

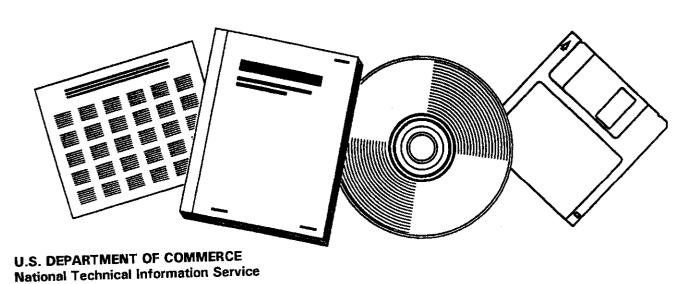
DE85013709



DEVELOPMENT OF AN ADVANCED WATER-GAS SHIFT CONVERSION SYSTEM. FINAL REPORT

BATTELLE PACIFIC NORTHWEST LABS. RICHLAND, WA

APR 1985



DOE/MC/80871-1906 (PNL-5468) (DE85013709) Distribution Category UC-90c

Development of an Advanced Water-Gas Shift Conversion System

Final Report

By
L.J. Sealock, Jr.
D.C. Elliott
R.S. Butner

Work Performed Under Field Task Proposal Agreement No. 80871

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
P.O. Box 880
Morgantown, West Virginia 26507-0880

By Pacific Northwest Laboratory Richland, Washington 99352

April 1985

ACKNOWLEDGMENTS

The authors wish to thank the U.S. Department of Energy and the Morgantown Energy Technology Center (METC) for support of this research. We appreciate the encouragement of Dr. Hsiao-Ya L. Lai, the METC Technical Project Officer, for her encouragement during the project. We would also like to acknowledge Dr. John Cox and Dr. Charles Nelson of the Basic Research Department of the Gas Research Institute whose support of our earlier research provided the technical foundation for the concept investigated in this project. Finally, we would like to express our appreciation to Gary G. Neuenschwander, whose help in the design, fabrication, and execution of the experimental phase of this work was invaluable.

CONTENTS

EXECUTIVE SUMMARY INTRODUCTION AND BACKGROUND Batch Reactor Tests Process Chemistry Concept Advantages Equilibrium Considerations Range of Catalyst Choice . Relationship to Coal Gasif	. ,			•							•		•		2
Batch Reactor Tests Process Chemistry Concept Advantages Equilibrium Considerations	• •	•	-	•											
Process Chemistry	. ,		-						•		٠.	•			4
Concept Advantages Equilibrium Considerations Range of Catalyst Choice .					•										5
Equilibrium Considerations Range of Catalyst Choice .				•										_	7
Range of Catalyst Choice .	s .												_	_	7
Range of Catalyst Choice .									_	_	-		_	•	8
										_	Ī	•	•	•	8
Refactionship to Coal Gasii		tion	Te	chn	olo	av.			•	•	•	•	•	•	11
PROJECT OBJECTIVE					_		_		•	_		•	•	•	14
EXPERIMENTAL SYSTEM AND ANALYTI	· CAI	MET	חטטי.	c			•	-	-	-	•	•	•	•	
	. UAL	. №[.]	תטט.	2	•	•	•	٠	•	Þ	•	•	٠	•	15
RESULTS	•	•	•	•	•	•	•	•	•	•	•	•		•	26
Parameter Studies		•	•					•							28
Gas Contacting Studies .		•		•		•									33
Catalyst Studies		•										•			36
Use of Preheated Feed Gas		•													39
Phase Equilibrium Consider	ati	ons													41
DISCUSSION		_	.=									-	•	•	48
Catalyst Turnover Rates .	-	•	•	•	•	•	•	•	•	•	•	•	•	•	
Reaction Rate Expressions	•	•	•	•	•	•	•	•	•	•	•	•	•	•	48
D	•	•	•	•	•	•	•	•	•	•	•	•	•	•	54
				•	•	•	•	•	•	•	•	•	•	•	60
Engineering Evaluation of	the	Hig	h-Pr	ess.	ure	Wa	ter	Ga	s S	Shif	t	Sys	tem	•	61
ACCOMPLISHMENTS AND CONCLUSIONS	•	•	•												72
RECOMMENDATIONS			•	-	•	•							•	•	74
Phase Equilibria and Proces	ssi	ng Co	ond i	tio	ns										74
Catalyst Concentration Effe	ects	· .													75
Use of Hot Gas Feed						•								_	75
Diluent Gas Effects											•				76
Methodology Changes												•		•	76

CONTENTS (cont'd)

Final -	Recommendati	ons .						77
REFERENCES .						• • •		78
APPENDIX A -	CYDEDIMENTAL	ΔΤΔΠ						82
					00000000	755 AQUEQUE	•	•
APPENDIX B	PRELIMINARY WATER-GAS SH	EVALUAT IFT CON'	ION OF VERSION	THE PNL CONCEP	T. PRESSURI	ZED AQUEOUS		99
		÷						
				•				
	•		•					
				r				
;			•					
A								
, ·•								•
,	*							
· 23			, ,	·				
; F"	•							
, v.			-					
27						; ;		
₹ <u>₹</u>	•		. ,	1	7013 ¹ 14		* · · · ·	÷ .
	¢ -		-	•		* * 1 · 1 ·		:
					2		. :	
76	, •		en e			· 3630 ·	٠,	

FIGURES

1	Effect of Temperature on the Catalytic Conversion of Carbon Monoxide by the Water-Gas Shift Reaction (Batch Data)	9
2	Effect of Sodium Carbonate Concentration on the Catalytic Conversion of Carbon Monoxide by the Water-Gas Shift Reaction (Batch Data) I	.2
3	Schematic Drawing of the Major Components of the Continuous Flow Water-Gas Shift Reactor System	.6
4	Detailed Drawing of the One-Liter Autoclave Configured for Use as a Continuous Flow Water-Gas Shift Reactor	7
5	Simplified Cutaway Drawing Illustrating the Flow of Gas in the Water-Gas Shift Reactor	9
6	Cross-Sectional View of the Externally Heated Packed Tube Feed-Gas Preheater	1
7	Photograph Indicating the Arrangement of the Secondary Condenser System, as Well as Gas Monitoring Apparatus	3
8	Overall View of the Reactor Facilities	5
9	Effect of Catalyst Temperature on the Conversion of Carbon Monoxide by the Water-Gas Shift Reaction at 2500 psig	0
10	Effect of Catalyst Temperature on the Conversion of Carbon Monoxide by the Water-Gas Shift Reaction at 3000 psig	1
11	Effect of Catalyst Temperature on the Conversion of Carbon Monoxide by the Water-Gas Shift Reaction at 1500 psig	2
12	Effect of System Pressure on the Conversion of Carbon Monoxide by the Water-Gas Shift Reaction at 300°C	4
13	Effect of Agitation Rate on the Catalyst Turnover	5
14	Effect of Catalyst on the Conversion of Carbon Monoxide by the Water-Gas Shift Reaction	8
15	Pressure-Temperature Phase Diagram for Pure Water Adapted from the Steam Tables	2
16	Effect of Initial Sodium Carbonate Concentration on the Vapor Pressure of Heated Solutions	4
17	Effect of Initial Sodium Formate Concentration on the Vapor Pressure of Heated Solutions	5
18	Effect of Temperature on Catalyst Turnover Rates at 2500 psig 49	9
19	Effect of Temperature on Catalyst Turnover Rates at 3000 psig 50)

FIGURES (cont'd)

20	Effect of Temperature on Catalyst Turnover Rates at 1500 psig	•	51
21	Effect of Total System Pressure on Catalyst Turnover Rates at 300°C		52
22	Comparison of Turnover Rates for Various Catalysts		53
23	Effect of Catalyst Solution Temperature on Measured Average Rate Constant for 6% Sodium Carbonate Catalyst		57
24	Plot of $ln(k)$ versus Reciprocal Temperature		59
25	Effect of Operating Pressure on the Estimated Cost of Water-Gas Shift Reactors for a 1000 ton per hour Coal Gasification Plant .	•	66
26	Effect of Catalyst Temperature on the Estimated Cost of Water-Gas Shift Reactors for a 1000 ton per hour Coal Gasification Plant .	•	67
27	Effect of Required Exit Concentration of CO on the Estimated Cost of Water-Gas Shift Reactors for a 1000 ton per hour Coal Gasification Plant	•	69
28	Effect of Reactor Aspect Ratio on the Estimated Cost of Water-Gas Shift Reactors for a 1000 ton per hour Coal Gasification Plant .		70
29	Effect of Individual Reactor Volume on the Estimated Cost of Water-Gas Shift Reactors for a 1000 ton per hour Coal Gasification Plant		71

<u>TABLES</u>

1	Aqueous Catalysts for the Water-Gas Shift Reaction
2	Water-Gas Shift Experimental Parameters Studied
3	Effect of Dip Tube Size on Reaction Rate
4	Typical Gas Analyses
5	Catalyst Turnover Numbers for Water-Gas Shift Catalysts
6	Rate Constant for Various Catalysts
7	Gas Composition for Pressurized Texaco Gasifier
8	Process Calculations for Water-Gas Shift at Several Conditions 61