Column operates adiabatically, and constant molal overflow assumption is acceptable.

The average molecular weight of the gas can be taken as that of biphenyl or $C_6H_5 \cdot C_6H_5 = 154.2$.

The average specific gravity of the liquid in the column is 0.72.

The tray spacing is 24 in. with a 2-in. slot liquid seal.

Assume the surface tension of the liquid is 20 dyne/cm.

Size and cost the column, using an 85 percent safety factor on the maximum allowable vapor velocity.

Problem 13. Design of Reactor for Coal Conversion to Nonpolluting Fuel Oil (Plus Partial Solution)[†]

A plant is being designed to produce low-sulfur oil from coal under the conditions outlined below. A major concern in the design is to minimize the volume of the reactor, and you are to carry out some preliminary studies for the reactor system. Specifically, you are to determine the total volume of the reactor if it is operated isothermally at 800°F for the case of a single, ideal, plug-flow reactor operation and for the case of a single, back-mix (continuous stirred-tank reactor) reactor system with the conditions and assumptions as outlined in the following.

Operating Conditions Plant is to produce 50,000 bbl/day (based on 60°F) of low-sulfur oil (0.4 weight percent sulfur) from coal. Table C-16 gives the specifications for the coal feed and the product oil.

Coal in the slurry is 35 percent by weight with the balance being recycled oil of the same composition as the product oil.

A nickel-molybdenum on alumina catalyst in the form of $\frac{1}{8}$-in. spheres is used with a desulfurization activity A_s of 1.25 and a bulk density of 42.0 lb/ft^3.

The following assumptions apply for the reactor system:

Pressure of 2500 psia and negligible pressure drop across the reactor.

25,000 ft^3 of gas at SC (SC = 60°F and 1 atm) flows to the reactor per barrel of slurry feed (based on 60°F).

The gas to the reactor contains 85 percent hydrogen; the other 15 percent is methane with negligible H_2S content.

Yield of product is 4.2 bbl of product oil (at 60°F) per ton of coal (as received).

Average molecular weight of fuel oil is 301.

No hydrogen, methane, or hydrogen sulfide is dissolved in the slurry.

Necessary heating and cooling units are available so reactors can be assumed to operate isothermally at 800°F.

Partial pressure of hydrogen for plug-flow reactor can be assumed as constant at the arithmetic average of entrance and exit pressures.

[†] Adapted from 1976 AIChE Student Contest Problem.

Table C-16

Coal feed		Oil product	
Bulk density, lb/ft^3 = 45.0		4.4° API = density of 64.97 lb/ft^3 at 60°F Density = 44.8 lb/ft^3 at 800°F	
[†]Proximate analysis, weight percent		Boiling distribution: true boiling point cut, weight percent	
Moisture	1.5	C_5, 400°F	8.1
Ash	10.3	400–650°F	32.1
Volatile matter	35.5	650–975°F	22.1
Fixed carbon	52.7	975°F+	37.7
Total	100.0	Total	100.0
[†]Ultimate analysis, weight percent		Ultimate analysis, weight percent	
Carbon	70.2	Carbon	90.2
Hydrogen	4.6	Hydrogen	8.5
Nitrogen	1.0	Nitrogen	0.8
Sulfur	3.6	Sulfur	0.4
Oxygen	10.5	Oxygen	—
Ash	10.1	Ash	0.1
Total	100.0	Total	100.0

[†] See *Perry's Chemical Engineers' Handbook* for discussion of these and other methods of analysis (6th ed., p. 9-4). Proximate and ultimate analyses in this case were carried out with air-dried coal samples; so the oxygen and hydrogen in the "moisture" reported in the proximate analysis are included in the ultimate analysis.

Assume the term $1 + K_{HS}\bar{p}_{HS}$ in the rate equation stays constant for the plug-flow reactor at the arithmetic average of the entering and exit values.

Assume negligible volume change during the reaction so that $C_s = C_{s_o}(1 - X_s)$.

Of the fuel oil passing through the reactor, 15 weight percent is vaporized in the reactor section, and this can be doubled to 30 percent on a molal basis considering different volatilities of the components.

The carbon in the coal that is lost to the gas stream is converted to CH_4, C_2H_6, C_3H_8, and C_4H_{10} in equal-volume amounts so that the average carbon/hydrogen ratio of the resultant gas is 0.35714 on a mol basis considering hydrogen as being 1.008 lb/lb mol of hydrogen.

All the nitrogen in the coal that is lost is converted to gaseous NH_3.

All the sulfur in the coal that reacts goes to H_2S.

Reactor sizing will be based on the rate equation for the desulfurization reaction

$$-r_s = k_s A_s \frac{C_s^2 \bar{p}_H}{C_{S_o}(1 + K_{HS}\bar{p}_{HS})}$$

where

$-r_s$ = rate of sulfur removal, lb mol/h·lb catalyst

k_s = reaction rate constant, ft^3/h·lb cat·psia

$k_s = \exp(14.76 - 55.000/RT) = 7.405 \times 10^{-4}$ at 800°F

K_{HS} = adsorption constant for H_2S inhibition (psia)$^{-1}$

$= 0.10 \exp(1200/RT) = 0.162$ at 800°F

R = 1.987 Btu/lb mol·°R
T = temperature, °R
A_s = desulfurization activity
C_s = sulfur concentration in slurry, lb mol/ft^3
$\bar{p}_H$ = hydrogen partial pressure, psia
$\bar{p}_{HS}$ = hydrogen sulfide partial pressure, psia

The reactor performance equations are as follows:

For plug-flow

$$\frac{W}{Q} = C_{s_o} \int_{X_{s_i}}^{X_{s_f}} \frac{dX_s}{-r_s}$$

For back-mix (CSTR)

$$\frac{W}{Q} = C_{s_o} \frac{X_{s_f} - X_{s_i}}{-r_s}$$

where

W = catalyst charge, lb
X_s = fractional conversion of sulfur
C_{s_o} = concentration of sulfur in slurry feed to reactor, lb mol/ft^3
Q = volumetric feed rate of slurry, ft^3/h
i = inlet value
f = final value

Suggestions Base material balances on 1 ton (2000 lb) of coal as received. Integrate rate expression for plug flow analytically (not graphically or by approximations). See information as provided for initial part of solution presenting necessary material balances for the conditions given for this problem, and understand what was done.

Problem 13. Partial Solution

Figure C-1 shows the first part of the solution to Problem 13 dealing with the design of a reactor for coal conversion to nonpolluting fuel oil.

Material Balances Choose as basis 1 ton of coal as received (2000 lb) to produce 4.2 bbl of product oil at 60°F

$$\text{Fuel produced} = 4.2\ \text{bbl}\left(42\,\frac{\text{gal}}{\text{bbl}}\right)\left(\frac{1}{7.48}\,\frac{\text{ft}^3}{\text{gal}}\right)\left(64.97\,\frac{\text{lb}}{\text{ft}^3}\right) = 1532\,\frac{\text{lb prod. oil}}{\text{ton coal}}$$

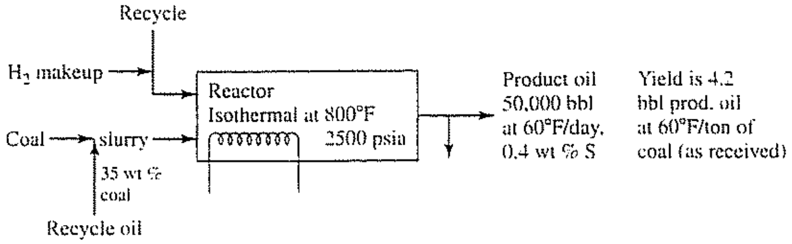

Figure C-1

Table C-17 Material balance, overall—2000 lb coal

Component	Feed		Prod. oil		Difference, lb	
	wt %	lb	wt %	lb		
C	70.2	1404	90.2	1381.95	22.05	
H	4.6	92	8.5	130.23	−38.23	gain in H
N	1.0	20	0.8	12.26	7.74	
S	3.6	72	0.4	6.13	68.87	
O	10.5	210	—	—	—	
Ash	10.1	202	0.1	1.53	200.47	
Total	100	2000	100	1532.1		

Hydrogen Material Balance 22.05 lb of C in coal is burned to CH_4, C_2H_6, C_3H_8, or C_4H_{10} as 0.35714 mol C per mol H.

$$\text{Hydrogen used to burn C} = \left(\frac{22.05}{12.011}\,\text{mol C}\right)\left(\frac{1}{0.35714}\,\frac{\text{mol H}}{\text{mol C}}\right)\left(1.008\,\frac{\text{lb H}}{\text{mol H}}\right)$$

$$= 5.19\ \text{lb H}$$

$$\text{Hydrogen used to make } NH_3 = \left(\frac{7.74}{14.007}\,\text{mol N}\right)\left(3\,\frac{\text{mol H}}{\text{mol N}}\right)\left(1.008\,\frac{\text{lb H}}{\text{mol H}}\right)$$

$$= 1.67\ \text{lb H}$$

$$\text{Hydrogen used to make } H_2S = \left(\frac{65.87}{32.064}\,\text{mol S}\right)\left(2\,\frac{\text{mol H}}{\text{mol S}}\right)\left(1.008\,\frac{\text{lb H}}{\text{mol H}}\right)$$

$$= 4.14\ \text{lb H}$$

$$\text{Hydrogen used to make } H_2O = \left(\frac{210}{16}\,\text{mol O}\right)\left(2\,\frac{\text{mol H}}{\text{mol O}}\right)\left(1.008\,\frac{\text{lb H}}{\text{mol H}}\right)$$

$$= 26.46\ \text{lb H}$$

$$\text{Hydrogen gain} = 38.23\ \text{lb}$$

$$\text{Total H used} = 75.69\ \text{lb H}$$

$$\frac{75.65}{2.016} = 37.544\ \text{lb mol } H_2$$

Material Balance, at Reactor Inlet, for Slurry Concentration Basis—2000 lb Coal. For slurry, 35 wt % is coal and 65 wt % is oil.

$$(2000\ \text{lb coal})\left(\frac{0.65\ \text{lb oil}}{0.35\ \text{lb coal}}\right) = 3714\ \text{lb of recycle oil}$$

$$= \frac{3714\ \text{lb}}{44.8\ \text{lb/ft}^3\ \text{at}\ 800^\circ\text{F}}$$

$$= 82.9\ \text{ft}^3\ \text{oil at}\ 800^\circ\text{F}/2000\ \text{lb coal}$$

$$\text{Volume of coal} = 2000\ \text{lb}/(45\ \text{lb/ft}^3) = 44.44\ \text{ft}^3$$

Total volume of slurry to reactor

$$= 82.9 + 44.44 = 127.34 \text{ ft}^3/2000 \text{ lb of coal fed}$$

Sulfur content of fuel oil in slurry

$$= (3714)(0.004) = 14.856 \text{ lb S}$$

Sulfur content of coal in slurry

$$= (2000)(0.036) = 72.00 \text{ lb S}$$

$$\text{Total} = 86.86 = \frac{86.86}{32.066} = 2.709 \text{ lb mol S}$$

Concentration of sulfur entering reactor in slurry

$$= C_{s_o} = \frac{2.709}{127.34} = 0.0213 \text{ lb mol/ft}^3$$

At Reactor Outlet

$$\text{Oil} = \overset{\text{Recycl.}}{3714} + \overset{\text{Prod.}}{1532} = 5246 \text{ lb} = \frac{5246 \text{ lb}}{44.8 \text{ lb/ft}^3} = 117.1 \text{ft}^3 \text{at } 800°\text{F}$$

$$\text{Sulfur in outlet oil} = (5246)(0.004) = 20.98 \text{ lb} = \frac{20.98}{32.066} = 0.65444 \text{ lb mol}$$

Concentration of sulfur in oil leaving reactor

$$= C_{s_f} = \frac{0.65444}{117.1} = 0.00559 \text{ lb mol/ft}^3$$

$$X_{S_f} = 1 - \frac{C_{S_f}}{C_{S_o}} = 1 - \frac{0.00559}{0.0213} = 0.738 \cong 0.74$$

$$X_{S_f} = \frac{C_{S_o} - C_{S_f}}{C_{S_o}} \qquad \text{assuming constant fluid volumetric flow rate}$$

Material Balance for Gas at Entrance and Exit of Reactor Basis—2000 lb Coal. 25,000 SCF of gas/bbl of slurry at 60°C is given as the condition

$$\text{Bbl of slurry at } 60°\text{F/2000 lb coal} = \left(\overset{\text{ft}^3 \text{ coal}}{\frac{2000}{45}} + \overset{\text{ft}^3 \text{ oil at } 60°\text{F}}{\frac{3714}{64.97}}\right)\left(7.48\frac{\text{gal}}{\text{ft}^3}\right)\left(\frac{1 \text{ bbl}}{42 \text{ gal}}\right)$$

$$= 18.1 \text{ bbl/2000 lb coal}$$

$$\text{Gas to reactor} = (25,000)(18.1) = 452,450 \text{ SCF of gas/2000 lb coal}$$

Gas is 85% H_2; so

$$(0.85)(452{,}450) = 384{,}583\ \text{SCF } H_2/2000\ \text{lb coal.}$$

$$\frac{359(520)}{492} = 380\ \text{ft}^3/\text{mol at SC of } 60°\text{F and 1 atm}$$

$$\frac{384{,}583}{380} = 1014\ \text{lb mol } H_2/2000\ \text{lb coal}$$

Gas is 15% CH_4; so

$$452{,}450\left(\frac{0.15}{380}\right) = 179\ \text{lb mol } CH_4/2000\ \text{lb coal}$$

$$\text{Total} = 1193\ \text{lb mol } (H_2 + CH_4)/2000\ \text{lb coal}$$

$$p_H \text{ at entrance to reactor} = \frac{1014}{1193}(2500) = 2125\ \text{psia}$$

$$p_H \text{ at entrance} = 0\ \text{(given)}$$

Material Balance, Gas at Exit of Reactor Basis—2000 lb Coal. Amount of fuel oil entering reactor is 3714 lb, or

$$\frac{3714}{\text{avg mol wt } 301} = 12.34\ \text{lb mol}/2000\ \text{lb coal}$$

Fuel oil is 15 wt % or 30 mol % vaporized; so 12.34(0.30) = 3.7 mols of fuel oil are vaporized in reactor, leaving 8.64 mols of fuel oil in liquid and 3.7 mols of fuel oil in gas at reactor exit.

Assume no mols of H_2 or CH_4 or NH_3 or H_2S are dissolved in the liquid.

$$\text{Total mols of } H_2 \text{ in gas at exit} = 1014 - \underset{\text{used in reactor}}{37.544} = 976.5\ \text{lb mols}$$

$$\text{Total mols of } H_2O \text{ in gas at exit} = \frac{26.46}{2.016} = 13.1\ \text{lb mols}$$

$$\text{Total mols of } NH_3 \text{ in gas at exit} = \frac{7.74}{14.007} = 0.55\ \text{lb mols}$$

$$\text{Total mols of } H_2S \text{ in gas at exit} = \frac{4.14}{2.016} = 2.06\ \text{lb mols}$$

$$\text{Total mols of } CH_4 \text{ in gas at exit} = \quad = 179.0\ \text{lb mols}$$

$$\text{Total mols of fuel oil in gas at exit} = \quad \underline{3.7}\ \text{lb mols}$$

$$\text{Total exit gas, mols} = \quad 1174.91\ \text{lb mols}/2000\ \text{lb coal}$$

Total entering gas, mols = 1193 lb mols/2000 lb coal

p_H at reactor exit = $\dfrac{976.5}{1174.91}(2500) \cong 2075$ psia

p_{HS} at reactor exit = $\dfrac{2.06}{1174.91}(2500) \cong 4.4$ psia

This completes the major work on material balances needed for solving this problem.

Now proceed, using these results and other information given in the problem, to complete the reactor design analysis requested.

Problem 14. Material Balance for Alkylation Plant Evaluation[†]

The simplified diagram of a catalytic alkylation unit is shown in Figure C-2. In the reactor, butylene and isobutane react to form C_8 "alkylate" according to the following reaction:

$$C_4H_8 + C_4H_{10} \longrightarrow C_8H_{18}$$

The unit is to produce product alkylate at a rate of 1700 m^3/day (10,693 bbl/day).

The yield is 1.72 m^3 alkylate per m^3 butylene consumed; 1.10 m^3 of isobutane are consumed per 1.0 m^3 butylene consumed.

The reactor effluent is to contain 75 volume % isobutane.

It may be assumed that the recycle is pure isobutane and that propane, alkylate, and *n*-butane are completely recovered as pure products in the columns. Propane and *n*-butane do not react.

Under these conditions,

a. How much of each feed stream is required in m^3/day and in bbl/day?

b. How much isobutane must be recycled in m^3/day and in bbl/day?

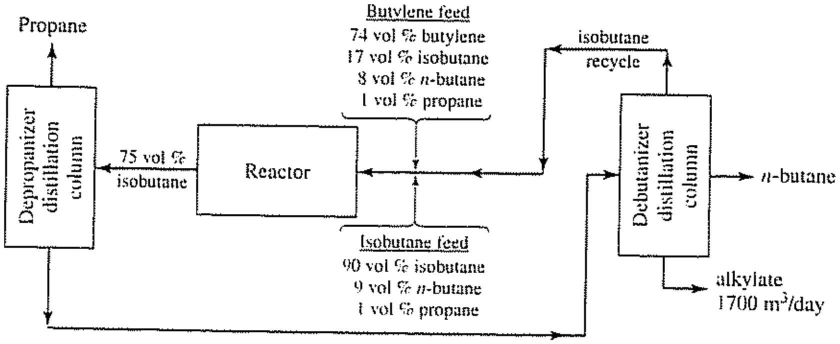

Figure C-2

[†] Adapted from 1977 AIChE Student Contest Problem.