MSFC-573_ Abstract

Simulation Of Unique Pressure Changing Steps And Situations In Psa Processes

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A more rigorous cyclic adsorption process simulator is being developed for use in the development and understanding of new and existing PSA processes. Unique features of this new version of the simulator that Ritter and co-workers have been developing for the past decade or so include: multiple absorbent layers in each bed, pressure drop in the column, valves for entering and exiting flows and predicting real-time pressurization and depressurization rates, ability to account for choked flow conditions, ability to pressurize and depressurize simultaneously from both ends of the columns, ability to equalize between multiple pairs of columns, ability to equalize simultaneously from both ends of pairs of columns, and ability to handle very large pressure ratios and hence velocities associated with deep vacuum systems. These changes to the simulator now provide for unique opportunities to study the effects of novel pressure changing steps and extreme process conditions on the performance of virtually any commercial or developmental PSA process.

This presentation will provide an overview of the cyclic adsorption process simulator equations and algorithms used in the new adaptation. It will focus primarily on the novel pressure changing steps and their effects on the performance of a PSA system that epitomizes the extremes of PSA process design and operation. This PSA process is a sorbent-based atmosphere revitalization (SBAR) system that NASA is developing for new manned exploration vehicles.

This SBAR system consists of a 2-bed 3-step 3-layer system that operates between atmospheric pressure and the vacuum of space, evacuates from both ends of the column simultaneously, experiences choked flow conditions during pressure changing steps, and experiences a continuously changing feed composition, as it removes metabolic CO_2 and H_2O from a closed and fixed volume, i.e., the spacecraft cabin. Important process performance indicators of this SBAR system are size, and the corresponding CO_2 and H_2O removal efficiencies, and N_2 and O_2 loss rates. Results of the fundamental behavior of this PSA process during extreme operating conditions will be presented and discussed.

MSFC-573_Presentation

Simulation of Unique Pressure Changing Steps and Situations in PSA Processes

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Introduction

1. Rigorous cyclic adsorption process simulator (Ddaspk-Fortran) being developed to assist in the design, development and understanding of new and existing PSA processes.
2. Unique features of this simulator include:
   - Multiple absorbent layers and columns
   - Pressure drop in the column
   - Entering and exiting flows defined by constant flow, valve equations, or choke flow approaches (Isentropic, Fanno, etc.)
   - Interaction with other processes: cabin, distillation units, etc.
   - Simultaneous feed, exit, pressure varying steps through multiple ports
   - Ability to handle large P ratios and v's associated with deep vacuum systems.
   - Equalization between pairs of columns (single and dual ended) in progress.

These features provide for unique opportunities to study the performance of virtually any commercial or developmental PSA process under extreme process conditions.

Objectives

- Focus primarily on a particular PSA system that NASA is developing: referred to as the sorbent-based atmosphere revitalization (SBAR) system
  - **this PSA system is unique because it uses deep space vacuum for regeneration *in lieu* of processed air as purge**

- Describe NASA's PSA System, with emphasis on the alternative regenerative steps that NASA has developed to further improve performance: single, dual, and triple ended blowdown
- Show validation of the PSA process simulator against NASA's experimental data of an 8.8 L dual blowdown system
- Use the simulator to discuss the role of these regenerative steps on PSA performance in terms of H_2O and CO_2 removal efficiencies

This SBAR system might be used in a new Crew Exploration Vehicle (CEV) to remove metabolic H_2O and CO_2 from cabin air.

Schematic of Base Case Column Simulated for Water and Carbon Dioxide Removal from Cabin Air

MSFC SBAR

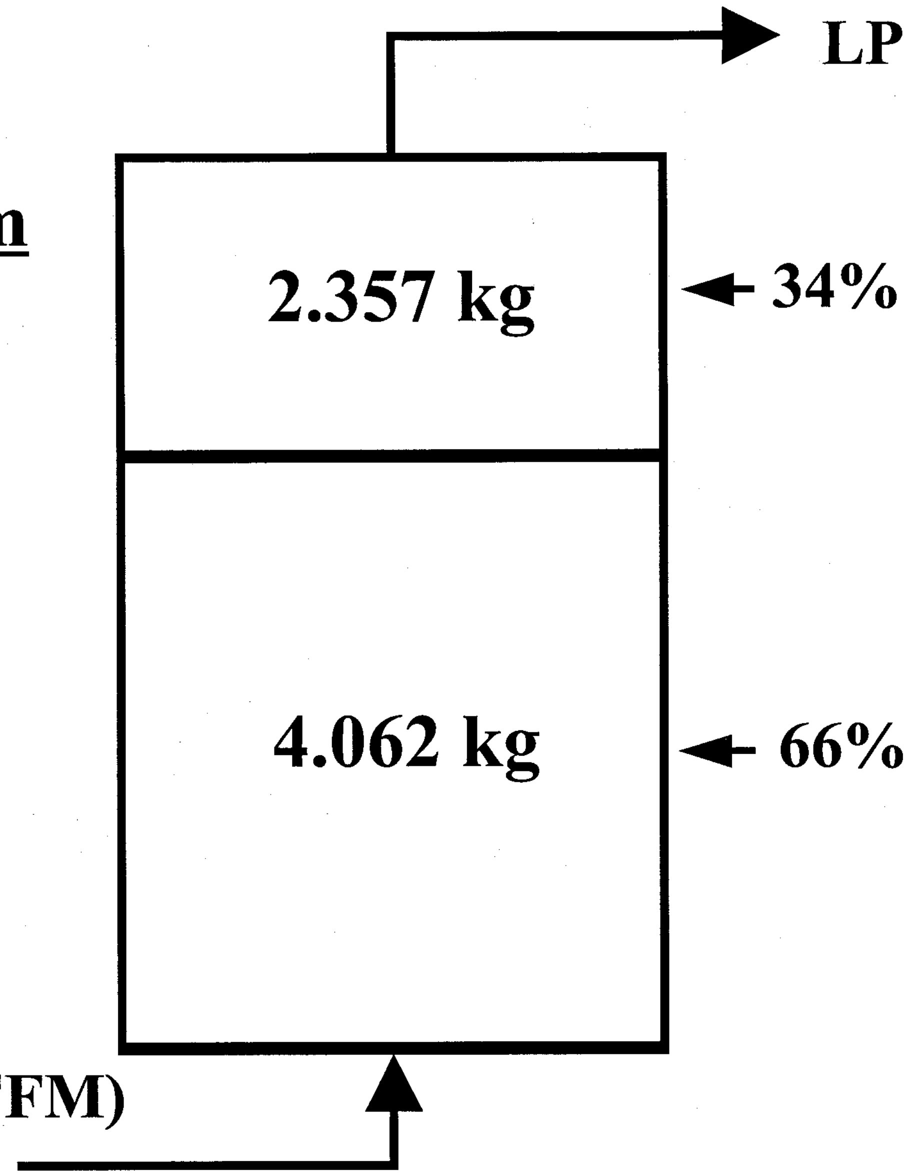
Experimental System

V_b = 8.88 L

L_b = 0.2654 m

r_b = 0.1032 m

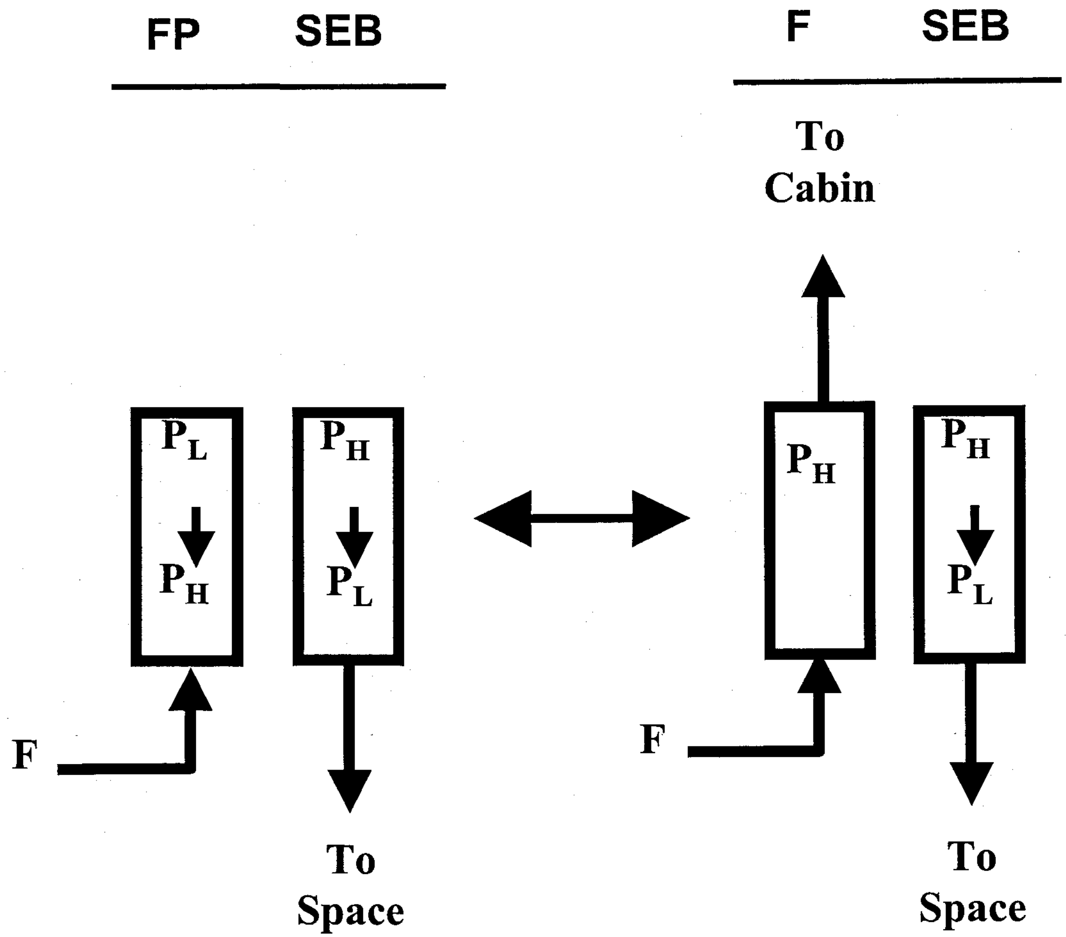
HCT = 450 s

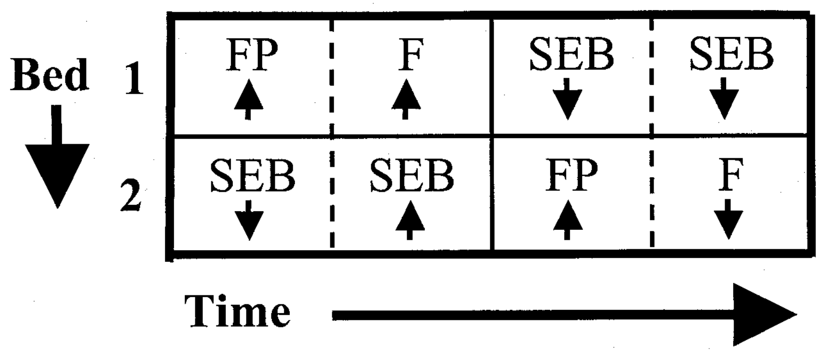


☐ Zeolite 13X

☐ Zeolite 5A

Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization



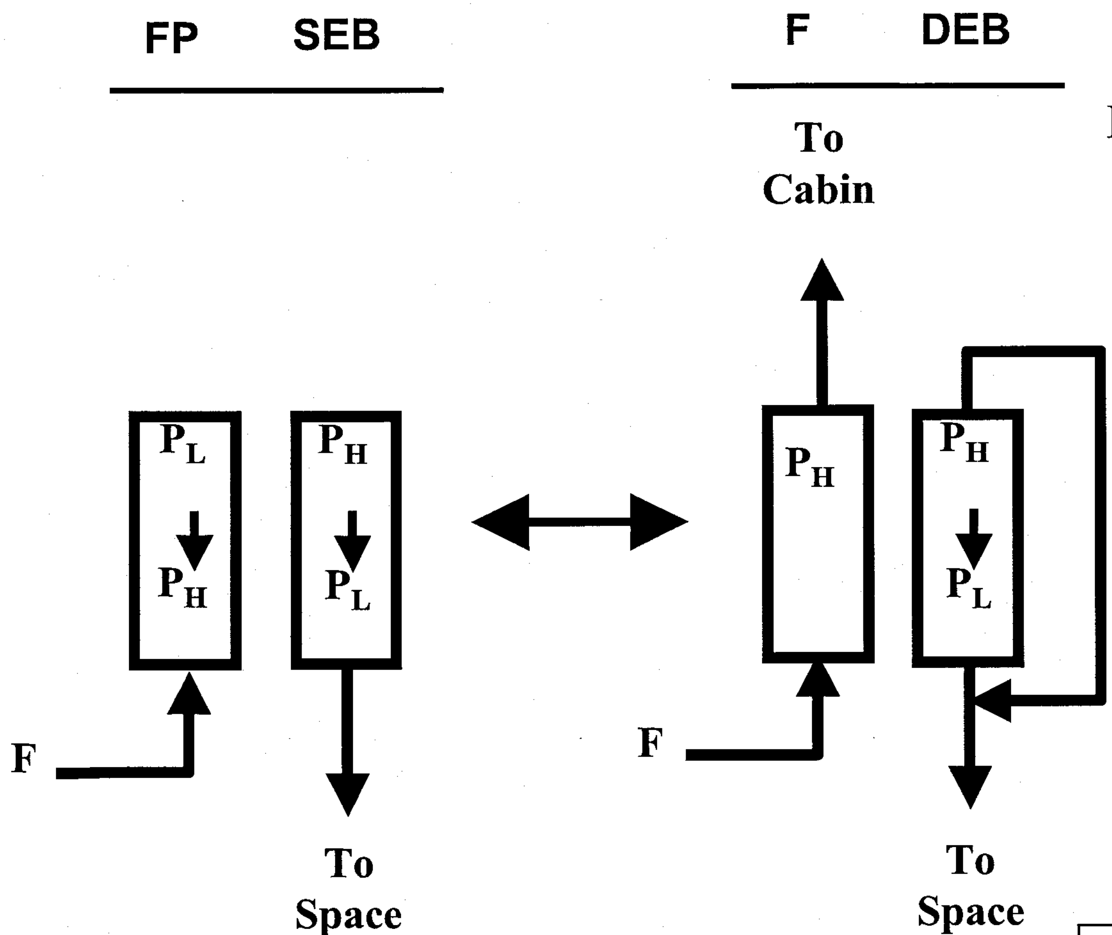


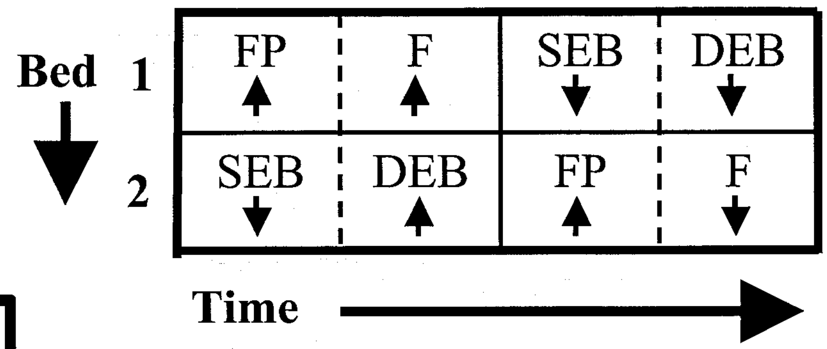
SBAR Cycle Step Times

$t_F = 420$ s
$t_{SEB} = 30$ s
$t_{SEB} = 420$ s
$t_{FP} = 30$ s

SEB: single ended blowdown

Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization



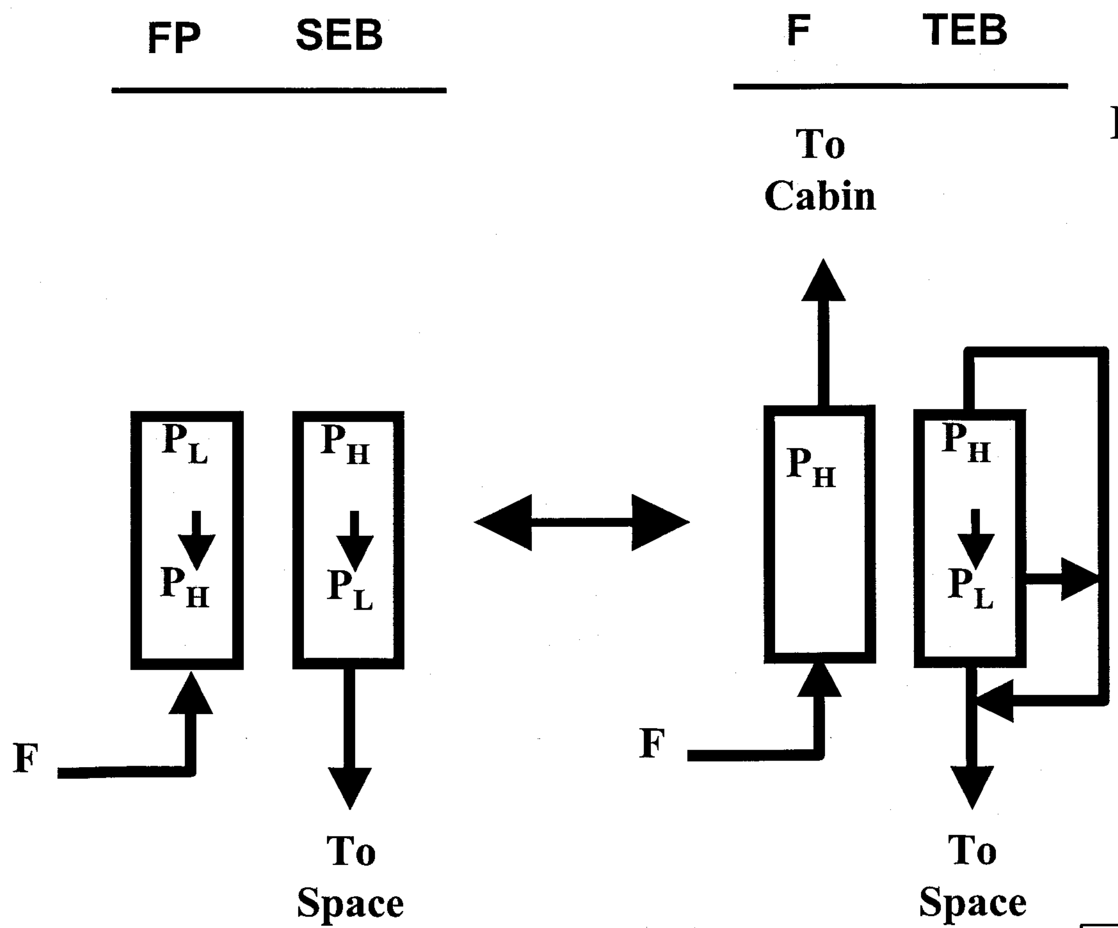


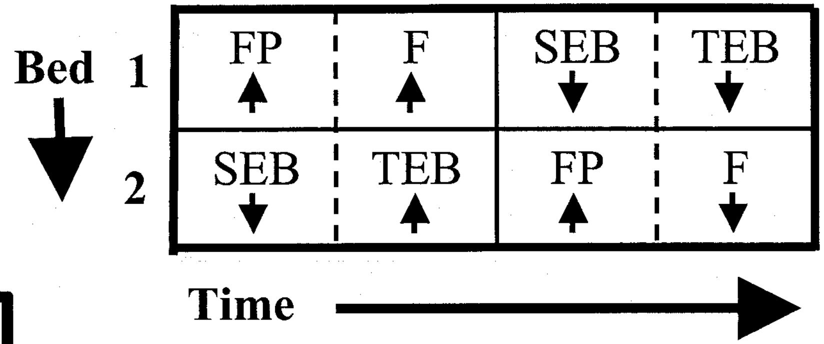
SBAR Cycle Step Times

$t_F = 420$ s
$t_{SEB} = 30$ s
$t_{DEB} = 420$ s
$t_{FP} = 30$ s

SEB: single ended blowdown
DEB: dual ended blowdown

Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization





SBAR Cycle Step Times

$t_F = 420$ s

$t_{SEB} = 30$ s

$t_{TEB} = 420$ s

$t_{FP} = 30$ s

SEB: single ended blowdown

TEB: triple ended blowdown

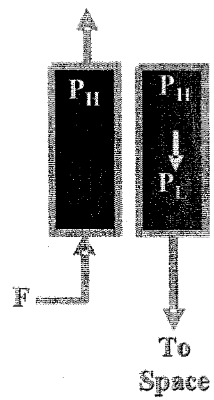
Simulator Input
Bed Characteristics and Transport Properties
MSFC SBAR Experimental System

	13X	5A
bed layer fraction (%)	66%	34%
porosity	0.26	0.35
pellet density (kg m^{-3})	1100	1201
heat capacity (kJ kg^{-1} K^{-1})	1.10	0.84
heat transfer coefficient (kW m^{-2} K^{-1})[a]	0.0017	0.0017
mass transfer coefficients (s^{-1})		
H_2O	0.00550	0.00310
CO_2	0.00150	0.00067
O_2	0.001	0.001
N_2	0.001	0.001
$r_{p,eff}$[b] (mm)	3.3	2.1

Motivation: Single vs Dual Ended Blowdown

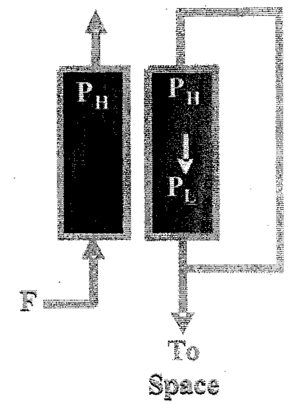
Pressure profiles @ End of Blowdown Step

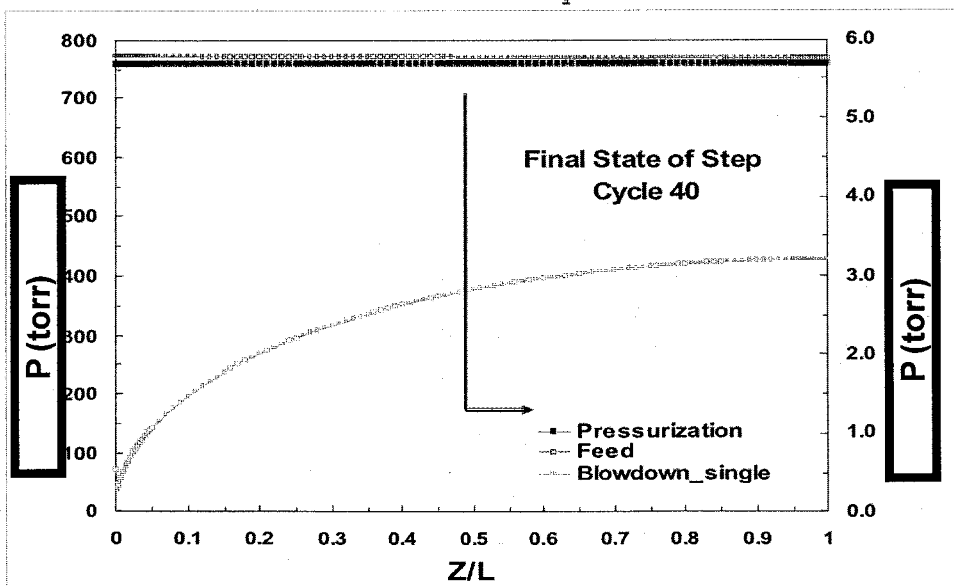
Single

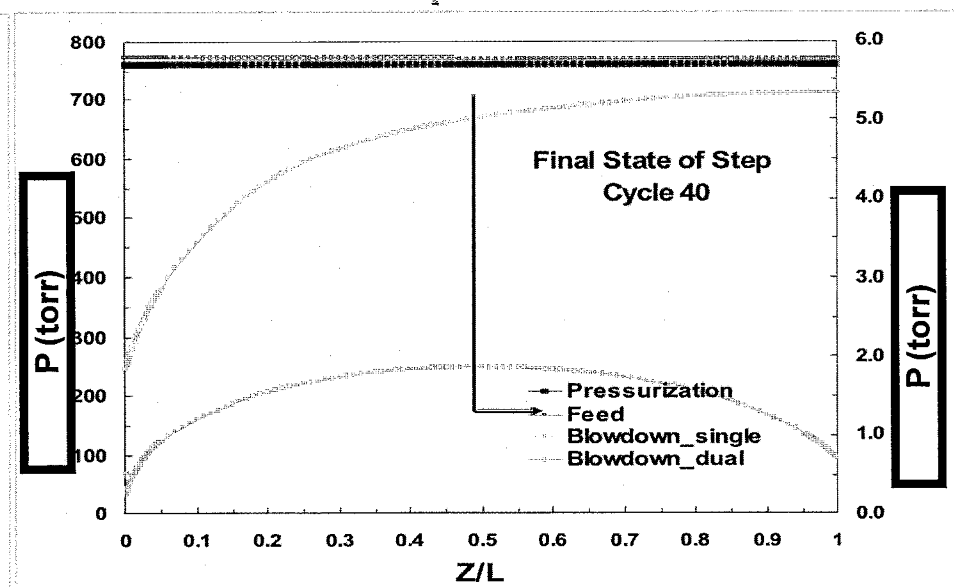


15 SCFM

Dual



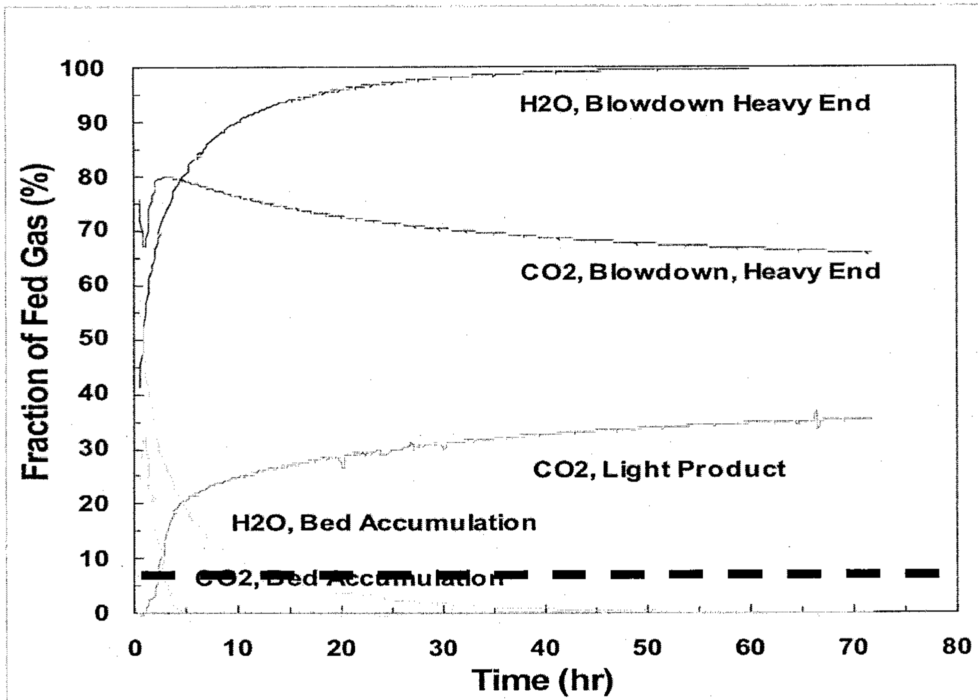




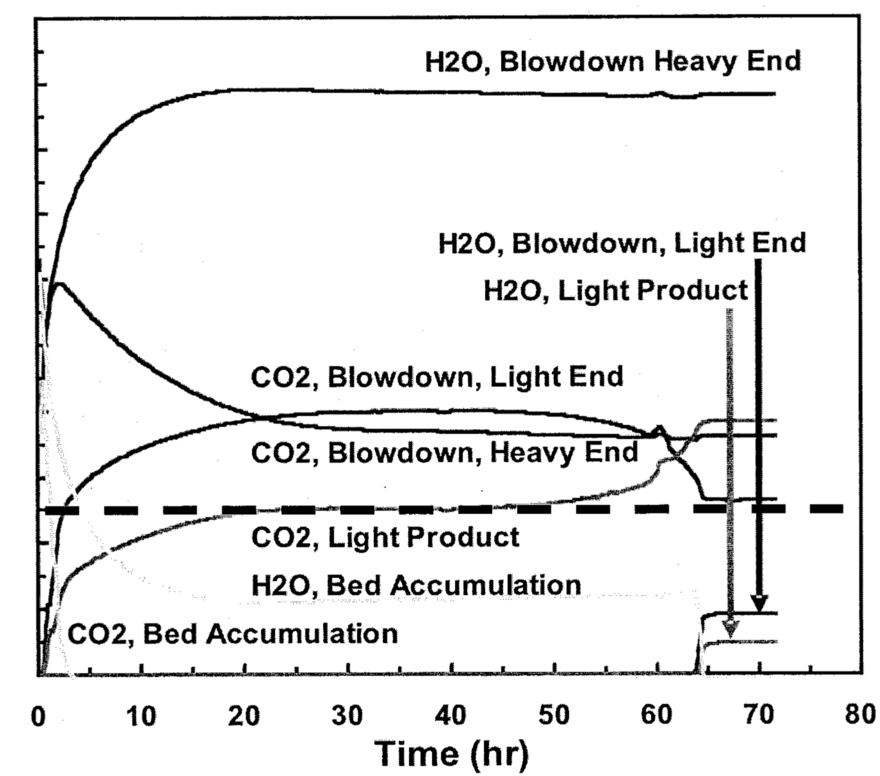
Motivation: Single vs Dual Ended Blowdown
Cycle Performance Parameters Zeolite System

15 SCFM

Single

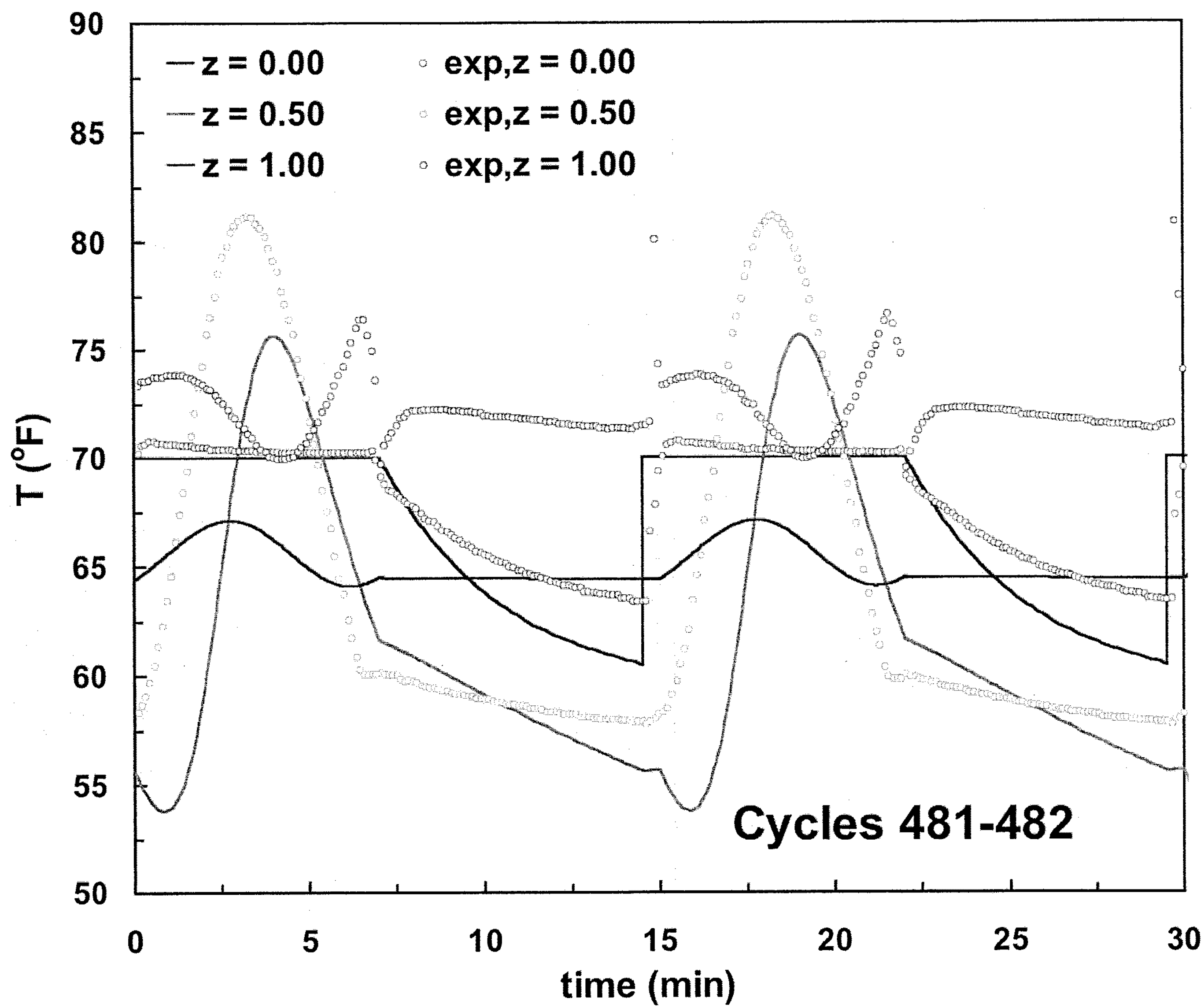


Dual



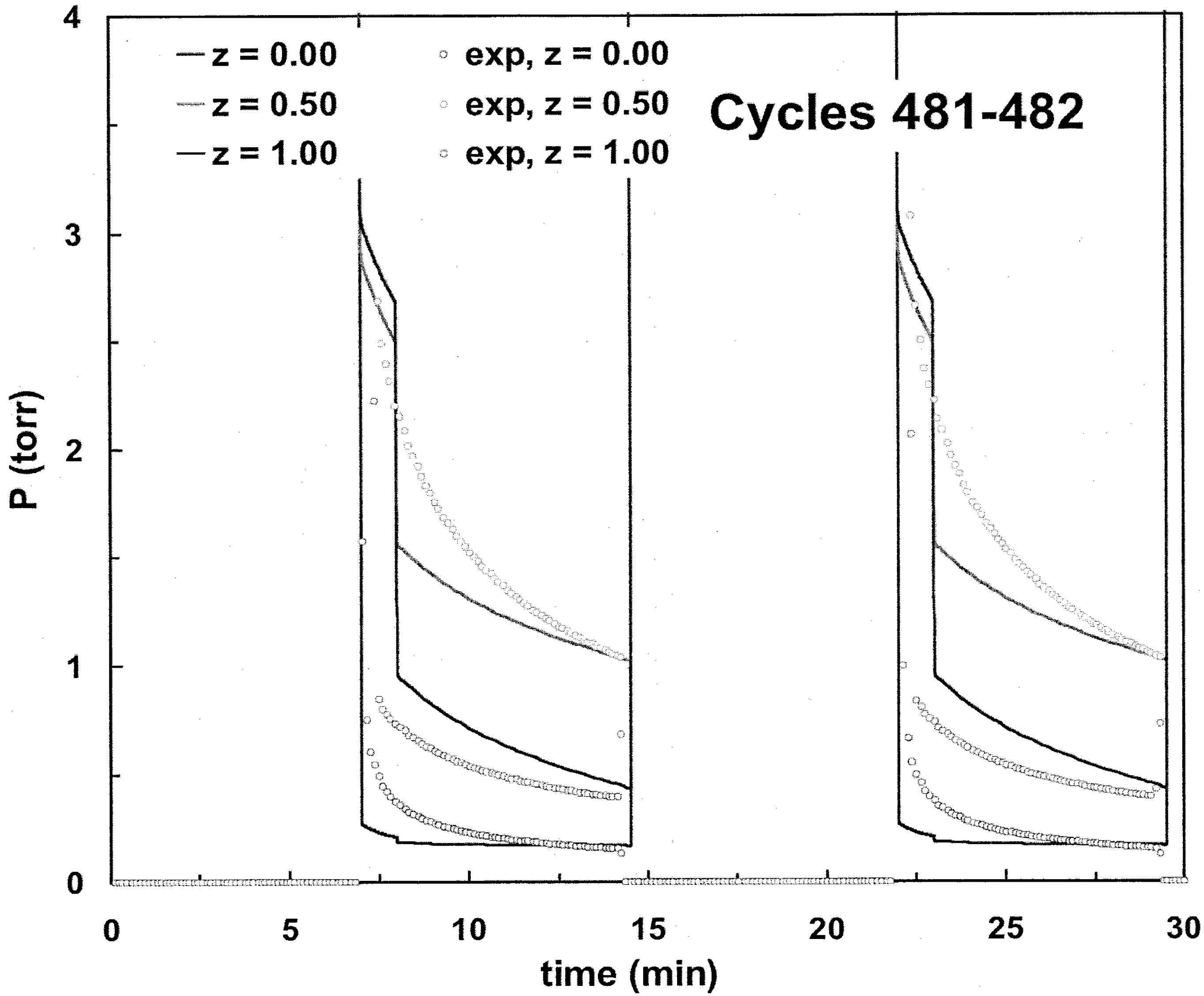
Modeling the SBAR DEB Experimental System
Temperature History Profiles at Three Bed Locations

120 h
F = 13.5 SCFM
V_b = 8.88 L
HCT= 450 s
t_F = 420 s
t_{SEB} = 30 s
t_{DEB} = 420 s
t_{FP} = 30 s



Modeling the SBAR DEB Experimental System
Pressure History Profiles at Three Bed Locations

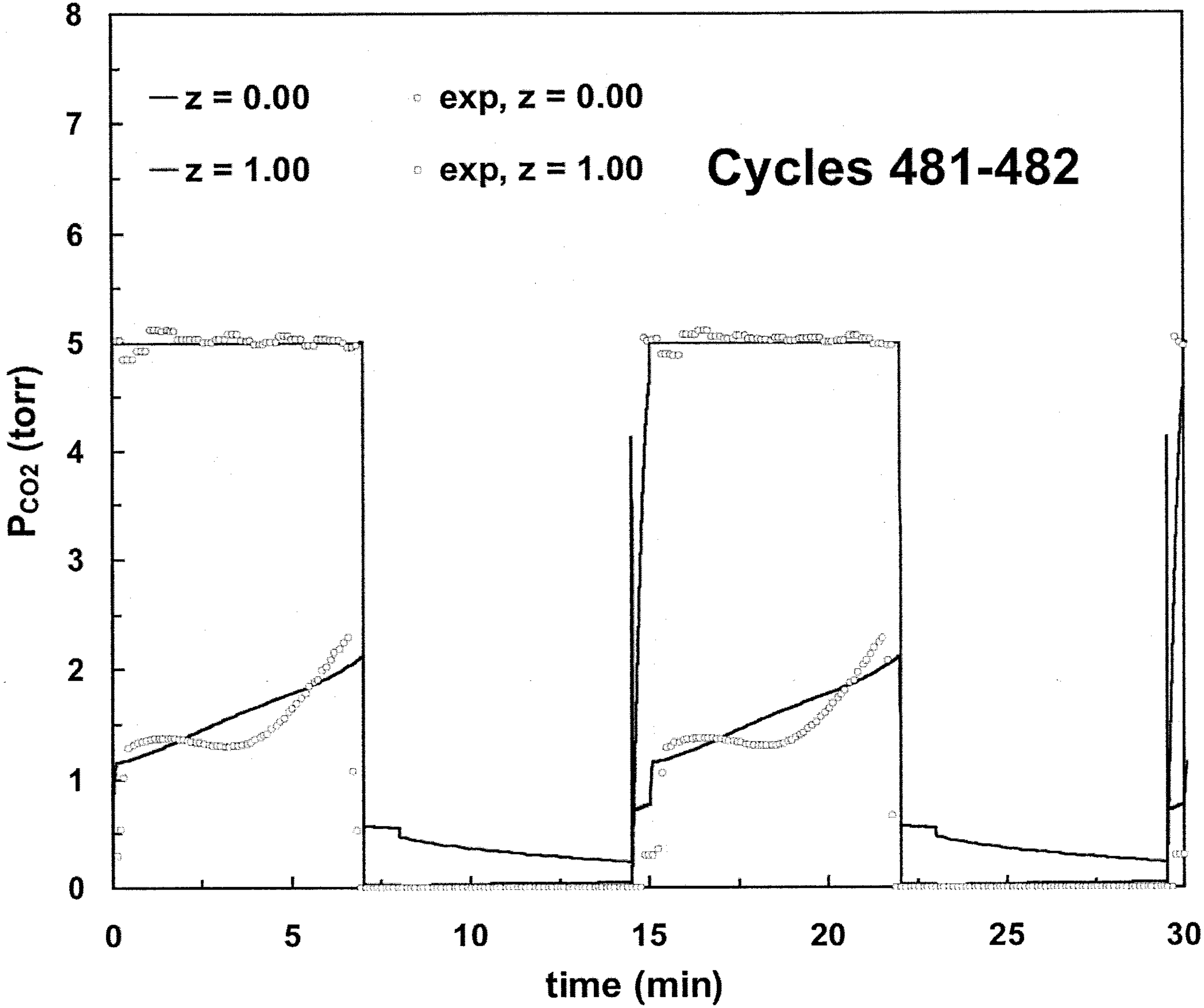
120 h
F = 13.5 SCFM
V_b = 8.88 L
HCT= 450 s
t_F = 420 s
t_{SEB} = 30 s
t_{DEB} = 420 s
t_{FP} = 30 s



Modeling the SBAR DEB Experimental System

P_{CO2} History Profiles at Two Bed Locations

120 h		
F =	13.5 SCFM	
V_b	=	8.88 L
HCT=		450 s
t_F	=	420 s
t_{SEB}	=	30 s
t_{DEB}	=	420 s
t_{FP}	=	30 s



Modeling the SBAR DEB Experimental System

Bed Profiles at End of Steps for P, T, P_{H2O} and P_{CO2}

120 h

F = 13.5 SCFM

V_b = 8.88 L

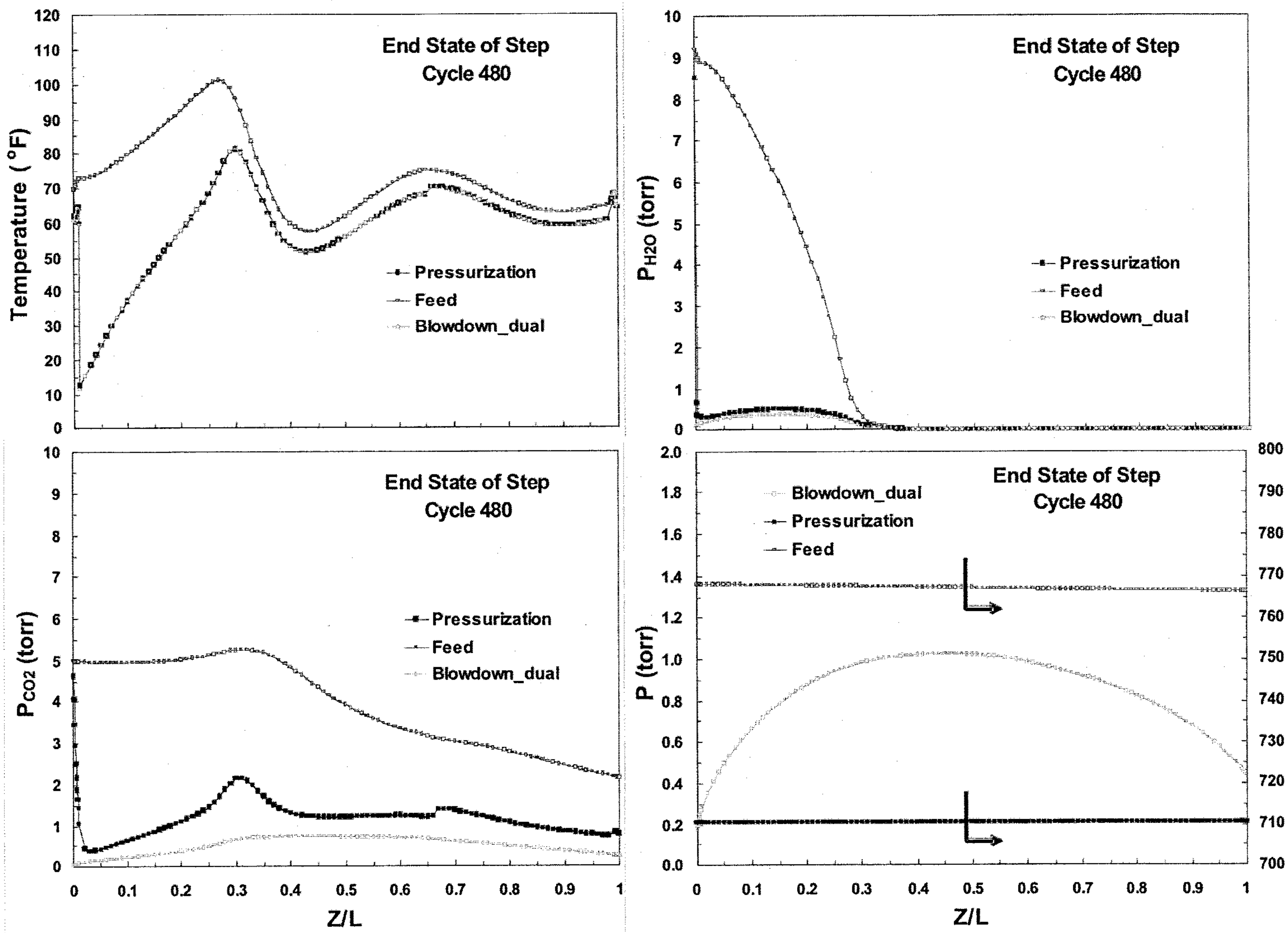
HCT = 450 s

t_F = 420 s

t_{SEB} = 30 s

t_{DEB} = 420 s

t_{FP} = 30 s



Modeling the SBAR DEB Experimental System

Summary of Modeling vs Experimental Results of Eight Different Test Runns

	Experimental Conditions							Experimental Results						Modeling Results					
Test Point	Bed Size, L	Half cycle Time, min	DED Time, min	Inlet ppCO2, torr	Inlet ppH2O, torr	Flow Rate, scfm	Inlet Temp, degF	CO2 Removal, lb/hr	CO2 Removal Eff	H2O Removal, lb/hr	H2O Removal Eff	Bed Temp High, degf	Bed Temp Low, degf	CO2 Removal, lb/hr	CO2 Removal Eff	H2O Removal, lb/hr	H2O Removal Eff	Mid Bed Temp High, degf	Mid Bed Temp Low, degf
12	8.88	7.5	7.0	5.0	9.1	12.0	67.8	0.45	0.76	0.44	1.00	78.9	48.4	0.48	0.83	0.44	1.00	76.1	50.5
18	**8.88**	**7.5**	**7.0**	**5.0**	**9.1**	**13.5**	**69.9**	**0.48**	**0.72**	**0.50**	**1.00**	**81.4**	**57.8**	**0.49**	**0.74**	**0.49**	**1.00**	**82.3**	**50.1**
20	8.88	7.5	7.0	5.1	9.1	14.0	69.6	0.47	0.68	0.51	1.00	81.4	57.6	0.50	0.69	0.51	1.00	86.2	56.6
23	8.88	7.5	7.0	5.0	9.1	14.5	70.0	0.35	0.49	0.53	1.00	81.6	56.8	0.48	0.68	0.53	1.00	84.2	51.0
42	8.88	7.5	6.0	7.0	13.1	10.0	77.0	0.52	0.75	0.53	1.00	85.3	73.3	0.52	0.84	0.57	1.00	83.9	61.1
43	8.88	7.5	6.0	3.0	13.1	10.0	79.2	0.20	0.68	0.53	1.00	88.2	76.4	0.26	0.87	0.51	1.00	97.0	62.1
52	8.88	7.5	6.0	7.0	9.1	13.5	70.0	0.70	0.75	0.50	1.00	85.1	44.6	0.65	0.71	0.49	1.00	80.2	49.6
54	8.88	7.5	6.0	3.0	9.1	13.5	70.4	0.26	0.64	0.50	1.00	86.0	51.6	0.32	0.81	0.49	1.00	87.1	49.7

Modeling the SBAR DEB Experimental System

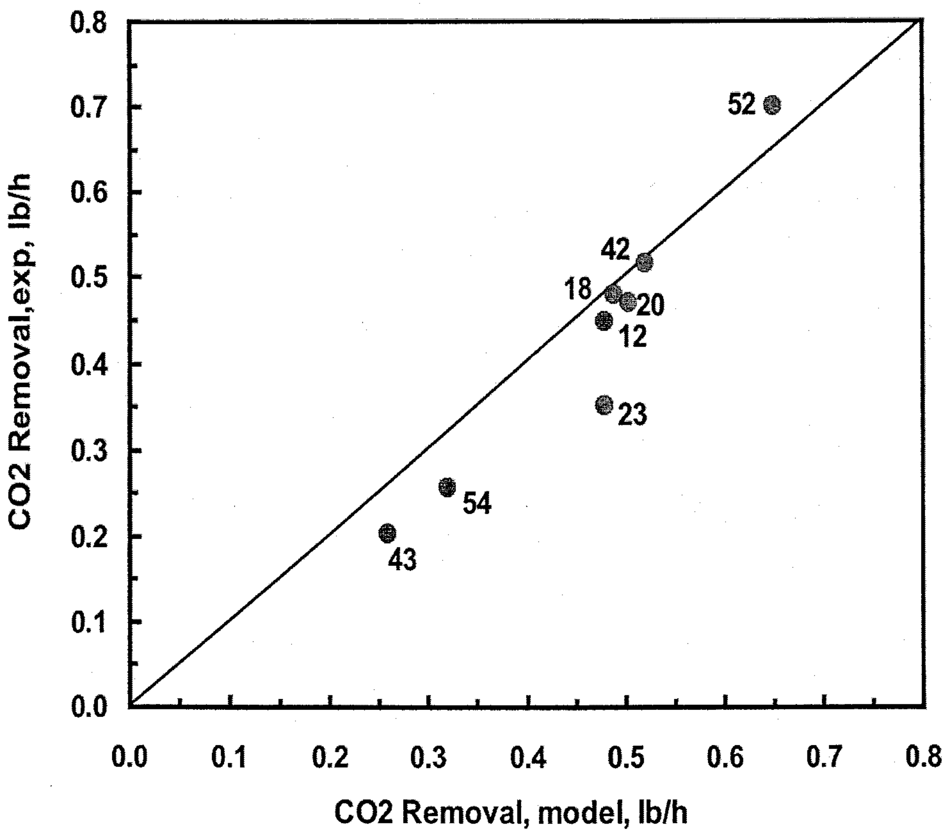
Summary of Modeling vs Experimental Results of Eight Different Test Runs: H_2O Removal

	Experimental Conditions							Experimental Results						Modeling Results					
Test Point	Bed Size, L	Half cycle Time, min	DED Time, min	Inlet ppCO2, torr	Inlet ppH2O, torr	Flow Rate, scfm	Inlet Temp, degF	CO2 Removal, lb/hr	CO2 Removal Eff	H2O Removal, lb/hr	H2O Removal Eff	Bed Temp High, degf	Bed Temp Low, degf	CO2 Removal, lb/hr	CO2 Removal Eff	H2O Removal, lb/hr	H2O Removal Eff	Mid Bed Temp High, degf	Mid Bed Temp Low, degf
12	8.88	7.5	7.0	5.0	9.1	12.0	67.8	0.45	0.76	0.44	1.00	78.9	48.4	0.48	0.83	0.44	1.00	76.1	50.5
18	**8.88**	**7.5**	**7.0**	**5.0**	**9.1**	**13.5**	**69.9**	**0.48**	**0.72**	**0.50**	**1.00**	**81.4**	**57.8**	**0.49**	**0.74**	**0.49**	**1.00**	**82.3**	**50.1**
20	8.88	7.5	7.0	5.1	9.1	14.0	69.6	0.47	0.68	0.51	1.00	81.4	57.6	0.50	0.69	0.51	1.00	86.2	56.6
23	8.88	7.5	7.0	5.0	9.1	14.5	70.0	0.35	0.49	0.53	1.00	81.6	56.8	0.48	0.68	0.53	1.00	84.2	51.0
42	8.88	7.5	6.0	7.0	13.1	10.0	77.0	0.52	0.75	0.53	1.00	85.3	73.3	0.52	0.84	0.57	1.00	83.9	61.1
43	8.88	7.5	6.0	3.0	13.1	10.0	79.2	0.20	0.68	0.53	1.00	88.2	76.4	0.26	0.87	0.51	1.00	97.0	62.1
52	8.88	7.5	6.0	7.0	9.1	13.5	70.0	0.70	0.75	0.50	1.00	85.1	44.6	0.65	0.71	0.49	1.00	80.2	49.6
54	8.88	7.5	6.0	3.0	9.1	13.5	70.4	0.26	0.64	0.50	1.00	86.0	51.6	0.32	0.81	0.49	1.00	87.1	49.7

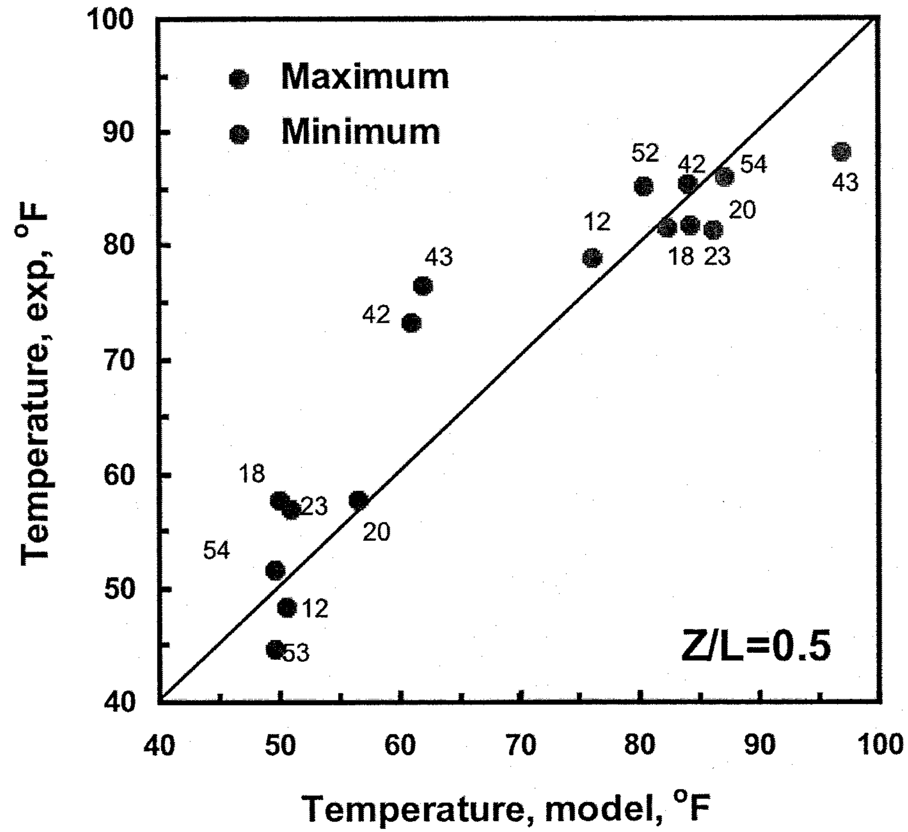
Modeling the SBAR DEB Experimental System

Summary of Modeling vs Experimental Results of Eight Different Test Runs

CO_2 Removal

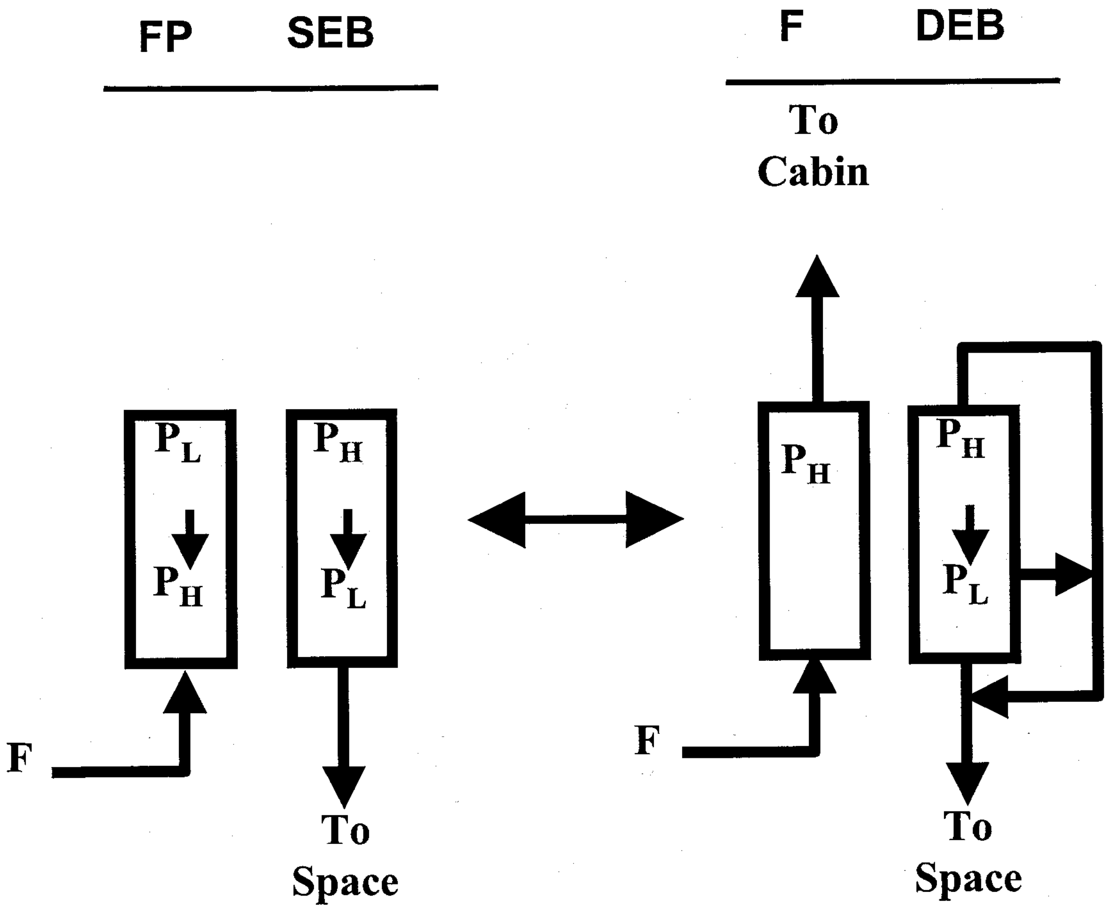


Cycle Bed Temperatures



Triple Ended Blowdown

Effect of Location of Third Exhaust Port



Test Run 18

F	=	13.5 SCFM
V_b	=	8.88 L
HCT	=	450 s
t_F	=	420 s
t_{SED}	=	30 s
t_{DED}	=	420 s
t_{FP}	=	30 s

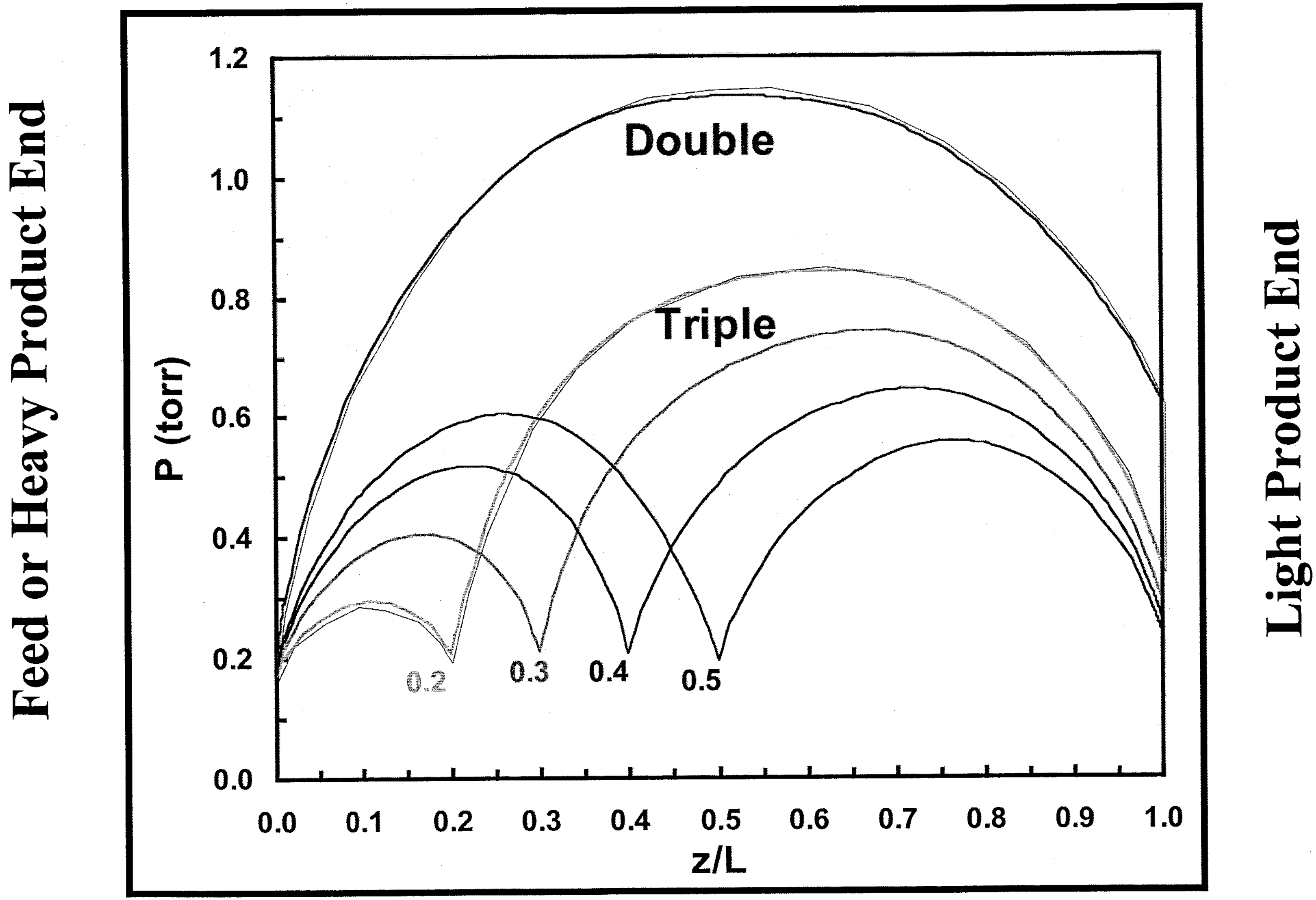
Third Port Location

z/L = 0.2, 0.3, 0.4, or 0.5

Triple vs Dual Ended Blowdown

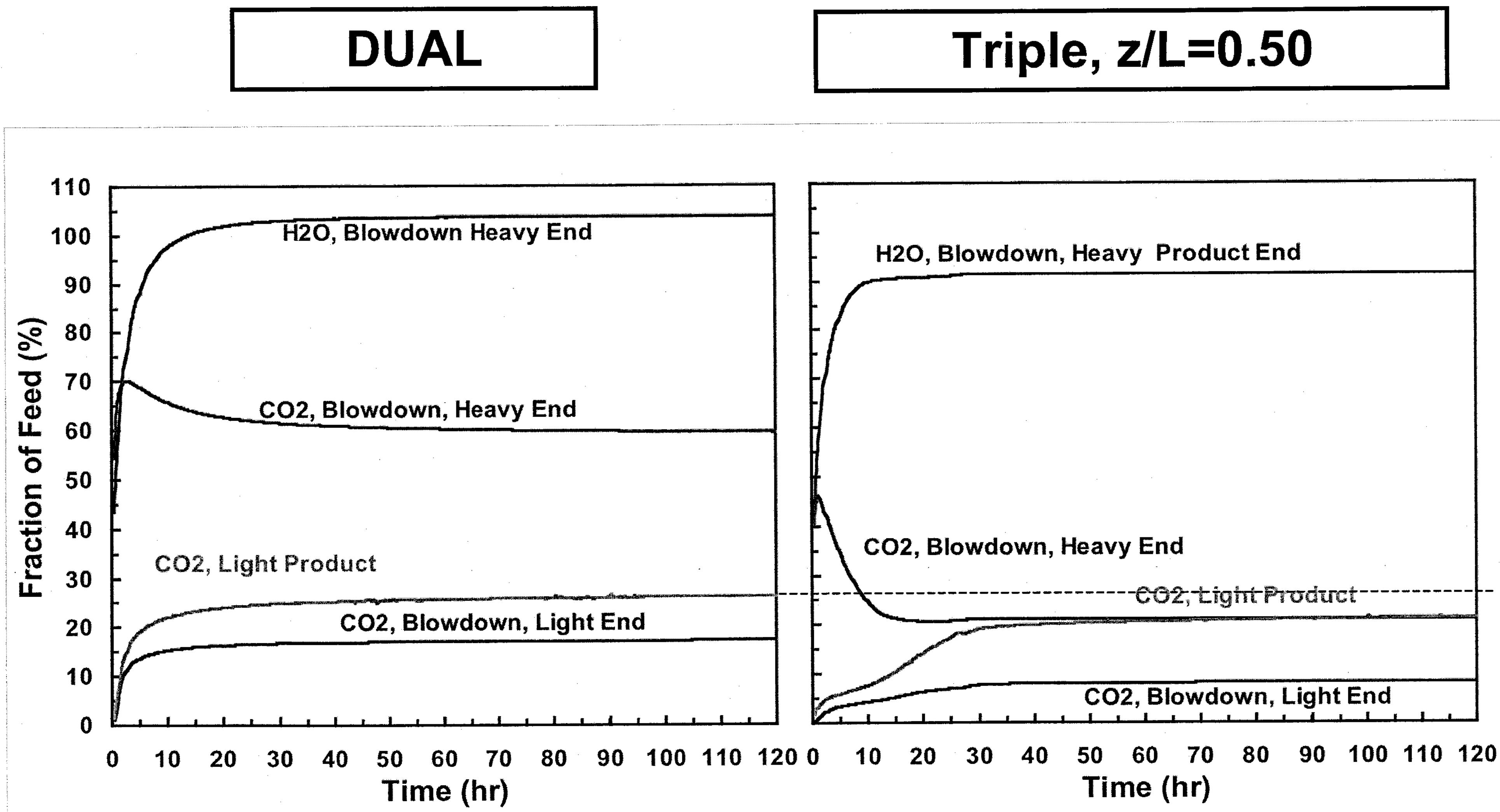
Bed Pressure Profiles at the End of the Blowdown step

Significant Increase of Driving Force



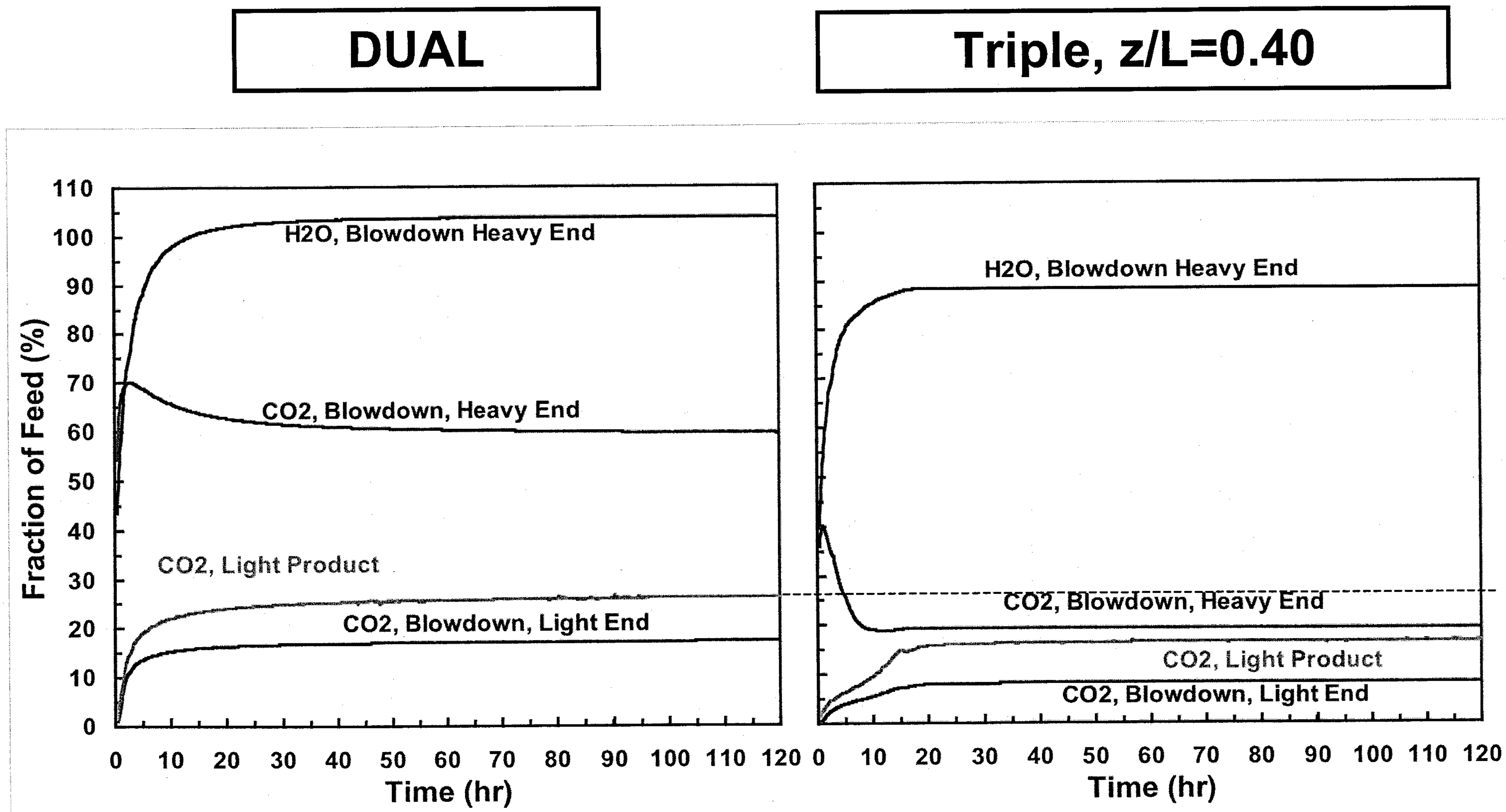
Triple vs Dual Ended Blowdown

History of H_2O and CO_2 Removal Per Cycle



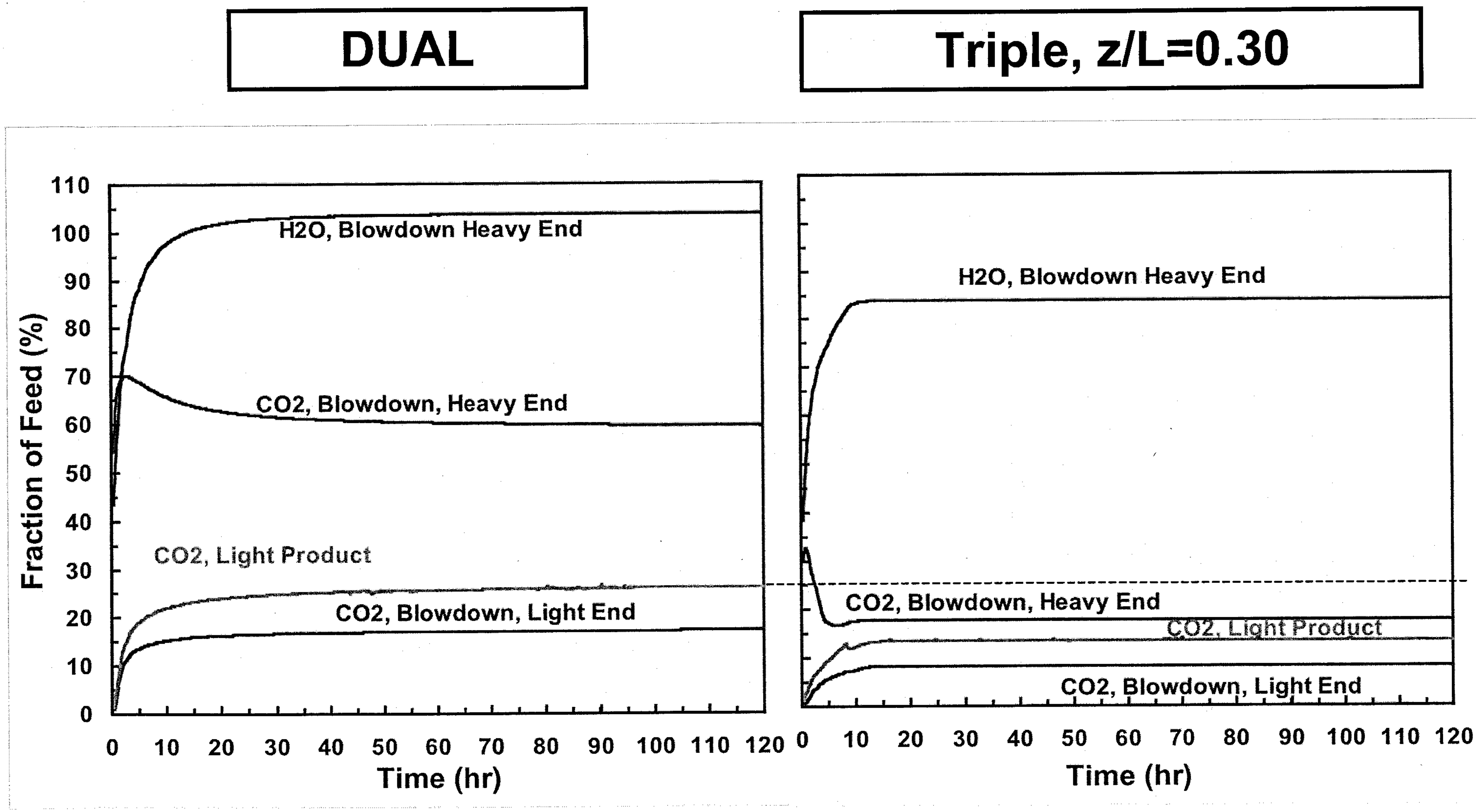
Triple vs Dual Ended Blowdown

History of H_2O and CO_2 Removal Per Cycle

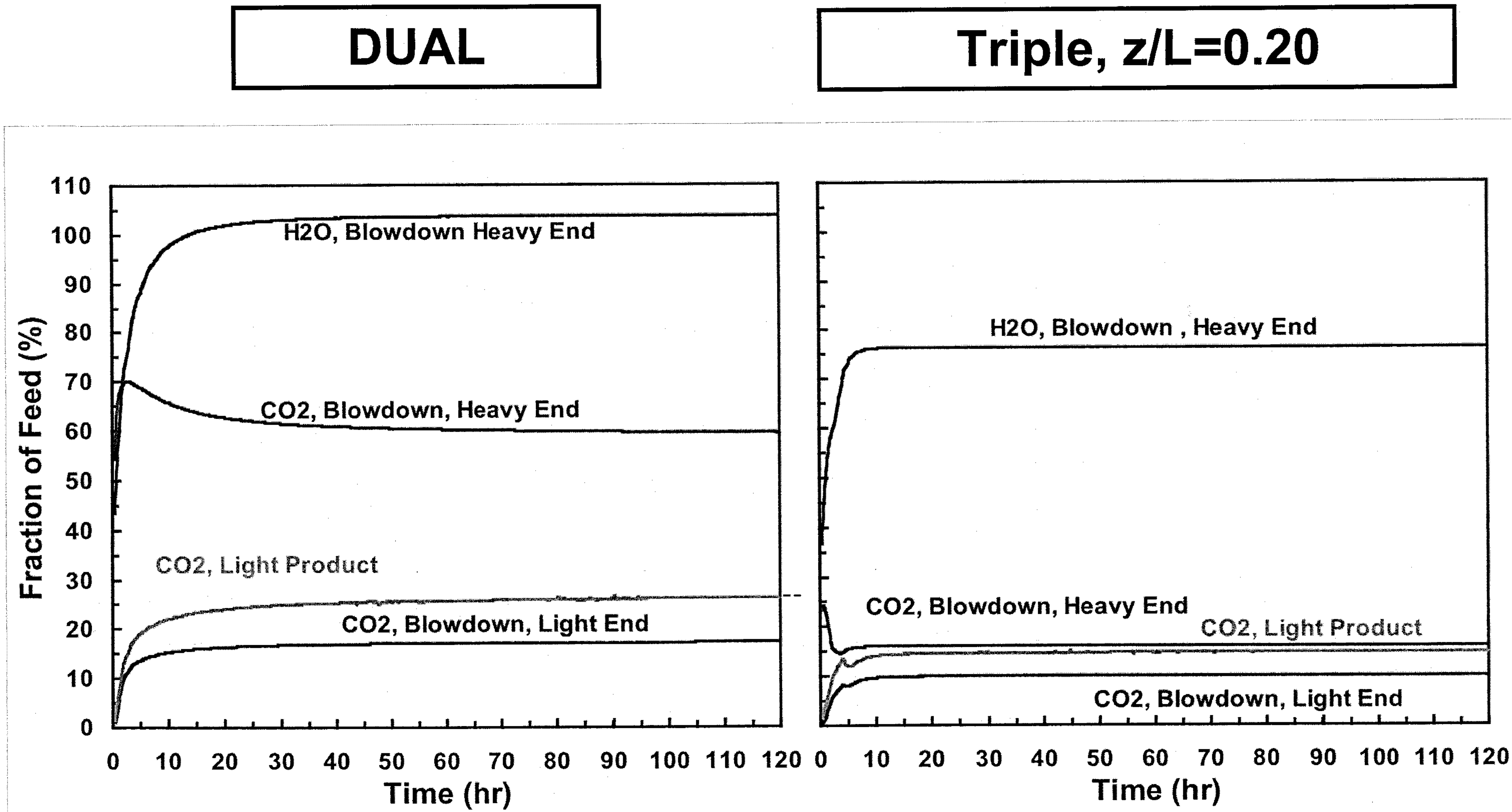


Triple vs Dual Ended Blowdown

History of H_2O and CO_2 Removal Per Cycle



Triple vs Dual Ended Blowdown
History of H_2O and CO_2 Removal per Cycle



Triple vs Dual Ended Blowdown

H_2O and CO_2 Removal after 120 hr

Optimal Third Port Location

	Conditions									Modeling Results			
Test Point	Third Port location z/L	Bed Size, L	Half cycle Time, min	DED Time, min	TED Time, min	Inlet ppCO2, torr	Inlet ppH2O, torr	Flow Rate, scfm	Inlet Temp, degF	CO2 Removal, lb/hr	CO2 Removal Eff	H2O Removal, lb/hr	H2O Removal Eff
18		**8.88**	**7.5**	**7.0**	**-**	**5.0**	**9.1**	**13.5**	**69.9**	**0.47**	**0.74**	**0.49**	**1.00**
Triple	**0.5**	8.88	7.5	-	7.0	5.0	9.1	13.5	69.9	**0.50**	0.79	0.49	1.00
	0.4	8.88	7.5	-	7.0	5.0	9.1	13.5	69.9	**0.53**	0.83	0.49	1.00
	0.3	8.88	7.5	-	7.0	5.0	9.1	13.5	69.9	**0.55**	0.86	0.49	1.00
	0.2	8.88	7.5	-	7.0	5.0	9.1	13.5	69.9	**0.54**	0.85	0.49	1.00

Conclusions

- A description of the new NASA SBAR PSA system for H_2O and CO_2 removal, with particular emphasis on its purgeless deep vacuum regenerative steps has been given
- Regeneration consisted of blowdown steps subject to deep vacuum through an increasing number of evacuation ports, i.e., single, dual and triple ended blowdown was studied.
- The USC PSA process simulator, for which adsorbent and adsorbate properties were independently obtained, successfully predicted NASA's experimental results of a dual ended system.
- The USC PSA process simulator was also used to discern the role of the regenerative steps on the performance of NASA's SBAR PSA system.

The USC PSA process simulator is currently being used in other projects of equal complexity.

Acknowledgements

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NASA MSFC
is greatly appreciated!

Thank You!

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