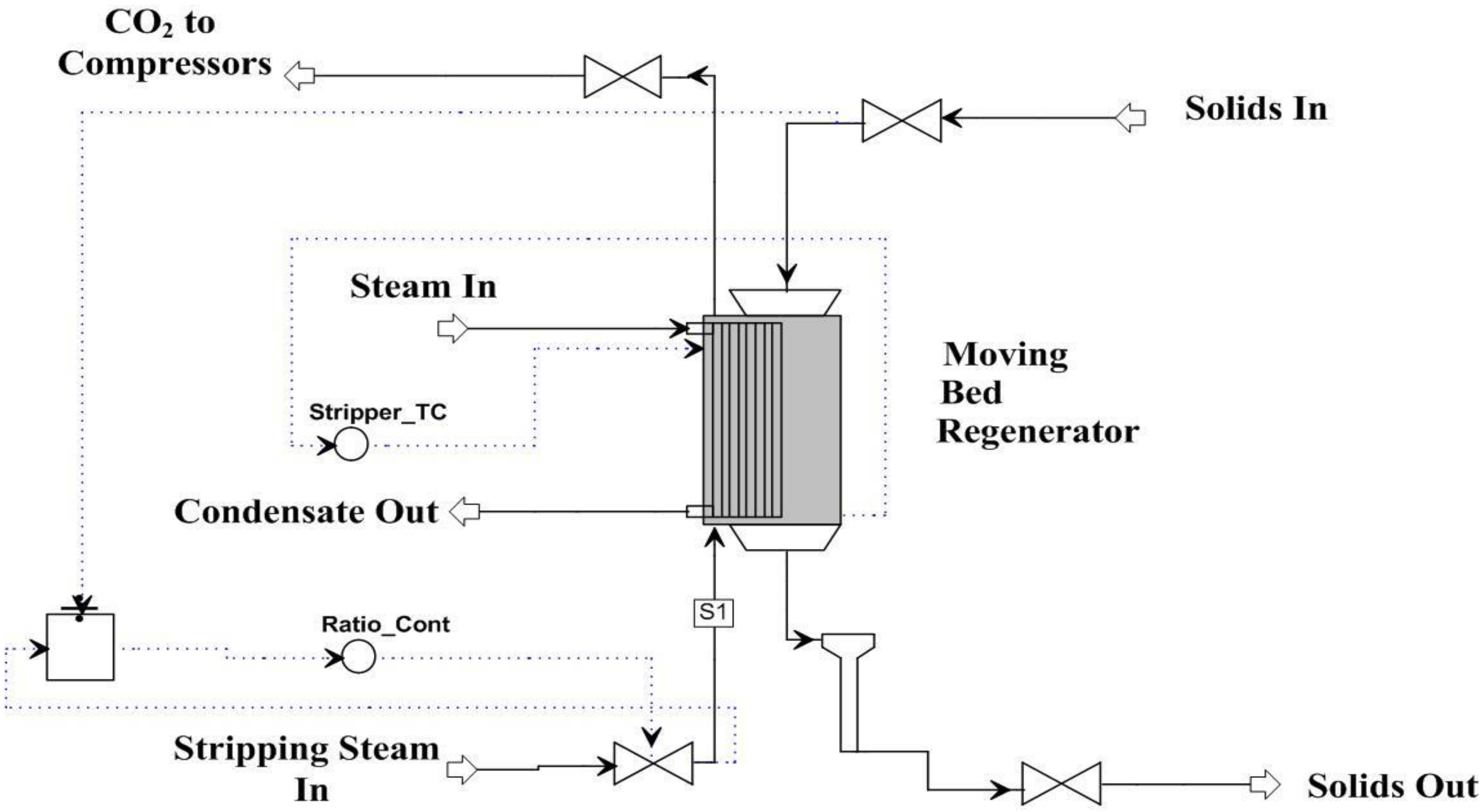
	ΔH_j $[J/mol]$	ΔS_j $[J/K/mol]$
H_2O	-52,100	-78.5
Bic	-36,300	-88.1
Car	-64,700	-174.6

	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.

Modeling of Balance of the Unit

Pressure flow-network developed along with the control valves



Regenerator Parameters and Operating Conditions

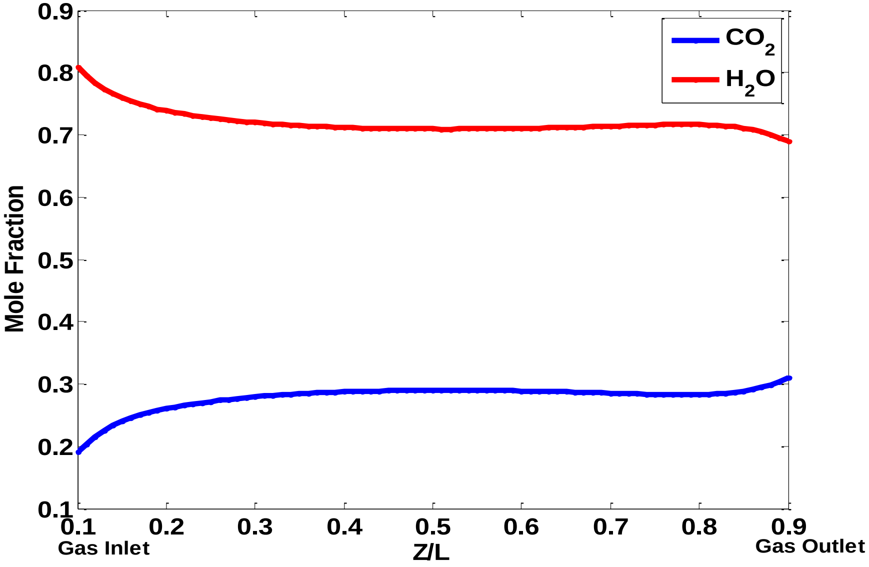
Variable	**Base Value**	**Units**
Reactor Diameter	9	m
Reactor Height	7	m
Average voidage	0.6	
Steam inlet flow rate	1000	kmol/hr
HX steam flow rate	2983.09	kmol/hr
Diameter of HX tube	0.015	m
Solids inlet flow rate	550000	Kg/hr
Solids inlet temperature	52.32	^{o}C
Initial loading of bicarbonate	0.263	mol/kg sorbent
Initial loading of carbamate	1.797	mol/kg sorbent
Initial loading of water	0.651	mol/kg sorbent

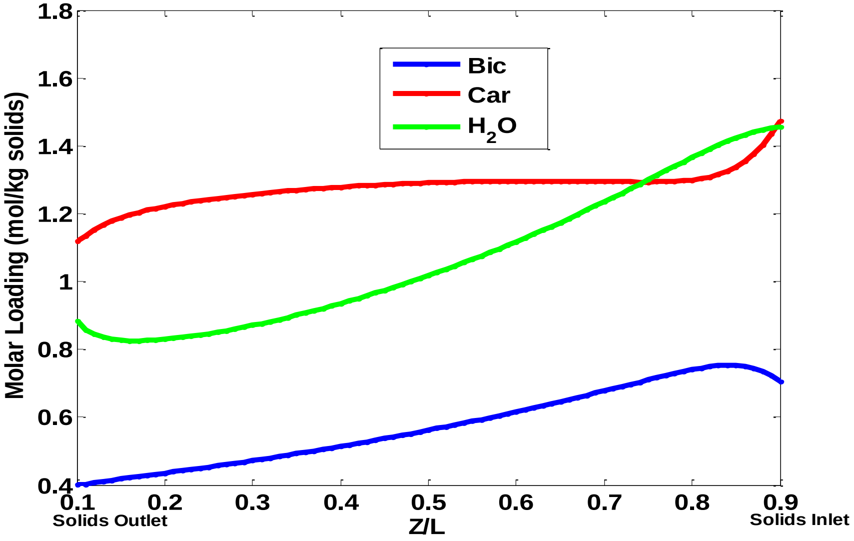
SOLUTION METHODOLOGY

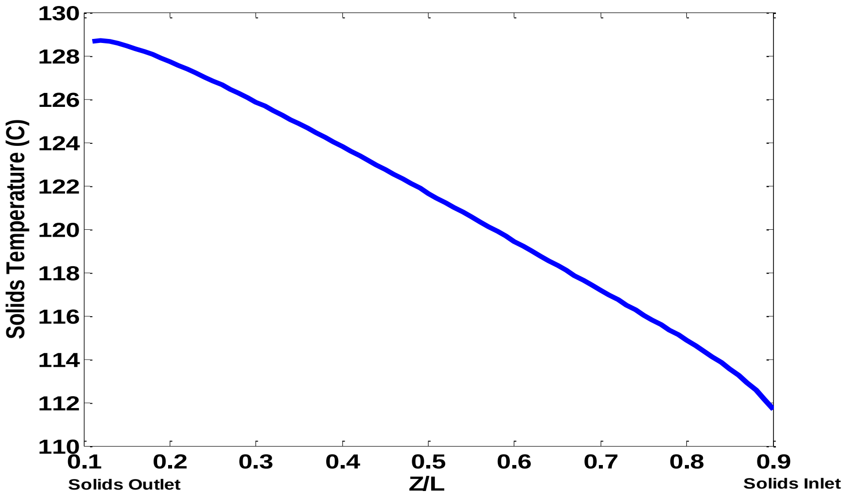
- All the equations are written and solved in Aspen Custom Modeler

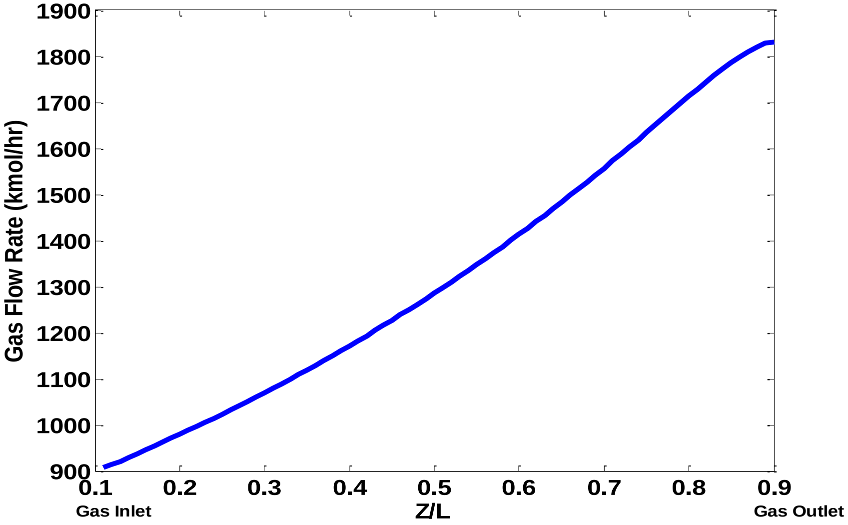
- The dynamic model is solved using the Method of Lines

Moving Bed Regenerator: Results

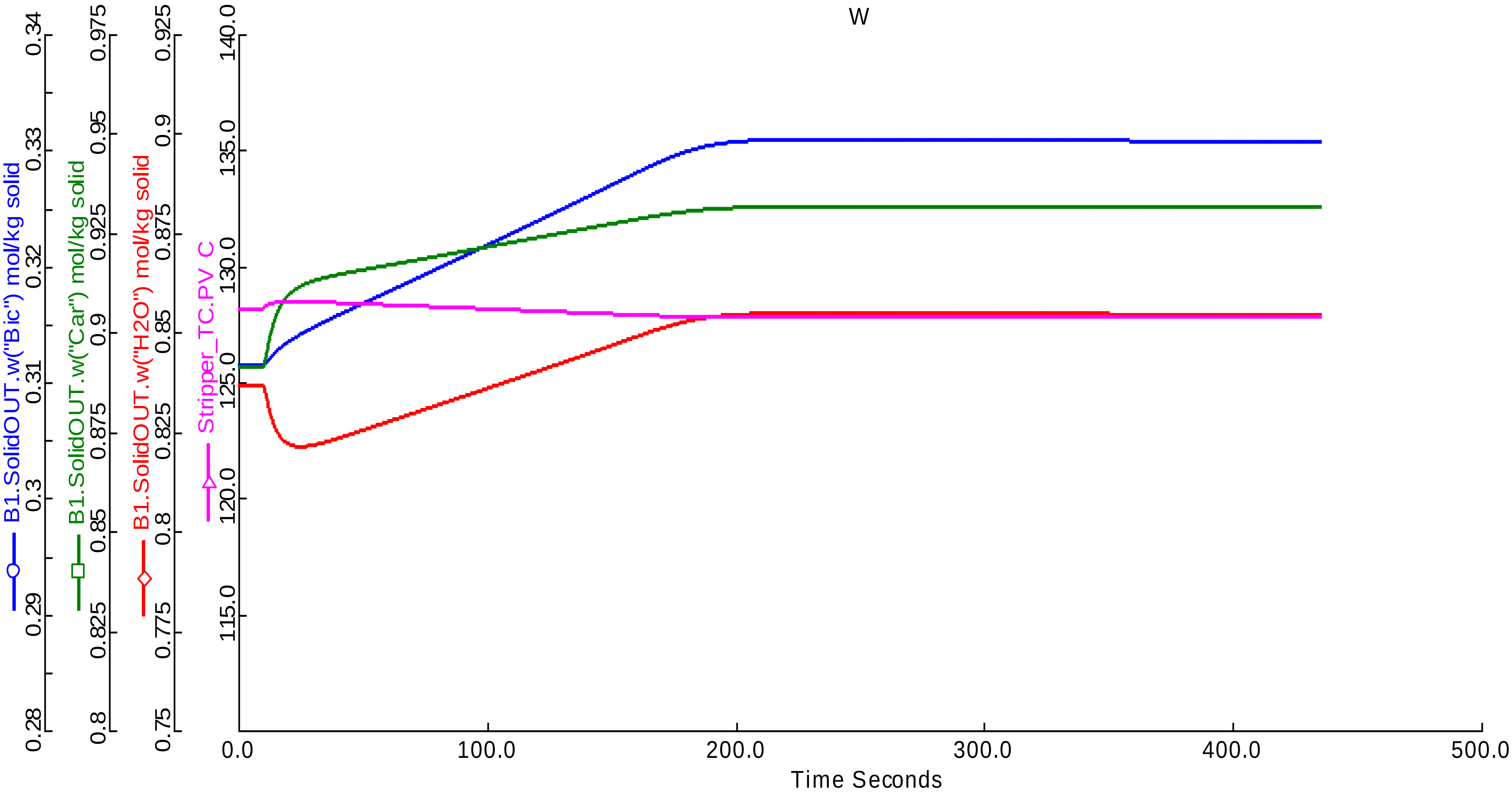




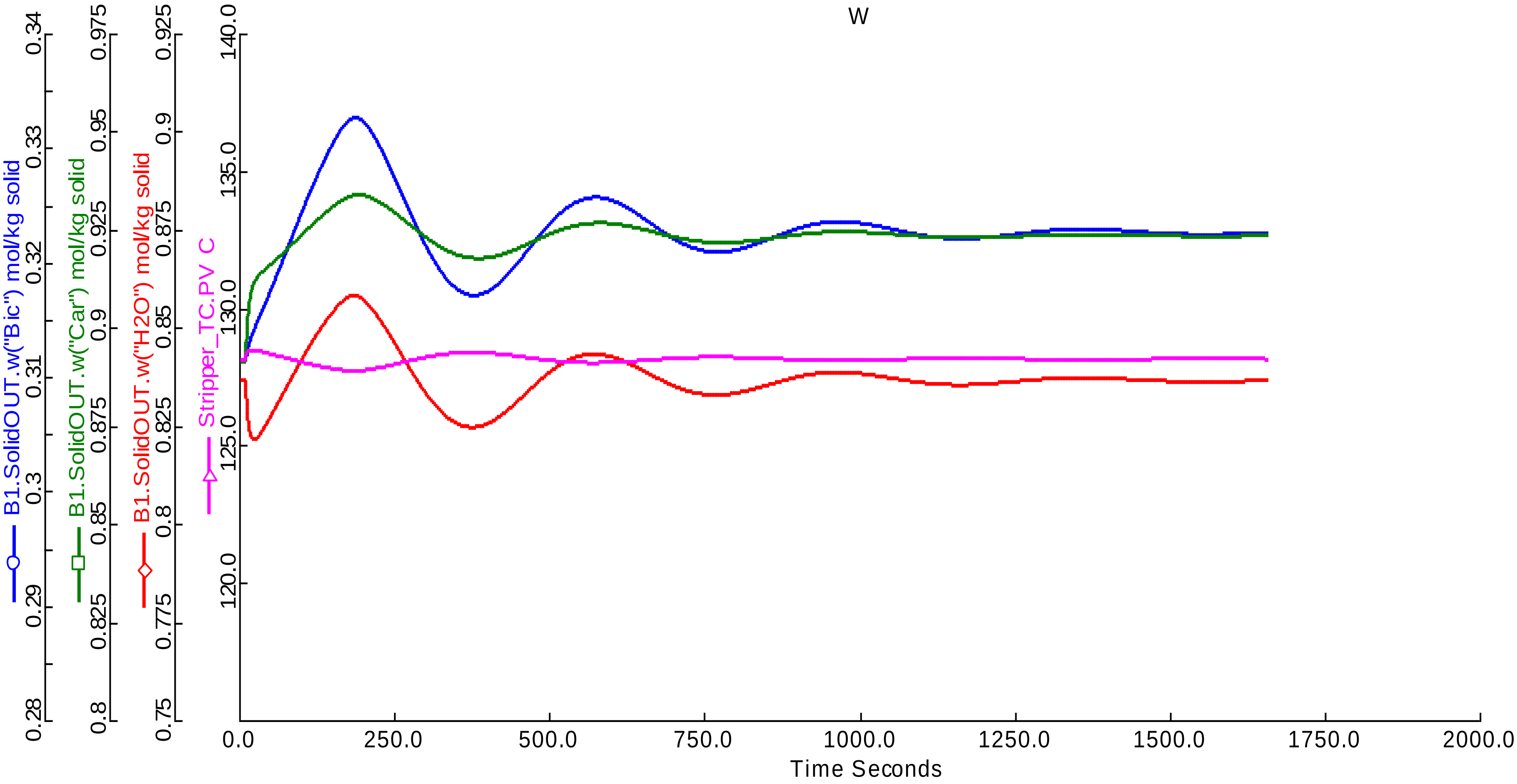




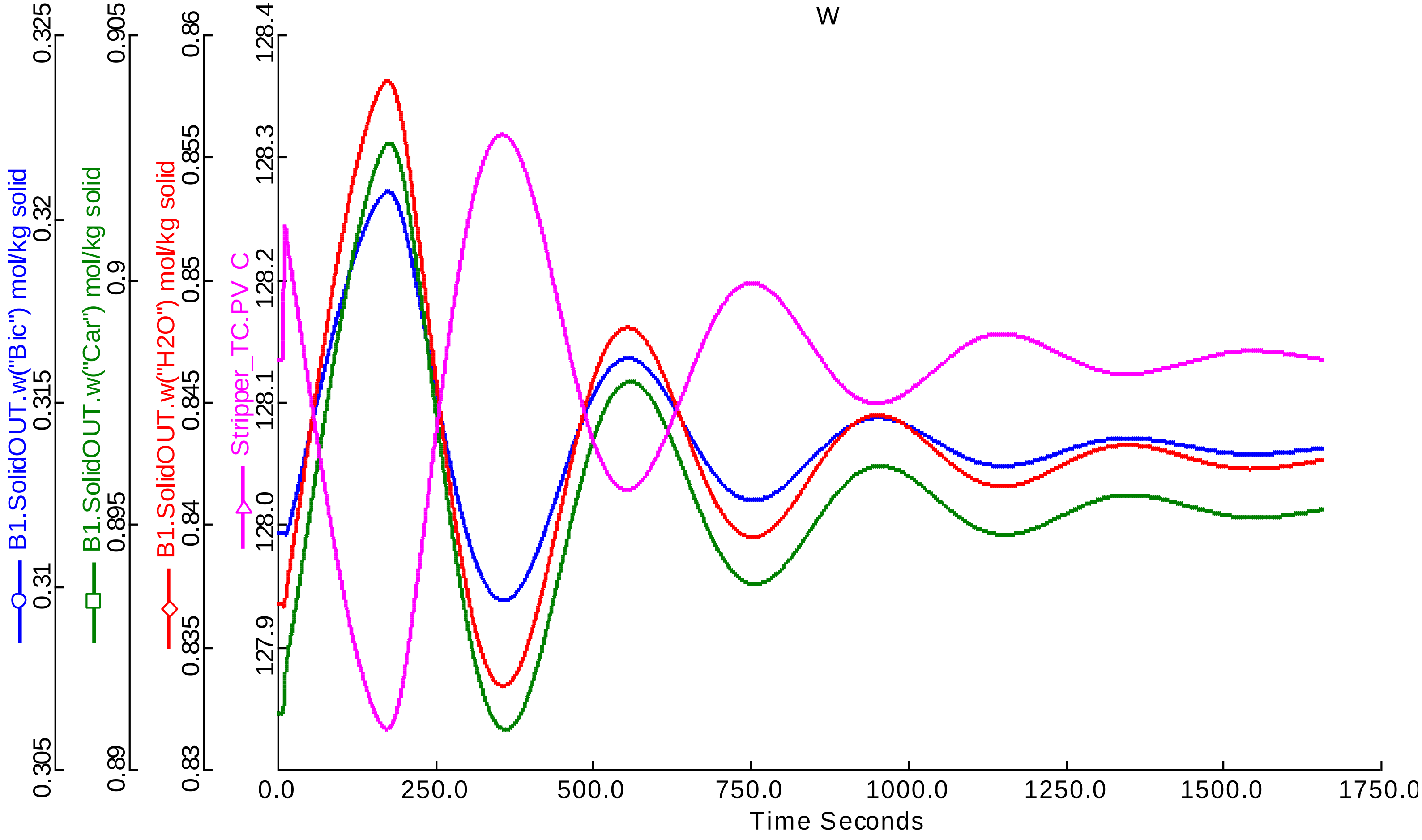
Transient Response of Key Regenerator Variables Due to 10% Step Increase in Sorbent Flowrate (open- loop)



Transient Response of Key Regenerator Variables Due to 10% Step Increase in Sorbent Flowrate (Only Outlet Temperature Controlled)



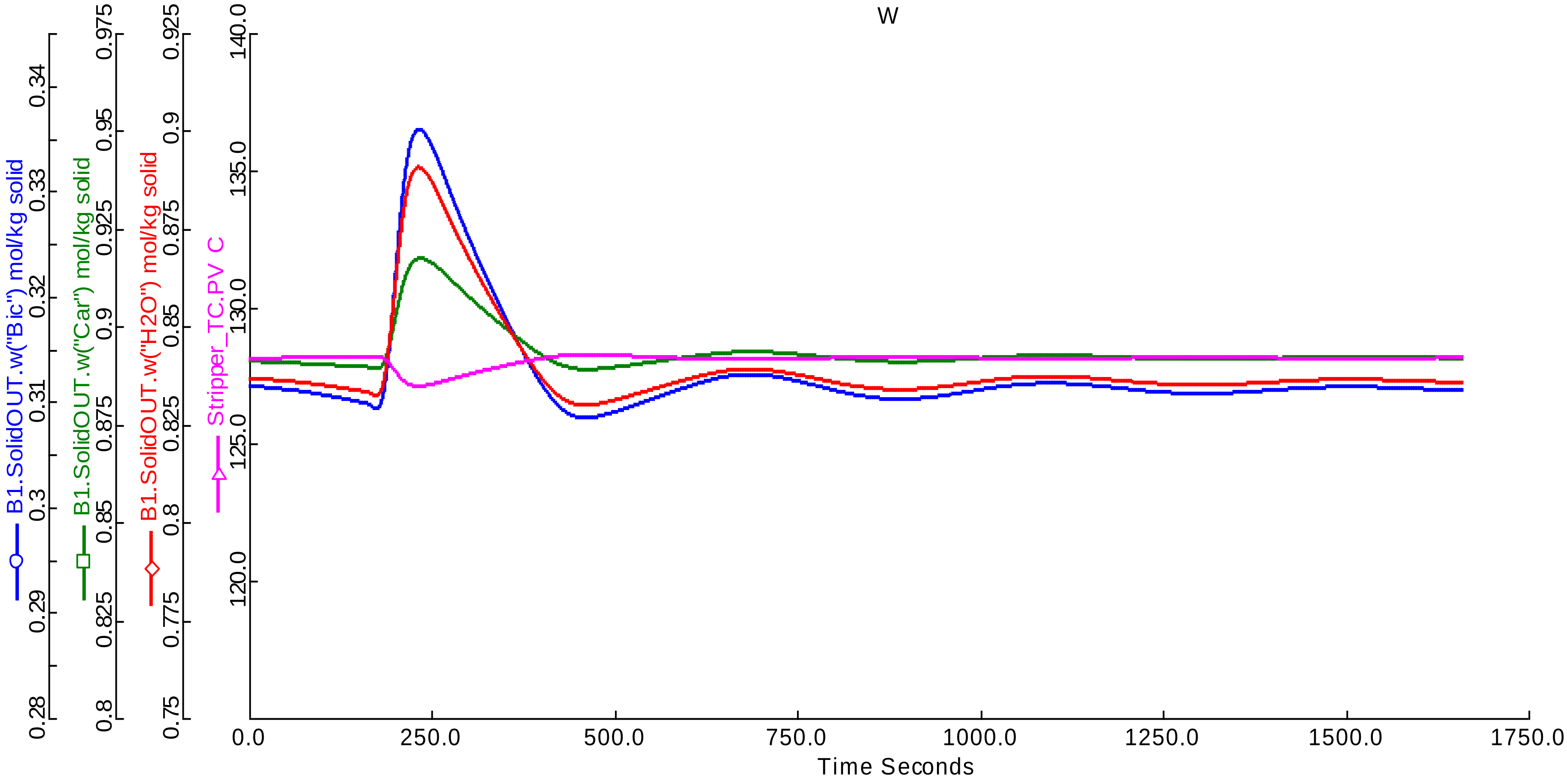
Transient Response of Key Regenerator Variables Due to 10% Step Increase in Sorbent Flowrate (Both Outlet Temperature and Steam to Sorbent Ratio Controlled)



Comparison of Initial Steady State Conditions to the Steady State Conditions After 10% Step Increase in Sorbent Flowrate

	Bicarbamate (mol/kg solid)	Carbamate (mol/kg solid)	Physiosorbed Water (mol/kg solid)
Initial	0.311	0.891	0.837
Only Outlet Temperature Control	0.322	0.923	0.836
Both Outlet Temperature and Ratio Controlled	0.313	0.895	0.842

Transient Response of Key Regenerator Variables Due to 20% Step Increase in Carbamate Loading (Both Outlet Temperature and Ratio Controlled)



CONCLUSIONS

1. A one-dimensional, non-isothermal, pressure-driven dynamic model of a moving bed reactor mainly to be used as the regenerator has been developed in ACM.

2. The model has been developed in analogy to fixed bed and fluidized bed reactors.

3. When both the outlet temperature and the ratio of the stripping steam flowrate to the solids flowrate are controlled, the reactor is found to reject disturbances satisfactorily.

Acknowledgements:

- As part of the National Energy Technology Laboratory's Regional University Alliance (NETL-RUA), a collaborative initiative of the NETL, this technical effort was performed under the RES contract DEFE0004000.

Disclaimer:

Thank you