

APPENDIX A

COST QUOTATION FOR KATALCO 7-2 ACTIVATED CARBON

Katalco

CORPORATION

Process Catalysts

2900 Butterfield Rd. • Oak Brook, Ill. • 60451 • Tel. 312-585-1100

Plant Telephone
312-767-6884

November 7, 1977

Mr. Martin Lieberman
Exxon Research and
Engineering Company
Post Office Box 8
Linden, New Jersey 07036

Katalco Quotation #K-77-74

Dear Mr. Lieberman:

As per our recent telephone conversation, I am submitting a quotation for Katalco 7-2, activated carbon. The following quotation contains price, delivery, packaging, and shipping information.

Unfortunately, Katalco does not, nor do I know of anyone who purchases spent carbon. It would be advantageous to include a facility to steam-air regenerate the carbon on site, or to investigate the use of another sulfur removal system, such as cobalt-moly/zinc oxide. Katalco would be pleased to investigate these alternatives with you.

Thank you for your interest in Katalco catalysts. If I can be of any further service, please do not hesitate to contact me.

Very truly yours,

A. V. Kinal

A. V. Kinal,
Sales and Service Representative

AVK/jh

Attachment

KATALCO CORPORATION

EXXON RESEARCH AND ENGINEERING COMPANY
LINDEN, NEW JERSEY

CATALYST AND QUANTITY

Katalco 7-2 Impregnated Activated Carbon - Approximately 3,600 ft³
(To be Utilized over a Period of One Year)

Size: 12 x 30 Mesh Bulk Density: 33 lbs/ft³

PRICE

The price of Katalco 7-2 is \$40.00 per cubic foot, f.o.b. Pittsburgh
(This Price is Applicable to Quantities Over 900 ft³)

Total Price for 3,600 ft³ - \$144,000, f.o.b. Pittsburgh

DELIVERY

Delivery can be made to the Bruceton, Pennsylvania site four weeks
after receipt of purchase order. Delivery can be adjusted to
accommodate your requirements, i.e., one delivery per month (300 ft³)
for one year, or as required.

PACKAGING

The Activated Carbon is packaged in 55 gallon fiber drums, each drum
containing 6.7 ft³ of carbon. Net weight of carbon per drum is 220 lbs.

TERMS

Our usual terms are Net 30 Days.

APPENDIX B

COST ESTIMATES FOR RECTISOL AND BENFIELD
SULFUR GAS REMOVAL PROCESSES

EXXON RESEARCH AND ENGINEERING COMPANY

P.O. BOX 8, LINDEN, N. J. 07036

GOVERNMENT RESEARCH LABORATORIES
M. BERGER
Director
J. W. HARRISON
Director
Energy and Environmental Research Laboratory

November 26, 1975

Mr. H. Haberland
LOTEPRO Corporation
1140 Avenue of the Americas
New York, New York 10036

Dear Mr. Haberland:

Per our conversation of October 10, I would like to request your estimate of both investment and operating costs, in as much detail as conveniently possible, of a Rectisol plant to purify the gas stream described in the attached table. These estimates are requested in connection with our contract (No. E(36-2)-0059) with the United States Energy Research and Development Administration. In this regard, we are endeavoring to establish methods and costs for lowering the sulfur content of a gas stream generated by a "Synthane" coal gasification system to a level of less than 0.1 ppm required for feeding to methanation. We understand that the Rectisol system is probably capable of achieving such a requirement.

Along with the cost information described above, I would appreciate your estimate of the compositions of streams leaving the Rectisol system (product gas, as well as CO₂ and H₂S-enriched regenerator effluents) and a general description of the facilities comprising the system (including, if possible, your recommendation for a sulfur recovery system to handle regenerator effluent).

I would be most grateful for any priority that you could assign this matter. Again, thank you for your regard and cooperation.

Very truly yours,

C. D. Kalfedelis / RFA

C. D. Kalfedelis

CDK/cab

Attachment

cc: E. P. Iaccarino
E. Shaw

Feed Gas to Acid Gas Treatment

Flow Rate = 74,000 molc /hr
Pressure = 965 psig
Temperature = 225°F

Composition

H₂ = 27.9%
CO = 9.0
CO₂¹ = 35.9
CH₄ = 21.9
C₂H₆ = 0.7
N₂ = 1.6
H₂O = 2.0

Sulfur
Comp'ds.* = 1.0

*Hydrogen Sulfide = 9800 ppm
Carbonyl Sulfide = 150
Thiophene = 31
Methyl Thiophene = 10
Dimethyl Thiophene = 10
Carbon Disulfide = 10
Methyl Mercaptan = 60

¹Treated gas should contain < 1-ZK CO₂.



1140 AVENUE OF THE AMERICAS • NEW YORK, N. Y. 10025 • (212) 575-7875

December 31, 1975

EXXON Research and Engineering Co.
P.O. Box 8
Linden, New Jersey 07036

Attn: Mr. C. D. Kalfadalis

Re: Rectisol System for Sulfur and CO₂
Removal from Synthene - Coal Gasification Gas
Your letter dated Nov. 26, 1975

Dear Mr. Kalfadalis:

We have prepared a material balance and utility list for a Rectisol system designed to purify the given gas stream. This system has been especially designed for high methan recovery.

We estimate the following utility consumption.

Refrigeration:	54 MMBTU/HR @ -49°F
Steam:	84 MMBTU/HR @ 50 psig
	48 MMBTU/HR @ 100 psig
Cooling Water:	2178 USGPM @ 18°F temp. rise
	does not include the refrigeration unit.
Electric Energy:	9510 KW, does not include the
	refrigeration unit.
Methanol Losses:	400 LBS/HR

The large flows that have to be handled require to build the plant in three parallel trains. Based on that assumption we estimate the investment cost for the turnkey unit to be

\$35,000,000.-

The accuracy of this estimate is $\pm 20\%$
Each train consists of:

- 1 Wash tower for sulfur removal
- 1 Wash tower for CO₂ removal
- 2 Regeneration towers for CH₄- Recovery
- Pumps
- 1 Refrigeration unit
- 1 Recycle compressor
- Heat exchangers
- 1 Water Methanol separation

LOTEPRO CORPORATION

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The Rectisol system can purify the gas stream to a sulfur level of less than .1 ppm. It also can enrich the sulfur in a sulfur fraction that can be fed directly to a Claus-unit for conversion into elemental sulfur.

The CO₂-tailgas will contain no more than 5 ppm of sulfur.

Rectisol also dries the gas. Therefore, the material balance has been set up for dry gas. The water is removed and delivered as pure water at battery limits.

If you have any questions please feel free to call the undersigned.

Best regards,
LOTEPRO CORPORATION

Juergen Bokemper

Juergen Bokemper

JB/ub
Encl.

PROJECT: EXXON SYNTHANE
 DATE: 12/30/75 BY:
 PAGE 1 OF 1 PAGES

LOTTECO CORP.

MATERIAL-BALANCE

TOTAL GAS FLOW RATE 74,000 LPMH

Gas Component	Feedgas		Purified gas		Sulfur-tailgas		CO ₂ -tailgas	
	Vol. %	LPMH	Vol. %	LPMH	Vol. %	LPMH	Vol. %	LPMH
N ₂	28.5		45.1		0.1		0.4	
CO	9.2		14.7		0		0.1	
CH ₄	22.4		35.5		0.2		0.2	
C ₂ H ₆	0.7		0.2		0.4		1.7	
N ₂	1.6		2.5		0		0	
CO ₂	36.6		2.0		74.3		97.5	
Total Sulfur Compound	1.0		<.1 ppm		25.0		<5 ppm	
	100.0	72,618	100.0	45,638	100.0	2,904	100.0	24,076
Feeds		965		935		20		2
BY		100		90		100		90

EXXON RESEARCH AND ENGINEERING COMPANY

P.O. BOX 8, LINDEN, N.J. 07036

GOVERNMENT RESEARCH LABORATORIES

M. BERGER
Director

J. W. HARRISON
Director
Energy and Environmental Research Laboratory

November 26, 1975

Dr. Homer Benson
Benfield Corporation
615 Washington Road
Pittsburgh, Pennsylvania 15228

Dear Dr. Benson:

Per our conversation of October 10, I would like to request your estimate of both investment and operating costs, in as much detail as conveniently possible, of a Benfield plant to purify the gas stream described in the attached table. These estimates are requested in connection with our contract (No. E (36-2)-0059) with the United States Energy Research and Development Administration. In this regard, we are endeavoring to establish methods and costs for lowering the sulfur content of a gas stream generated by a "Synthane" coal gasification system to a level of less than 0.1 ppm required for feeding to methanation. We understand that the Benfield system alone is not capable of achieving such a requirement but would require an ancillary sulfur guard system.

Along with the cost information described above, I would appreciate your estimate of the compositions of streams leaving the Benfield system (product gas, as well as CO₂ and H₂S-enriched regenerator effluents) and a general description of the facilities comprising the system (including, if possible, your recommendation for a sulfur recovery system to handle regenerator effluent).

I would be most grateful for any priority that you could assign this matter. Again, thank you for your regard and cooperation.

Very truly yours,

C. D. Kalfadelis / 11/23

C. D. Kalfadelis

CDK:da
Attachment

cc: E. P. Laccarino
H. Shaw

Feed Gas to Acid Gas Treatment

Flow Rate = 74,000 moles/hr
Pressure = 965 psig
Temperature = 225°F

Composition

H₂ = 27.9%
CO = 9.0
CO₂¹ = 35.9
CH₄ = 21.9
C₂H₆ = 0.7
N₂ = 1.6
H₂O = 2.0

Sulfur
Comp'ds.* = 1.0

*Hydrogen Sulfide = 9800 ppm
Carbonyl Sulfide = 150
Thiophene = 31
Methyl Thiophene = 10
Dimethyl Thiophene = 10
Carbon Disulfide = 10
Methyl Mercaptan = 60

¹Treated gas should contain \leq 1-2% CO₂.

Benfield

CORPORATION • 615 WASHINGTON RD., PITTSBURGH, PA.

January 12, 1976

Exxon Research and Engineering Company
P. O. Box 8
Linden, New Jersey 07035

Attention: Mr. C. D. Kalfadelis

Reference: Your letter of November 26, 1975, CDK/jep; our PS-1601

Subject: Benfield Unit Information for your ERDA Contract E(36-2)-0059

Gentlemen:

On the basis of the process information accompanying your referenced letter we offer the following information on a Benfield unit to satisfy your product specifications:

a. Estimated total plant installed cost - \$26.7 M:

This is a preliminary budget estimate with a range of plus or minus 15%. It is on a battery limits basis without including offsite steam or power generation, cooling water, compressed air, etc. facilities. Installed cost includes equipment (towers, pump, tanks, exchangers, etc.), plus electrical, piping, insulation, instruments, concrete, painting, field labor and indirect costs.

b. Estimate utility requirements per hour:

Steam	0.646 MM lbs.
Power (pumps and fans)	15917 KWH
Cooling water (25°F rise)	3.25 MM U.S. Gal.
Chemical make-up for losses	\$7.29

c. Estimated solution inventory \$392,000

The analyses of the inlet and outlet gas of the Benfield unit are:

<u>Component</u>	<u>Inlet Volume Percent</u>	<u>Outlet Volume Percent</u>
H ₂	28.47	45.6
CO	9.18	14.7
CO ₂	36.63	0.15
CH ₄	22.35	35.8
C ₂ H ₆	0.71	1.1
H ₂	1.64	2.6
H ₂ S	9800 ppm	40.5 ppm

Exxon Research & Engineering Company
January 12, 1976
Page 2

<u>Component</u>	<u>Inlet Volume Percent</u>	<u>Outlet Volume Percent</u>
COS	150 ppm	< 3 ppm
CS ₂	10 ppm	< 2 ppm
Methyl mercaptans	60 ppm	20 ppm
Thiophenes	51 ppm	80-85 ppm
Total mole (dry)	72520	44886
Water	26663 lbs.	1195 lbs.
Temperature	225°F	122 °F
Pressure	980 psia	973 psia

The analysis of the regenerator effluent is (total regenerator effluent will be approximately 27645 lb. mols/hr.):

<u>Component</u>	<u>Volume Percent</u>
CO ₂	96.1
H ₂ S	2.65
Methyl mercaptan	80 ppm
Other (H ₂ , CO, CH ₄ , etc.)	1.2

The Benfield system would consist of two identical trains, each train containing two absorber and two regenerators plus pumps, exchangers, reboilers and condensers.

We have assumed bulk removal of CO₂, H₂S and COS with no selectivity. As a guard chamber and for further removal of the organic sulfur from the product gas we suggest consideration of activated carbon and zinc oxide to reduce the sulfur components to tolerable levels for methanation. If residual COS becomes a problem in downstream purification, we could, at a reasonable extra plant investment, decrease the residual COS to about 0.1 ppm.

If selective removal of H₂S is of interest, we could provide an acid gas that would contain H₂S in the range of 13-20% that would be suitable for a Claus unit feed.

We trust that the foregoing is of some help to you.

Very truly yours,

THE BENFIELD CORPORATION

Homer E. Benson, President

Feed Gas to Acid Gas Treatment

Flow Rate = 74,000 moles/hr
Pressure = 965 psig
Temperature = 225°F

Composition

H₂ = 27.9%
CO = 9.0
CO₂¹ = 35.9
CH₄ = 21.9
C₂H₆ = 0.7
N₂ = 1.6
H₂O = 2.0

Sulfur
Comp'ds.* = 1.0

*Hydrogen Sulfide = 9800 ppm
Carbonyl Sulfide = 150
Thiophene = 31
Methyl Thiophene = 10
Dimethyl Thiophene = 10
Carbon Disulfide = 10
Methyl Mercaptan = 60

¹Treated gas should contain \leq 1-2% CO₂.

APPENDIX C

ADSORPTION OF SULFUR COMPOUNDS FROM SYNTHESIS GAS
THEORETICAL ANALYSIS

Nicholas Kafes

August, 1976

NSF Faculty Research Participation Project
Grant No. SER 76-04548

Exxon Research and Engineering Company
Government Research Laboratories
Linden, New Jersey 07036

BACKGROUND

An ERDA-sponsored development program was conducted at Exxon's Government Research Laboratories to recommend and define the sulfur guard system to be employed on a coal derived synthesis gas prior to methanation. The contaminants of concern are H_2S , COS , CH_3SH , CS_2 , C_4H_4S in the 10 to 100 ppm range. The intent was to effect removal of the organic sulfur compounds by physical adsorption on an activated carbon surface and to effect chemisorption removal of the H_2S by converting a metal oxide impregnant of the carbon to the sulfide. The experimental program that was conducted consists of obtaining dynamic adsorption data for each of the contaminants separately in a synthetic synthesis gas blend. Data was also subsequently obtained with all of the contaminants in the gas blend.

The task assigned to the writer concerned the scaleup of the laboratory data being generated so that a reliable design could be implemented for a large scale commercial operation. An extensive review of the literature was undertaken in order to evaluate methods that could be employed to establish a design basis for such a multi-component adsorption system. Most of the workers in the field, however, have focused their efforts on single component systems under a variety of limiting constraints. The literature is replete with mathematical analyses in an attempt to define the sorbate concentrations as a function of time and distance along the bed. Relatively very little experimental data are being generated. The failure, in general, of these solutions to predict the behavior of adsorption beds with accuracy is a measure of the complexity of the phenomena being analyzed.

For the adsorption of one component from an inert fluid the rate of adsorption at the interface is usually so rapid that it is normally ignored in comparison with boundary layer and solid phase diffusion. These latter two mechanisms have been examined by numerous investigators; however, the relatively rigorous solutions of Rosen (1954) and Vermaeker, et. al. (1973) appear most tractable for numerical evaluation. Approximate approaches, depending on a simplification of the transfer mechanisms or mathematical treatment have been proposed but the solutions are still cumbersome and of little direct value in design though they might be of utility in predicting the effect of a particular variable. Worth noting is the solution of Houghan and Marshall (1947), who assume that solid phase diffusion is not important and that the rate of mass transfer is a function of the sorbate concentration in the fluid and the average concentration in the particles. The solution is in graphical form and permits one to approximate the mass transfer breakthrough profile with reasonable effort.

For multicomponent systems, very little was found in the literature, where the interactive effect of the different species on one another is taken into account. A worthwhile piece of experimental work was that of Thomas (1971) on the binary adsorption of ppm levels of C_6H_6 and C_7H_8 on activated carbon. This appears to be on the right track toward the modeling of dynamic multicomponent systems even though the results have limited applicability for design purposes.

DESIGN APPROACH

The writer was asked to put together an approach for a multicomponent adsorption system design and to implement this with available information existing in the literature. The parameters involved could

then be subsequently modified as the data becomes available from the development program. The intent was to point up the key factors that dictate the design of the unit.

For a single component system, the determination of the adsorbent bed length requirement in practice, consists of defining the equilibrium zone, where the adsorbent is saturated with sorbate, and the mass transfer zone, where the concentration of the sorbate species falls from the saturation value to zero at the leading edge of the zone.

$$L_0 = L_{\text{Equil}} + L_{\text{MTZ}}$$

This approach is simplified somewhat, when a stable mass transfer front is exhibited by considering these two zones equivalent to a Length of Equivalent Equilibrium Section and a Length of Unused Bed, Collins (1968), Lukchis (1973). In the mass transfer zone approximately half the adsorbent can be considered to be at its saturation value and half completely unused (experimentally this fraction ranges between .4 to .6).

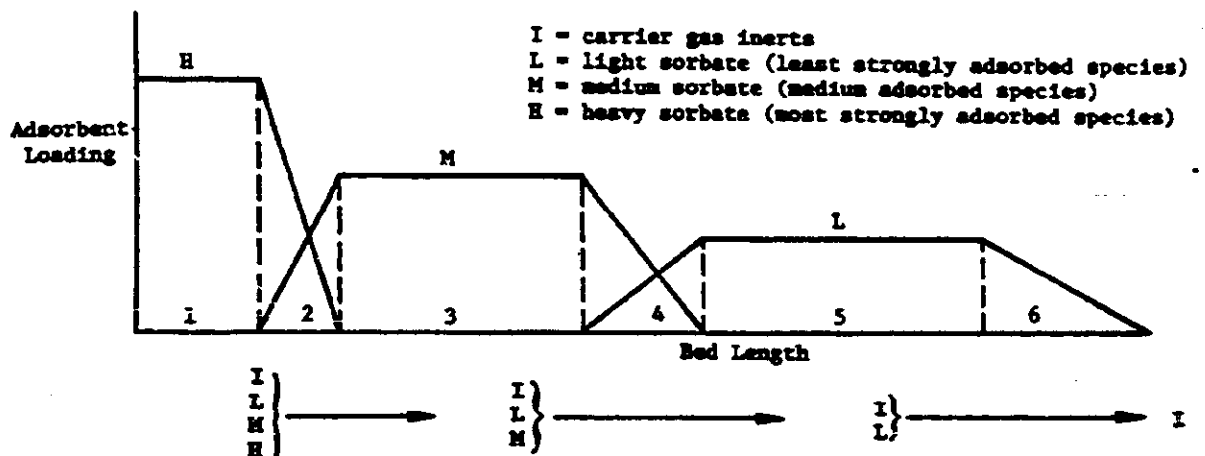
$$L = (L_{\text{Equil}} + \frac{L_{\text{MTZ}}}{2}) + \frac{L_{\text{MTZ}}}{2} = \text{LES} + \text{LUB}$$

The equivalent equilibrium section bed requirement can be defined using available isotherm loading data taken under static conditions. These values are frequently derated to account for the dynamic conditions prevailing in the bed. The length of the mass transfer zone is a function of the adsorbent properties, fluid properties, concentration and flow conditions. As previously indicated, the breakthrough profile, or MTZ length, can be reasonably approximated, under certain restricted conditions (isothermal, linear equilibrium relation) using available models such as that of Hougan and Marshall (1947) as described by Fair (1969). The use of a more complex model is not warranted. To establish a firmer basis for design

necessitates that the MIZ length be obtained experimentally along with the dynamic saturation loadings for the equilibrium section.

To provide a design basis for a multicomponent system, the approach taken was to account for the individual components of the system in a series fashion. Each of the species is treated in sequence, in the order of their molar polarizability, i.e., from the most strongly adsorbed species to the least strongly adsorbed species. This order is dependent on molecular weight, boiling point, and refractive index of the components involved. This additive procedure has been referred to in the literature, Conviser (1965), Manchanda (1973), Chi (1973), as being successfully employed in the prediction of molecular sieve bed performance for the drying and desulfurization of natural gas, though relatively little detailed information is given. This approach is also recommended by activated carbon vendors for the multicomponent systems where low concentration levels prevail and where no interactive effects are expected.

For a system in which the species are present at ppm levels it is reasonable to expect that a number of stable mass transfer fronts would be manifested as the fluid passes through the bed. If no interaction is assumed between the sorbates, a multicomponent system should exhibit the following type of behavior.



At the inlet side of the bed, zone 1 is completely saturated with the heavy sorbate. In zone 2, the medium sorbate which had previously been adsorbed is being replaced by the heavy sorbate. This zone is an interchange zone and can be considered to be occupied half by the heavy sorbate at its saturation value and half by the medium species at its saturation value. In zone 3 the medium sorbate saturates the bed having completely pushed off the light sorbate. Again in zone 4 an interchange takes place where the medium sorbate is pushing out the light sorbate. In zone 5 the light sorbate saturates the bed and in the zone 6 mass transfer zone the light sorbate concentration drops from its saturation value to zero at the leading edge. The breakthrough point (a measurable concentration level at the loading edge) for the light sorbate usually dominates the design of the bed.

The idealized front profiles shown above can then be replaced by equivalent equilibrium sections for all the species plus a length of unused bed for the least strongly adsorbed contaminant.

$$L = (LES)_{\text{Heavy}} + (LES)_{\text{Medium}} + (LES)_{\text{Light}} + (LUB)_{\text{Light}}$$

There are no lengths of unused bed for the heavy and medium sorbates since the mass transfer zones for the species involved are fully occupied.

The above model assumes that there are no interactive co-adsorption effects taking place. This is somewhat unrealistic, however the adsorbent requirement calculated by considering the individual species separately should be on the conservative side particularly if the components exhibit different adsorptive tendencies toward the adsorbent. The major uncertainty with the above approach, for the situation at hand, involves the so called inert constituents of the carrier gas. If the carrier

gas has a constituent with an adsorption affinity close to the lightest sorbate, these will be competition for the same adsorption sites such as to effect a much lower loading value for the light sorbate relative to the equilibrium isotherm value. This will result in a much larger adsorbent requirement when designing for light sorbate removal.

CASES INVESTIGATED

For the multicomponent system under consideration, a number of situations were calculated according to the possible modes of operation proposed for the sulfur guard system. Three base cases were implemented with further variations for contaminant level and design velocity.

Case I - involves the use of a virgin, unimpregnated activated carbon to remove all five sulfur species by physical adsorption.

Case II - involves the use of an impregnated activated carbon to remove the four organic sulfur species C_4H_4S , CS_2 , CH_3SH , COS by physical adsorption and the H_2S species by a parallel chemisorption mechanism.

Case III - involves the use of an impregnated activated carbon to remove the three heaviest organic sulfur species, C_4H_4S , CS_2 , CH_3SH by physical adsorption and the H_2S by chemisorption.

The cases were calculated for the following stream composition, contaminant levels, flow quantity and operating conditions.

For the adsorbent bed the following parameters were fixed*

Breakthrough time	$t_B = 24$ hours
Adsorbent mesh size	4 x 10 mesh
Superficial velocity	$V^* = 6.7$ cm/sec

*This is about 3x the design value used in the experimentation. However, this should have only a minor effect on predicted performance.

	<u>Mol. %</u>		<u>Contaminant (PPM)</u>	<u>Operating Conditions</u>
H ₂	45.0			
N ₂	2.7			
CO	14.7	Cl ₄ H ₄ S	45	T = 90°F P = 1000 psig
CO ₂	1.0	CS ₂	12	
CH ₄	35.4	CH ₃ SH	25	
C ₂ H ₆	1.0	COS	80 (10)	
H ₂ O	.2	H ₂ S	25	
	<u>100.0</u>		<u>187 (117)</u>	

Mols/hr. = 45000 (flow quantity for a 250 M SCFD plant).

Pressure drop considerations dictate the mesh size and superficial velocity employed. These values were set for Case II, the most important of the above cases with design velocity changes being considered for the other cases.

The adsorbent particle size employed in the Exxon development program is a 12 x 30 mesh impregnated activated carbon necessitated by the small diameter take being tested. For a large scale commercial unit, however, this particle size would not be practical. The ensuing pressure drop would be three to four times larger than for the 4 x 10 mesh size carbon. Alternately, a very low superficial velocity would have to be employed leading to an excessive vessel diameter or a large number of vessels. At the SYMBANE pilot unit, a very low velocity, .044 ft/sec., is to be employed with the 12 x 30 mesh impregnated activated carbon. The effect of particle size on the mass transfer characteristics is not too discernable. Equilibrium loadings are essentially unaffected, though a larger particle size will bring about a lengthening of the breakthrough profiles.

Values for the equilibrium loadings (static isotherm data) are available in the literature, Grant (1960, 1962) for H₂S, COS, CH₃SH and

CS_2 on a 4×10 mesh virgin activated carbon which has properties similar to the carbon being tested. The equilibrium loading for thiophene, C_4H_4S , was estimated using the generalized Polanyi correlation which fairly accurately describes the behavior of the other sulfur species of the system.

With these loadings and the mass rate of the individual species given, the adsorbent volume equilibrium requirement for each of the components is readily calculated for the chosen breakthrough time. For a specified superficial velocity the cross sectional area for the system is fixed and hence the lengths of the equivalent equilibrium sections can be determined. The length of the unused bed for the lightest sorbate is obtained from the breakthrough profile which can be calculated for a given superficial velocity and particle size.

For Case I, the above noted equilibrium values were used directly to establish the equivalent equilibrium section lengths. The length of the unused bed for H_2S , the lightest sorbate, was calculated from the Hougen, Marshall prediction for the breakthrough curve. Eight vessels with dimensions $D = 12$ ft, $L = 59$ ft, would be required (four adsorbing, four regenerating). The superficial velocity is .165 ft/sec with a bed pressure drop of 2.4 psi. The results for this case are subject to some uncertainty due to the coadsorption of the ethane and carbon dioxide constituents of the carrier gas, which have an adsorption affinity relatively close to H_2S .

For Case II the lengths of the equivalent equilibrium sections were calculated using the above noted equilibrium loading values for the organic sulfur species, derated by 10% to account for loss of adsorption surface due to the copper oxide impregnant. The length of the unused bed

for COS, the lightest sorbate, was calculated from the Hougen/Marshall model and added to the bed length. The equilibrium loading value for H_2S chemisorption was predicated by the stoichiometry of the copper present in the carbon. Six vessels with dimensions $D = 12$ ft, $L = 38$ ft would be required (three adsorbing, three regenerating). The superficial velocity is .22 ft/sec. with a bed pressure drop of 2.4 psi. The physical adsorption of the organic species controls the design the bed; the parallel chemisorption mechanism for H_2S removal utilizes less than 10% of the bed. The COS contaminant level for this case was taken at 80 ppm corresponding to a low performance Benfield operation located upstream of the sulfur guard system. If a high performance Benfield unit is installed, a 10 ppm COS level can be attained. The above dimensions for the six vessels can then be reduced to $D = 12$ ft, $L = 22$ ft. The reasonable confidence in these results can be expected since the carrier gas species, C_2H_6 and CO_2 have adsorption characteristics an order of magnitude different from COS, the lightest sorbate.

For Case III the calculations are the same as for Case II except that CH_3SH is the light sorbate breakthrough constituent. It is anticipated that COS will be removed with an HDS unit. This is a relatively easy cleanup operation requiring four vessels with dimensions $D = 12$ ft., $L = 17$ ft. (two adsorbing, two regenerating). The superficial velocity is .33 ft/sec. with a bed pressure drop of 1.9 psi. Again, as for Case II, physical adsorption of the organic species controls the design; the H_2S chemisorption mechanism utilizes less than a third of the bed. Confidence in the calculations for this case is high since essentially no interference is expected from C_2H_6 and CO_2 ; the CH_3SH has a considerably larger adsorption affinity than these two species.

The results for the three cases are summarized in the following tabulation. No over design is included at this point. If higher contaminant levels are encountered this would be compensated for, to a considerable degree, by higher equilibrium loadings. However, this loading increase is not directly proportional and extra bed length would be required or alternately a shorter breakthrough cycle can be used for the period of higher contaminant levels. For the impregnated carbon cases, the H_2S level is not controlling and a large concentration increase can be easily contained.

The superficial velocities employed, are in the ball park, and yield reasonable bed pressure drops (on low side) for the 4 x 10 mesh carbon chosen. Vessel diameter was limited to 12 feet; shop fabrication of a larger number of these vessels was assumed more economic than field fabrication of a lesser number of larger diameter vessels. Modifications in the system design, however, can be readily implemented for changes in superficial velocity/diameter/number of vessels.

Time ran out with regard to pursuing an investigation of interactive co-adsorptive effects of the carrier gas constituents. This type of data is simply not available for the species involved. However, co-adsorption equilibrium calculations of binary pairs by the methods of Myers (1965) or You (1971) might be combined to yield some prediction of these effects. The development program as it is presently constituted, single component runs plus five component runs, is suitable to provide a basis for direct scale up for a large commercial size unit. However, it will be difficult to ascertain specific interactive effects from the data. It would be informative if binary and ternary runs would be executed, par-

ticularly for the more critical light sorbates, H_2S , COS , CH_3SH , with and without the interfacing carrier gas species C_2H_6 and CO_2 .

<u>Case</u>	<u>Breakthrough Contaminant</u>	<u>Number of Vessels on Line</u>	<u>RESULTS</u>		<u>[4x10]</u>	<u>Design Confidence Level</u>
			<u>[D = 12 ft]</u>		<u>[mesh]</u>	
			<u>Vessel Length (ft)</u>	<u>Superficial Velocity (ft/sec)</u>	<u>Bed Pressure Drop (psi)</u>	
I	H_2S	4	59	.165	2.4	Low
II	COS 80 ppm (10 ppm)	3	38	.22	2.4	Good
III	CH_3SH	2	17	.33	1.9	High

REFERENCES

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APPENDIX
OF
CALCULATIONS

GAS - AVERAGE MOLECULAR WEIGHT AND DENSITY

89.6°F
 T = 32°C = 305°K
 P = 1014.7 psia = 69 atm

	<u>Mole %</u>	<u>M</u> <u>(lbs/mol)</u>	<u>Pc</u> <u>(atm)</u>	<u>Tc</u> <u>(°C)</u>	<u>Tc</u> <u>(°K)</u>
H ₂	45.0	2.016	12.8	-239.9	33
H ₂	2.7	28.02	33.5	-147.1	126
CO	14.7	28.01	35.0	-139.0	134
CO ₂	1.0	44.01	73.0	31.1	304
CH ₄	35.4	16.04	45.8	-82.5	190
C ₂ H ₆	1.0	30.07	48.8	32.1	305
H ₂ O	.2	18.016	218.4	374.15	647
	<u>100.0</u>				

$M_{aoe} = 12.24$

$(Pc)_{aoe} = 29.68 \text{ atm}$

$(Tc)_{aoe} = 113^\circ\text{K}$

Reduced Conditions

$P_r = \frac{P}{P_c} = 2.33$

$T_r = \frac{T}{T_c} = 2.70$

Compressibility

$Z = 1.02$

Density

$C = \frac{PM}{ZRT}$

$C = \frac{1014.7 (12.24)}{(1.02)(10.73)(549.6)} = 2.06 \frac{\text{lbs.}}{\text{ft}^3}$

VESSEL DIAMETERS - TO PROCESS GAS AT DIFFERENT VELOCITIES

T = 90°F
 P = 100 psig
 Molal rate
 Mass rate
 Volumetric rate
 Cross sectional Area
 Diameter

M = 12.24 lb/mol
 d = 2.06 lb/ft³
 $\mu_T = 45000$ Mols/hr.
 $\dot{m} = \mu M = 550800$ lbs/hr
 $Q = \frac{\dot{m}}{d} = 267000 \frac{\text{ft}^3}{\text{Hr}} = 74.27 \frac{\text{ft}^3}{\text{sec}}$
 $S = \frac{Q}{V}$
 $S = \frac{\pi D^2}{4}$ $D = (S/.785)^{\frac{1}{2}}$

<u>Multiple of SYNTHANE Value</u>	<u>Velocity $\frac{\text{ft}}{\text{sec}}$</u>	<u>Crosssection Area (ft²)</u>	<u>Diameter (Single Vessel) (ft)</u>	<u>(Two Vessels)</u>	<u>(Three Vessels)</u>	<u>(Four Vessels)</u>
1	.044	1688	46.4	32.8	26.8	23.2
2	.088	844	32.8	23.2	18.9	16.4
4	.176	422	23.2	16.4	13.4	11.6
5	.220	337	20.7	14.7	12.0	10.4
6	.264	281	18.9	13.4	10.9	9.5
8	.352	211	16.4	11.6	9.5	8.2

PRESSURE DROP - 4 x 10 MESH CARBON

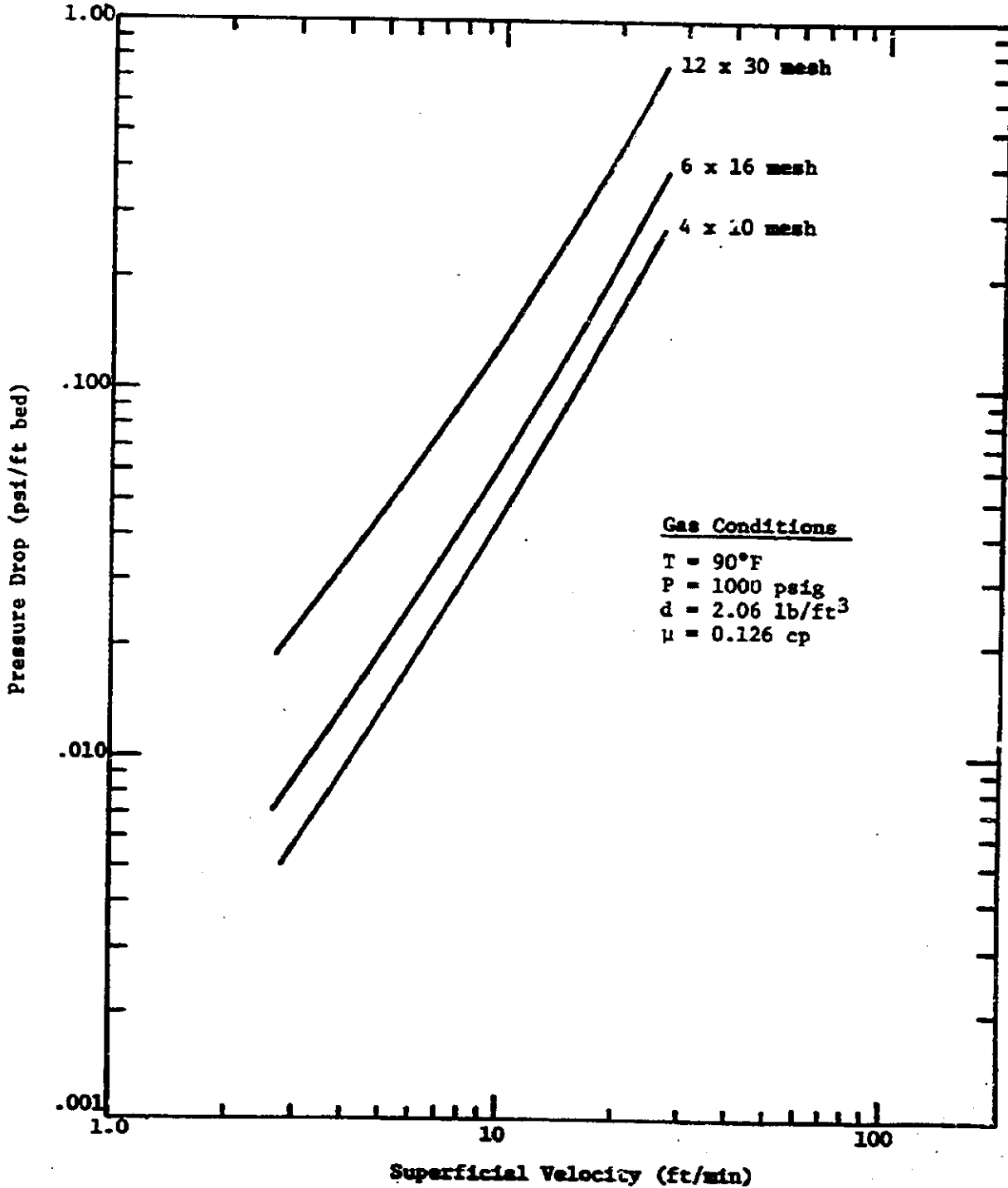
$$\begin{aligned} &= 90^{\circ}\text{F} & d &= 2.06 \frac{\text{lb}}{\text{ft}^3} & E &= .39 \text{ (bed voidage)} \\ &= 1000 \text{ psig} & \mu &= .0126 \text{ cp} & D_{Pa} &= 1.84 \text{ mm (adjusted mean particle diameter)} \\ & & v &= .22 \frac{\text{ft}}{\text{sec}} = 13.2 \frac{\text{ft}}{\text{min}} & & \text{(superficial velocity)} \end{aligned}$$

Equation

$$\begin{aligned} \Delta P &= (.934) \frac{(1-E)^2}{E^3} \left(\frac{\mu v}{D_{Pa}} \right) + 8.86 (10^{-4}) \frac{(1-E)}{E^3} \frac{v^2 d}{D_{Pa}} \\ &= (.934) \frac{(.61)^2}{(.39)^3} \frac{(.0126)(13.2)}{(1.84)^2} + (.000886) \frac{(.61)}{(.39)^3} \frac{(13.2)^2 (2.06)}{(1.84)} \\ &= .288 + 1.777 = 2.065 \frac{\text{inches H}_2\text{O}}{\text{ft-bed}} \\ &= \left(\frac{2.065}{1'} \right) \left(\frac{62.4}{144} \right) = .075 \frac{\text{psi}}{\text{ft-bed}} \end{aligned}$$

PRESSURE DROP VS. SUPERFICIAL VELOCITY

BPL Activated Carbon



ATTRITION OF ADSORBENT - DUE TO HIGH GAS VELOCITY

For granular alumina system attrition should not be a problem if momentum as calculated from following relation is less than 30,000.

Momentum = (V) (M) (P)

Superficial Velocity V = 13.4 ft/min (.22 ft/sec.)

Molecular Weight M = 12.2

System Pressure P = 69 atm (1014.7 psig)

Momentum = (13.4) (12.2) (69)

= 11,100

SULFUR COMPOUNDS - PROPERTIES

	<u>PPM</u> <u>Level</u>	<u>Pc</u> <u>(atm)</u>	<u>Tc</u> <u>(°C)</u>	<u>M</u> <u>(lb/mol)</u>	<u>Boiling Pt.</u> <u>°C</u> <u>(1 atm)</u>	<u>Liq.</u> <u>Sp.G.</u>
H ₂ S	25	88.9	100.4	34.08	-59.6	
C ₄ H ₄ S	45	48.0	317.0	84.13	84.4	1.070 15/4
CS ₂	12	76.0	273.0	76.13	46.3	1.263 20/4
CH ₃ SH	25	71.4	196.8	48.10	6.8	-89.6°
COS	80 or 10	61.0	105.0	60.07	-50.2	1.24 ⁻⁸⁷

187 (117)

EQUILIBRIUM LOADINGS

Activated Carbon

EPL 2026-54 (4x10 mesh)

Sulfur Compounds	(ppm)	(Mol. Fract) Y _i	(Partial Pressure) P _i Y _i P _t	[90°F and P _i]		[90°F P _i = 0.01 psig]
				Loading (%) lb/100 lb	Loading W lb/lb	Loading (%) lb/100
H ₂ S	25	.000025	.0254	.20	.002	.10
C ₄ H ₄ S	24	.000045	.0457	(36.5)	.305	21.5
CS ₂	12	.000012	.0122	10.0	.10	9
CH ₃ SH	25	.000025	.0254	3.4	.034	2
COS	80	.000080	.0812	2.5	.025	.78
	10	.000010	.0102	.78	.0078	

Loadings all from experimental data except for C₄H₄S value which was estimated from Polanyi correlation.

T = 90°F

P = 1014.7 psia

THIOPHENE - EQUILIBRIUM LOADING

Polanyi Correlation - Sulfur Family

C₄H₄S (45 ppm) T = 32°C
305°K P = 1000 psig

M = 84.13 P_i = .0457 psia (partial pressure)

P° = 2.116 psia (vapor pressure at 32°C)

SpG = 1.07 (at 15°C)

SpG = (1.13) est. (at P_i = .0457 psia, .00311 atm)

Liquid Molar Volume at
temperature where vapor
pressure equals adsorption
pressure

$$v_v = \frac{M}{d} = \frac{84.13 \left(\frac{\text{gm}}{\text{mol}} \right)}{1.13 \left(\frac{\text{gm}}{\text{cm}^3} \right)} = 74.45 \frac{\text{cm}^3}{\text{mol}}$$

Adsorption Potential
Parameter

$$\frac{T}{v} \log_{10} \frac{P^\circ}{P_i} = \left(\frac{305}{74.45} \right) \log \frac{2.116}{.0457}$$
$$= 6.83$$

Loading from Sulfur
Family Polanyi Plot

27 cm³ liq./100 gm carbon

w = .27 (1.13)

w = .305 gm liquid/gm carbon

(30.5% loading)

BENZENE - EQUILIBRIUM LOADING

Benzene used as a substitute for thiophene in Pittsburgh carbon computer program. Check to see if benzene loading data fall on Polanyi sulfur family plot.

$$\frac{C_6H_6}{C_6H_6} \quad (45 \text{ ppm}) \\ M = 78.11$$

$$T = 32^\circ\text{C} \\ 305^\circ\text{K}$$

$$P = 1000 \text{ psia}$$

$$P_1 = .0457 \text{ psia} \quad (\text{partial pressure})$$

$$P^\circ = 2.64 \text{ psia} \quad (\text{vapor pressure at } 32^\circ\text{C})$$

$$SpG = .879 \quad (\text{at } 20^\circ\text{C})$$

$$V_m = \frac{M}{d} = \frac{78.11}{.93} = 84.0$$

$$SpG = .93 \quad (\text{at } P_1 = .0451 \text{ psia}) \\ .00311 \text{ atm})$$

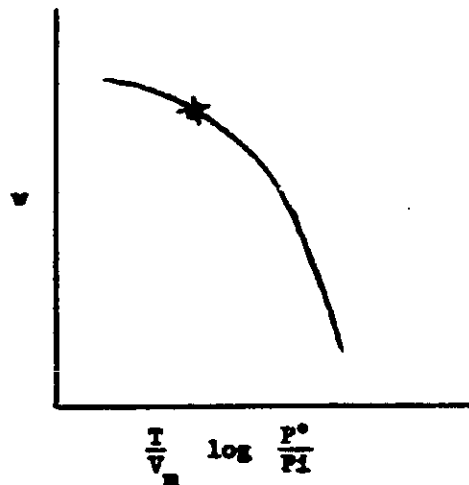
$$\frac{T}{V_m} \log_{10} \frac{P^\circ}{P_1} = \left(\frac{305}{84.0}\right) \log \frac{2.64}{.0457} = 6.40 \quad \left\{ \begin{array}{l} \text{Adsorption} \\ \text{Potential Parameter} \end{array} \right.$$

$$w = 25 \text{ gms } C_6H_6 / 100 \text{ gm carbon}$$

$$w = \frac{.25}{.89} = .281 \frac{\text{cm}^3 \text{ liquid}}{\text{gm carbon}}$$

$\left\{ \begin{array}{l} C_6H_6 \text{ loading} \\ \text{on BPL } (4 \times 10) \\ \text{activated carbon.} \end{array} \right.$

If this point is plotted on the Sulfur Family Polanyi correlation it falls on the curve drawn through the sulfur compound data.



EQUILIBRIUM FRONT CALCULATIONS

Breakthrough time	$\theta_0 = 24 \text{ hours}$
Total Molal Flow Rate	$W_T = 4500 \text{ lbs/hr.}$
Total Volumetric Flow Rate	$Q = 74.27 \text{ ft}^3/\text{sec.}$
Density of Adsorbent (lb/ft ³)	C_b
Molecular Weight of Contaminant Species (lb/mol)	M_i
Mole Fraction of Contaminant in Gas (mol/mol)	Y_i
Mass Rate of Contaminant (lbs/mol)	$R_{i1} = Y_i W_T M_i$
Pickup of Contaminant at Breakthrough (lbs)	$M_i \theta_0$
Equilibrium Loading of Contaminant (lb/lb carbon)	W_i
Carbon Requirement for Contaminant - Mass (lb)	$C_{vi} = M_i \theta_0 / W_i$
Carbon Requirement for Contaminant - Volume (ft ³)	$C_{vi} = C_{mi} / C_b$
Length of Equivalent Equilibrium Section (ft)	$(LES)_i = C_{vi} / S$

Cross sectional area S based on superficial velocity V chosen

For preliminary purposes
take $v = .22 \frac{\text{ft}}{\text{sec}}$

$$S = \frac{Q}{v} = \frac{74.27}{.22} = 337 \text{ ft}^2$$

Diameter if three vessels
operate in parallel

$$D = \left(\frac{S/3}{\pi/4} \right)^{1/2} = 12.0 \text{ ft.}$$

Total Length of Bed

$$L_0 = \sum_{i=1}^{i=N} (LES)_i + (LUB)_{i=N}$$

$$L_0 = \sum_{i=1}^{i=N} \left(\frac{Y_i W_T M_i \theta_0}{W_i C_b S} \right) + \frac{(LUB)_{i=N}}{2}$$

CASE I - Removal of all five sulfur compounds by Physical Adsorption with virgin unimpregnated BPL carbon (4 x 10 mesh)

$M_T = 45000 \text{ mols/Hr.}$

$\theta_b = 24 \text{ hr.}$

$C_b = 33 \text{ lb/ft}^3$

@ $v = 0.22 \frac{\text{ft}}{\text{sec}}$

$S = 337 \text{ ft}^2$

Three vessels in parallel
Diameter = 12.0 ft.

(@ $v = .165 \frac{\text{ft}}{\text{sec}}$)

$S = 450 \text{ ft}^2$

Four vessels in parallel
Diameter = 12.0 ft.

	Contaminant		M_1 $Y_1 M_T M_1$ (lbs/hr)	Pickup $\theta_b M_1$ (lbs)	Loading W_1 (lb/lb carbon)	Carbon Requirement		LES C_b/S (ft)
	Conc. Level (ppm)	Y_1				C_m $\theta_b M_1 / W_1$ (lbs)	C_v C_m / C_v (ft ³)	
C_4H_4S	45	.000045	170.4	4089	.305	13405	405	1.2 (.9)
CS_2	12	.000012	41.1	987	.100	9870	305	.9 (.7)
CH_3SH	25	.000025	54.1	1299	.034	38200	1160	3.4 (2.6)
COS	80	.000080	216.3	5191	.025	207600	6290	18.7 (14.0)
H_2S	25	.000025	38.3	920	.002	460080	13940	41.4 (31.0)

(LES) = 65.6 (49.2)

(LUB) H_2S - Determined from calculation of Breakthrough Curve for H_2S

(LUB) = 6.3 (4.8)
 H_2S

$L_o = 71.9 (54.0)$

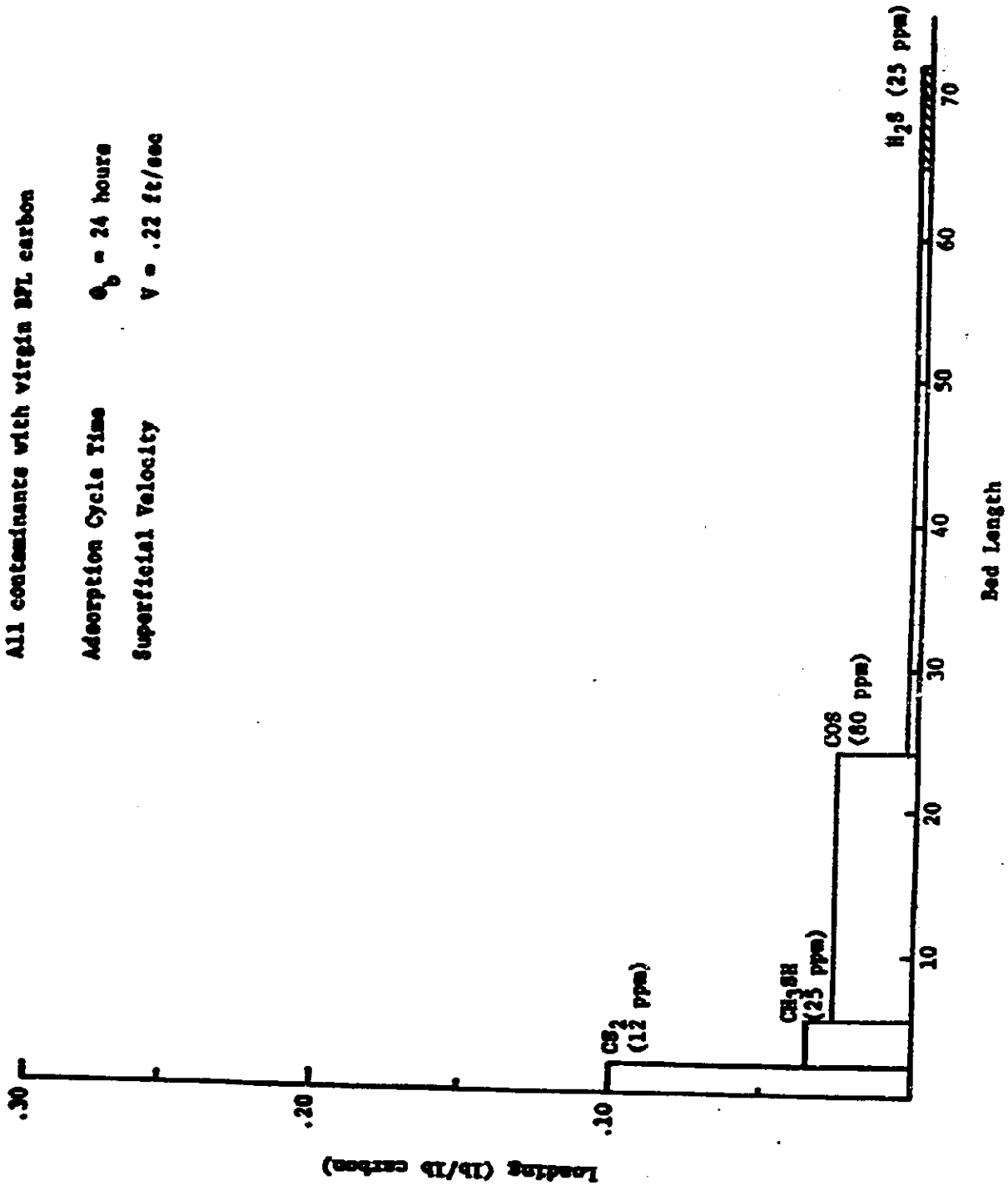
$v = .22 \frac{\text{ft}}{\text{sec}}$ $v = .165 \frac{\text{ft}}{\text{sec}}$

CASE I - PHYSICAL ADSORPTION

All contaminants with virgin BPL carbon

Adsorption Cycle Time $t_b = 24$ hours

Superficial Velocity $V = .22$ ft/sec



$$v = .22 \frac{\text{ft.}}{\text{sec}} \text{ (5 * SYNTHANE pilot plant)}$$

$$D = 12.0 \text{ ft.}$$
$$L = 77.0 \text{ ft.}$$



Three Vessels in Parallel - Operating
Three Vessels in Parallel - Regenerating/
Cooling

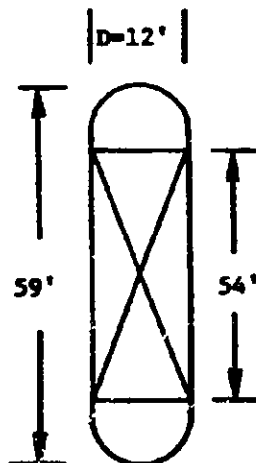
$$\text{Pressure Drop} = .075 \text{ psi/ft (4x10 mesh)}$$

$$\Delta P = .075 (72) = 5.4 \text{ psi}$$

In this case a slightly lower velocity should be used.

$$v = .165 \frac{\text{ft.}}{\text{sec}}$$

$$D = 12.0 \text{ ft.}$$
$$L = 59.0 \text{ ft.}$$



Four Vessels in Parallel - Operating
Four Vessels in Parallel - Regenerating/
Cooling

$$\text{Pressure Drop} = .045 \text{ psi/ft (4x10 mesh)}$$

$$\Delta P = .045 (54) = 2.4 \text{ psi}$$

PROPERTIES OF ACTIVATED CARBON
(Granular Form)

Mesh Size		4 x 10	12 x 30 (estimated)
Particle Density	C_p (lbs/ft ³)	50	
Bulk Density	C_B (lbs/ft ³)	30	33
Effective Diameter	D_p (ft)	.0110	.0027
External Void Fraction	F_e	.40	.39
External Surface	A_v (ft ² /ft ³)	460	725 (.75)(970)
Specific Heat	C_p (Btu/lb°F)		
Pore Diameter	d_p (avg.)	20	

VISCOSITY OF GAS MIXTURE

	Mol.-%	90°F 14.7 psia M (cp)	90°F 1000 psia M (cp)
CH ₄	35		.013
H ₂	45	.009	(.0099) est.
CO	15	.018	(.0198) est.
	95		M _{ave} = .0126 cp x 2.42 = 0.30 $\frac{\text{lb}}{\text{ft/hr}}$

DIFFUSIVITY OF H₂S IN GAS MIXTURE

$$D_{H_2S} = \frac{.0043 T^{1.5} \sqrt{\frac{1}{M_{H_2S}} + \frac{1}{M_G}}}{P \left(\frac{v_{H_2S}}{1/3} + v_G \right)^{1/3}}$$

$M_{H_2S} = 34.08$
 $M_G = 12.24$
 $T = 32^\circ\text{C} = 305^\circ\text{K}$
 $P = 1014.7 \text{ psia} = 69 \text{ atm}$

Molar volume as a liquid at its boiling point } $v_{H_2S} = \frac{M_{H_2S}}{C_{H_2S}} = \frac{34.08 \left(\frac{\text{gm}}{\text{gm mole}} \right)}{.96 \left(\frac{\text{gm}}{\text{cm}^3} \right)} = 35.5 \frac{\text{cm}^3}{\text{gm mole}}$

$v_G = \frac{M_G}{C_G} = \frac{12.24 \left(\frac{\text{gm}}{\text{gm mole}} \right)}{.42 \left(\frac{\text{gm}}{\text{cm}^3} \right)} = 29.1 \frac{\text{cm}^3}{\text{gm mole}}$

$$D_{H_2S} = \frac{.0043 (305)^{1.5} \left(\frac{1}{34.08} + \frac{1}{12.24} \right)^{1/2}}{(69) (35.3^{1/3} + 29.1^{1/3})^2} = .00273 \frac{\text{cm}^2}{\text{sec}}$$

$$D_{H_2S} = .00273 \left(\frac{\text{cm}^2}{\text{sec}} \right) \frac{3600 \left(\frac{\text{sec}}{\text{hour}} \right)}{(30.48)^2 \left(\frac{\text{cm}}{\text{sec}} \right)^2} = .0106 \frac{\text{ft}^2}{\text{hr}}$$

BREAKTHROUGH PROFILE FOR H₂S - 4 x 10 MESH CARBON

T = 90°F	C = 2.06 lb/ft ³	C _b = 33 lb/ft ³
P = 1014.7 psia	μ = .030 lb/ft-hr	D _p = .0110 ft
V = .22 $\frac{\text{ft}}{\text{sec}}$	D _{H₂S} = .0106 $\frac{\text{ft}^2}{\text{hr}}$	a _o = 460 ft ² /ft ³

$N_{Re} = \frac{D_p G}{\mu} = \frac{.0110 (1632)}{.030} = 598$	G = VC
	G = (.22)(2.06)(3600)
	G = 1632 lb/hr-ft ²

T_D = .03 for 4 x 10 mesh

$N_{Sc} = \frac{\mu}{CD} = \frac{.030}{2.06 (.0106)} = 1.37$

$a = \frac{a_o T_D}{(H_{SC})^{2/3}} = \frac{460 (.03)}{(1.37)^{2/3}} = 11.2$

Slope of linear isotherm:

C = Y*/w

$C = \frac{6.97 (10^{-5})}{.002} = .035$

$b = \frac{acG}{C_b}$

$b = \frac{11.2 (.035) (1632)}{33} = 19.3$

Loading

w = .002 lb/lb carbon

Equilibrium
Gas Conc
(25 ppm)

$Y^* = \frac{PIM_1}{PM_G}$

$Y^* = \frac{.0254 (34.08)}{1014.7 (12.24)} = 6.97 (10^{-5})$

BREAKTHROUGH PROFILE - H₂S (25 ppm)

a = 11.2

	$\left(\frac{Y_{out}}{Y_{in}}\right)$	b0 z=41.4 az=464	0 b=19.3 (hr)	$\frac{Y_{act}}{Y_{in}}$	b0 Z=47.7 AZ=534	0 b=19.3 (hr)
O _b	.01	390	20.21	.01	470	24.30
	.10	420	21.76	.10	510	26.42
O _s	.50	460	23.83	.50	540	27.98
	.90	495	25.65	.90	600	31.09

$$LUB = L_o \left(\frac{O_s - O_b}{O_s} \right)$$

$$= 41.4 \left(\frac{23.83 - 20.21}{23.83} \right)$$

$$= 41.4 (.152)$$

LUB = 6.3 ft.

$$LES = 41.4 \left(\begin{array}{l} \text{Used this value} \\ \text{as initial estimate} \\ \text{of Z} \end{array} \right)$$

L_o = 47.7 ft.

$$LUB = L_o \left(\frac{O_s - O_b}{O_s} \right)$$

$$= 47.7 \left(\frac{27.98 - 24.30}{27.98} \right)$$

$$= 47.7 (.132)$$

LUB = 6.3 ft.

LES = 41.4

L_o = 47.7 ft.

$$\left. \begin{array}{l} \text{Superficial} \\ \text{Velocity} \end{array} \right\} v = .22 \frac{\text{ft.}}{\text{sec}}$$

$$\left. \begin{array}{l} \text{Front} \\ \text{Velocity} \end{array} \right\} U = \frac{L_o}{O_s}$$

$$U = \frac{47.7}{27.98} \frac{1}{3600}$$

$$U = .00047 \text{ ft/sec}$$

CASE II - CHEMISCRPTION - H₂S removal $w' = .04$ lb/lb carbon
(Loading value from development program)

PHYSICAL ADSORPTION - COS, CH₃SH, CS₂, C₄H₄S removal
(Equilibrium loadings of BPL derated)
 $10' = .90$ (co)

$ri_1 = 45000$ mols/hr

$\theta_b = 24$ hr.

$C_b = 33$ lb/ft³

@ V = 0.22 ft/sec

S = 337 ft²

(Three vessels in Parallel)
Diameter = 12.0 ft.

	Contaminant Conc. Level (ppm)	Y ₁	M ₁ Y ₁ N ₁ M ₁ (lbs/hr)	Pickup $\theta_b M_1$ (lbs)	Loading W ₁ (lb/lb carbon)	Carbon Requirement		
						C _m $\theta_b M_1 / W_1$ (lbs)	C _v C _m /C _v (ft ³)	LES C _v /S (ft)
2 ^S	25	.000025	38.3	920	.040	23000	697	2.1
4 ^{H₄S}	45	.000045	170.4	4089	.2745	14895	451	1.3
2	12	.000012	41.1	987	.090	10960	332	1.0
3 ^{SH}	25	.000025	54.1	1299	.0306	42440	1286	3.8
10	80 (10)	.000080 (.000010)	216.3 (27.0)	5191 (649)	.0225 (.00702)	230670 (92415)	6990 (2800)	20.8 (8.3)

Σ (LES) = 26.9 (14.4)

(LUB)_{cos} - Determined from calculation of
Breakthrough Curve for COS

(LUB)_{cos} = 5.6 (2.6)

L_o = 32.5 (17.0)

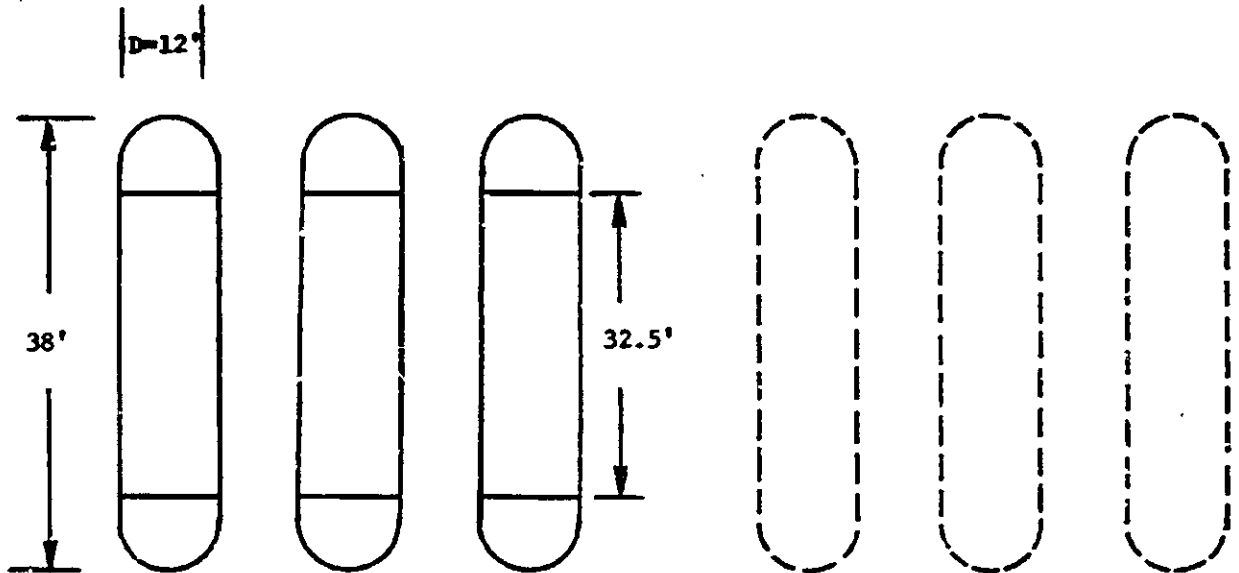
COS 80 ppm 10
ppm

Three Vessels in Parallel - Operating

(D = 12.0 ft.)

Three Vessels in Parallel - Regenerating/Cooling

(L = 38.0 ft.)



Pressure Drop = $.075 \frac{\text{psi}}{\text{ft bed}}$ for 4 x 10 mesh carbon

$$\Delta P = .075 (32.5) = 2.4 \text{ psi}$$

The above is for a COS level of 80 ppm.

For a COS level of 10 ppm

Vessel Dimensions would be D = 12.0 ft

L = 22.0 ft

$$\Delta P = .075 (17.0) = 1.3 \text{ psi}$$

DIFFUSIVITY OF COS IN GAS MIXTURE

$$D_{\text{COS}} = \frac{.0043 T^{1.5} \sqrt{\frac{1}{M_{\text{COS}}} + \frac{1}{M_{\text{G}}}}}{P (V_{\text{COS}}^{1/3} + V_{\text{G}}^{1/3})^2}$$

T = 32°C = 305°K

M_{COS} = 60.07

P = 1014.7 psia = 69 atm

M_G = 12.24

$$V_{\text{COS}} = \frac{M_{\text{COS}}}{CL_{\text{COS}}} = \frac{60.07}{1.17} = 51.3 \frac{\text{cm}^3}{\text{gm mol}}$$

Molar Volume as
a liquid at its
boiling point

$$V_{\text{G}} = \frac{M_{\text{G}}}{CL_{\text{G}}} = \frac{12.24}{.42} = 29.1$$

$$D_{\text{COS}} = \frac{.0043 (305)^{1.5} \left(\frac{1}{60.07} + \frac{1}{12.24} \right)^{1/2}}{(60) (51.3^{1/3} + 29.1^{1/3})^2} = .00226 \frac{\text{cm}^2}{\text{sec}}$$

$$D_{\text{COS}} = .0022 \left(\frac{\text{cm}^2}{\text{sec}} \right) \frac{3600 \left(\frac{\text{sec}}{\text{hr}} \right)}{30.48^2 \left(\frac{\text{cm}}{\text{ft}} \right)^2} = .00874 \frac{\text{ft}^2}{\text{hr}}$$

BREAKTHROUGH PROFILE FOR COS - 4 x 10 MESH

$$\begin{aligned} T &= 90^\circ\text{F} & C &= 2.06 \text{ lb/ft}^3 & C_b &= 33 \text{ lb/ft}^3 \\ P &= 1014.7 \text{ psia} & M &= .030 \text{ lb/ft-hr.} & D_p &= .0110 \text{ ft} \\ v &= .22 \text{ ft/sec.} & D_{\text{COS}} &= .00874 \frac{\text{ft}^3}{\text{hr}} & a_o &= 460 \text{ ft}^2/\text{ft}^3 \\ H_{\text{Re}} &= \frac{D_p G}{\mu} = \frac{.0110 (1632)}{.030} = 598 & G &= v_e \\ & & G &= (.22)(2.06)(3600) \\ & & G &= 1632 \text{ lb/hr-ft}^2 \\ & & \text{TD} &= .030 \text{ for } 4 \times 10 \text{ mesh} \\ H_{\text{SC}} &= \frac{\mu}{CD} = \frac{.03}{2.06 (.00874)} = .168 \\ a &= \frac{av \text{ TD}}{(H_{\text{SC}})^{2/3}} = \frac{460 (.03)}{(1.68)^{2/3}} = 9.75 \end{aligned}$$

Slope of linear isotherm:

$$\begin{aligned} c &= \frac{Y^*}{w'} & \text{Loading} & & w' &= .0225 \text{ lb/lb carbon} \\ c &= \frac{3.93 (10^{-4})}{.0225} = .0175 & \text{Equilibrium} & & & \\ & & \text{Gas Conc.} & & & \\ & & (80 \text{ ppm}) & & & \\ b &= \frac{acG}{C_b} \\ b &= \frac{9.75 (.0175)(1632)}{33} = 8.44 \end{aligned}$$

BREAKTHROUGH PROFILE - COS (80 FT)

$a = 9.75$

	$\frac{Y_{out}}{Y_{in}}$	b_0 $s=20.8$ $a_s=203$	Q $b=3.44$ (hr)	$\frac{Y_{out}}{Y_{in}}$	b_0 $s=25.8$ $a_s=252$	Q $b=3.44$
Q_b	.01	160	18.96		200	23.70
	.10	175			220	26.06
Q_s	.50	210	24.88		255	30.21
	.90				285	33.77

$$LUB = L_0 \left(\frac{Q_s - Q_b}{Q_s} \right)$$

$$= 20.8 \left(\frac{24.88 - 18.96}{24.88} \right)$$

$$= 20.8 (.238)$$

$$LUB = 5.0 \text{ ft.}$$

$$LES = 20.8 \text{ ft.} \quad (\text{used this value as initial estimate of } Z)$$

$$L_0 = 25.8 \text{ ft.}$$

$$LUB = L_0 \left(\frac{Q_s - Q_b}{Q_s} \right)$$

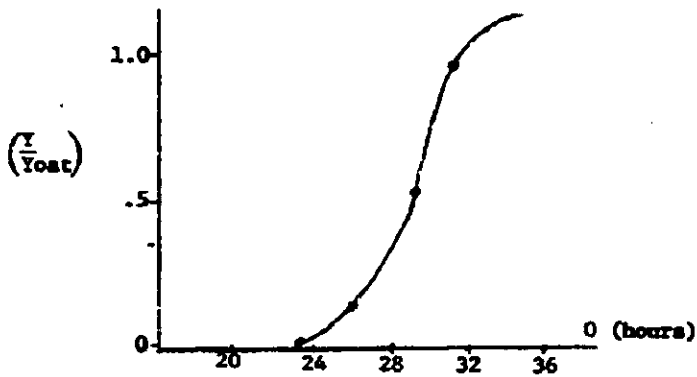
$$= 25.8 \left(\frac{30.21 - 23.70}{30.21} \right)$$

$$= 25.8 (.216)$$

$$LUB = 5.6 \text{ ft.}$$

$$LES = 20.8 \text{ ft.}$$

$$L_0 = 26.4 \text{ ft.}$$



$$\left. \begin{array}{l} \text{Superficial Velocity } \} \\ \text{Front Velocity } \} \end{array} \right\} V = .22 \text{ ft/sec.}$$

$$U = \frac{L_0}{Q_s}$$

$$U = \frac{26.4}{30.21} \frac{1}{3600}$$

$$U = .00024 \text{ ft/sec}$$

USE III - CHEMISORPTION - H₂S removal $w' = .04$ lb/lb. carbon.
(loading value from development program)

PHYSICAL ADSORPTION - CH₃SH, CS₂, C₄H₄S removal (Equilibrium loadings of BPL derated 10%) $w' = .90(10)$

$Q_T = 45000$ mols/hr.

$Q_L = 24$ hr.

$C_b = 33$ lb/ft³

$v = .22$ ft/sec

$S = 337$ ft²

Three Vessels in Parallel
Diameter = 12.0 ft.

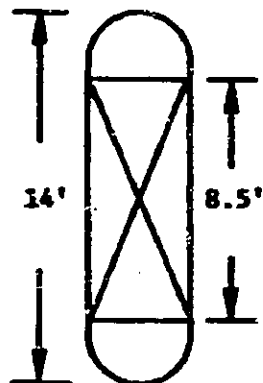
(@ $v = .33$ ft/sec. $S = 225$ ft²)
Two vessels in parallel $D = 12.0$ ft.

	Contaminant		M_1 $Y_1 K_r M_1$ (lbs/hr)	Pickup $G_p M_1$ (lbs)	Loading W_1 (lb/lb carbon)	Carbon Requirement		LES C_v/S (ft)	
	Conc. Level (ppm)	Y_c				C_m $G_p M_1/W_1$ (lbs)	C_v C_m/C_v (ft ³)		
H ₂ S	25	.000025	38.3	920	.040	23000	697	2.1	(3.1)
$\frac{1}{2}$ H ₂ S	45	.000045	170.4	4989	.2745	14895	451	1.3	(2.0)
CS ₂	12	.000012	41.4	987	.090	10960	332	1.0	(1.5)
CH ₃ SH	25	.000025	54.1	1299	.0306	42440	1286	3.8	(5.7)
								Σ (LES) = 6.1	(9.2)
								(LUB) = 2.2	(2.8)
								CH ₃ SH	—
								Lo = 8.3	(12.0)
								$v = .22$ $\frac{ft}{sec}$	$v = .33$ $\frac{ft}{sec}$

$v = .22 \frac{\text{ft}}{\text{sec}}$ (3rd STREAM pilot plant)

D = 12.0 ft.
L = 14.0 ft.

| D=12' |



Three Vessels in Parallel - Operating
Three Vessels in Parallel - Regenerating/
Cooling

Pressure Drop = .075 psi/ft (4x10 mesh)

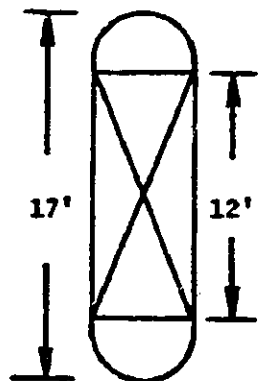
$\Delta P = .075 (8.5) = .64 \text{ psi}$

In this case a higher velocity can be used

$v = .33 \frac{\text{ft}}{\text{sec}}$

D = 12.0 ft.
L = 17.0 ft.

| D=12' |



Two Vessels in Parallel - Operating
Two Vessels in Parallel - Regenerating/
Cooling

Pressure Drop = .16 psi/ft (4x10 mesh)

$\Delta P = .16 (12) = 1.9 \text{ psi}$

DIFFUSIVITY OF CH₃SH IN GAS MIXTURE

$$D_{\text{CH}_3\text{SH}} = \frac{.0043 T^{1.5} \sqrt{\frac{1}{M_{\text{CH}_3\text{SH}}} + \frac{1}{M_G}}}{P (V_{\text{CH}_3\text{SH}}^{1/3} + V_G^{1/3})^2}$$

T = 32°C = 305°K

M_{CH₃SH} = 48.10

P = 1014.7 psia = 69 atm

M_G = 12.24

$$V_{\text{CH}_3\text{SH}} = \frac{M_{\text{CH}_3\text{SH}}}{CL_{\text{CH}_3\text{SH}}} = \frac{48.10}{.885} = 54.4$$

$$V_G = \frac{M_G}{CL_G} = \frac{12.24}{.42} = 29.1$$

$$D_{\text{CH}_3\text{SH}} = \frac{.0043 (305)^{1.5} \left(\frac{1}{48.10} + \frac{1}{12.24} \right)^{1/2}}{(69) (54.4^{1/3} + 29.1^{1/3})^2} = .00226 \frac{\text{cm}^2}{\text{sec}}$$

$$D_{\text{CH}_3\text{SH}} = .00226 \left(\frac{\text{cm}^2}{\text{sec}} \right) \frac{3600 \left(\frac{\text{sec}}{\text{hr}} \right)}{30.48^2 \left(\frac{\text{cm}}{\text{ft}} \right)^2} = .00874 \frac{\text{ft}^2}{\text{hr}}$$