

Title: Thermal Pollution Reduction by Adiabatic Degassing

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Abstract:

The reduction of thermal pollution by means of adiabatic degassing was studied by using a computer simulation of the process. The systems studied were hydrogen sulfide, ammonia, and sulfur dioxide in water. Each system was studied separately as aqueous unsaturated solutions. These systems are characteristic of possible thermal pollution streams, e.g. hydrogen sulfide and ammonia in water are both products of refinery operations as well as municipal sewage treatment plants; the sulfur dioxide in water would arise in power station flue gas scrubbing operations or in smelter flue gas scrubbing operations.

The results indicate that there is a range of gas concentrations for which adiabatic degassing would be an efficient means of reducing thermal pollution, provided there is available a supply of low cost, low pressure steam.

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I. Conclusions

1. Adiabatic degassing is a feasible method for reducing thermal pollution. Simulation of three binary gas-water systems show that a 5°F temperature drop can be achieved under a stipulated set of conditions at an operating cost of less than 0.158¢/gallon solution through the process.
2. For the three binary gas-water systems, the simulation of an adiabatic flash required good experimental vapor-liquid equilibrium data. A comparison of the simulation run using good experimental correlations and estimates using data corresponding to an ideal mixture approximation showed the latter to give a larger value by 30% in the value of the vapor-to-feed ratio. This effect is to show both an increased operating cost and capital equipment cost over what is needed.
3. For the three gases evaluated, e.g. hydrogen sulfide, ammonia and sulfur dioxide, hydrogen sulfide having the greatest solubility shows the least cost per degree of cooling. However this system requires the greatest solute removal because of the fact that hydrogen sulfide is a pollutant exclusive of any consideration of thermal pollution.
4. For systems being cooled less than 5°F (from 90°F to 85°F) vacuum pumps of the Nash Hytor type are competitive with ejectors in terms of operating costs. For greater cooling multistage ejectors are better.
5. Work should continue on the utilization of the sensible heat of thermal polluted water resources for agricultural or municipal

systems. This should be the primary consideration in the engineering analysis of the reduction of thermal pollution. If this is not feasible, then adiabatic degassing offers an alternative for thermal pollution reduction.

II. Recommendations

1. The physical properties of gas compounds dissolved in water need to be correlated and studied further. These properties are presently only available as binary systems. Multicomponent systems are important in thermal pollution as well as industrial and municipal utility processing.
2. The thermodynamic properties of water need to be reduced to a semi-empirical correlation suitable for computer usage. Such a correlation would serve many different engineering design efforts in water using processes, i.e. steam cycle power generation, sewage treatment process analysis, petro-chemical industrial operations, and electrochemical processes.
3. The Office of Water Resources Research should support efforts at developing agricultural and municipal use of thermal polluted water resources. This effort should include an educational effort directed at urban planners. This could be accomplished through preparation of a self-instructional packet supplemented by conferences.
4. The corrosion effects of gas-water systems should be studied. Particular emphasis should be placed on the mechanism of the corrosive action, followed by emphasis on protective coatings for the equipment.

III. Introduction

The Office of Water Resources Research of the U. S. Department of the Interior describes the thermal pollution problem as follows:

"With the expected increase in the number of electric generating plants and the consequent thermal loading of rivers, lakes, and estuaries, increased research attention is needed in physical mixing and thermodynamics of heated discharges; in development of economically competitive alternatives to use of once-through water as a heat-transfer medium; on biologic, ecologic, and environmental impacts; on types and quantities of data required to properly evaluate facility sites and to choose among alternative sites; an adequacy of regulations and procedures for site selection with respect to water use and management; and on possible ways of utilizing the heat for man's advantage." [1]

This statement places emphasis on electric power generating stations. If thermal pollution is considered in the broader definition of 'any increase in the sensible (or latent) heat of a naturally occurring water resource', then there are thermal pollution problems associated with almost all industrial processes. This report considers the broader definition which includes industry but considers only fluid streams. It evaluates one particular process, in detail, for reducing thermal pollution. This process is adiabatic degassing.

The reduction of thermal pollution requires an expenditure of energy unless a use can be found for the sensible heat of the water stream. Currently, there are two principal projects being evaluated for use of waste heat from power generating stations: (1) use for agricultural projects and (2) use within a municipality utility complex. Both projects could also be considered in conjunction with industrial waste heat. The limiting characteristic of the waste heat stream, i.e. an aqueous solution which is being discharged to a natural water resource, is that the temperature of the fluid is usually between 100-125°F. There are very few industrial processes which could use such a low temperature source of

sensible heat. However for agricultural use or for municipal utilities this temperature is sufficient. While this report is not primarily concerned with either use, each will be described because any new process, such as adiabatic degassing needs to be evaluated in terms of what processes are currently available.

A. Agricultural Use of Thermal Pollution

There are four possible uses of the sensible heat of thermal pollution for agricultural purposes. These are:

- (1) direct application of the heated water to the soil for irrigation,
 - (2) direct application of the heated water to agricultural crops by sprinkler systems,
 - (3) indirect application through humidity and temperature control to green-house or animal enclosures,
- and (4) direct application to fish production through fish farming or to algae growth for protein harvesting.

The effect of increasing the environmental temperature under controlled conditions for improving agricultural productivity is shown in Figures 1 and 2. Figure 1 shows the effect of temperature on the growth or production of food animals [2]. Figure 2 shows idealized growth curves for several crops. These figures indicate that positive benefits can be achieved from judicious use of thermal pollution; however with all operations there is the investment of scale and cost of operation which must be considered.

Specifically, it has been experimentally tested that surface irrigation with 100°F water has not resulted in any appreciable increase in crop production [3]. Apparently the ambient conditions in the test area were such that the sensible heat of the water was reduced through evaporation.

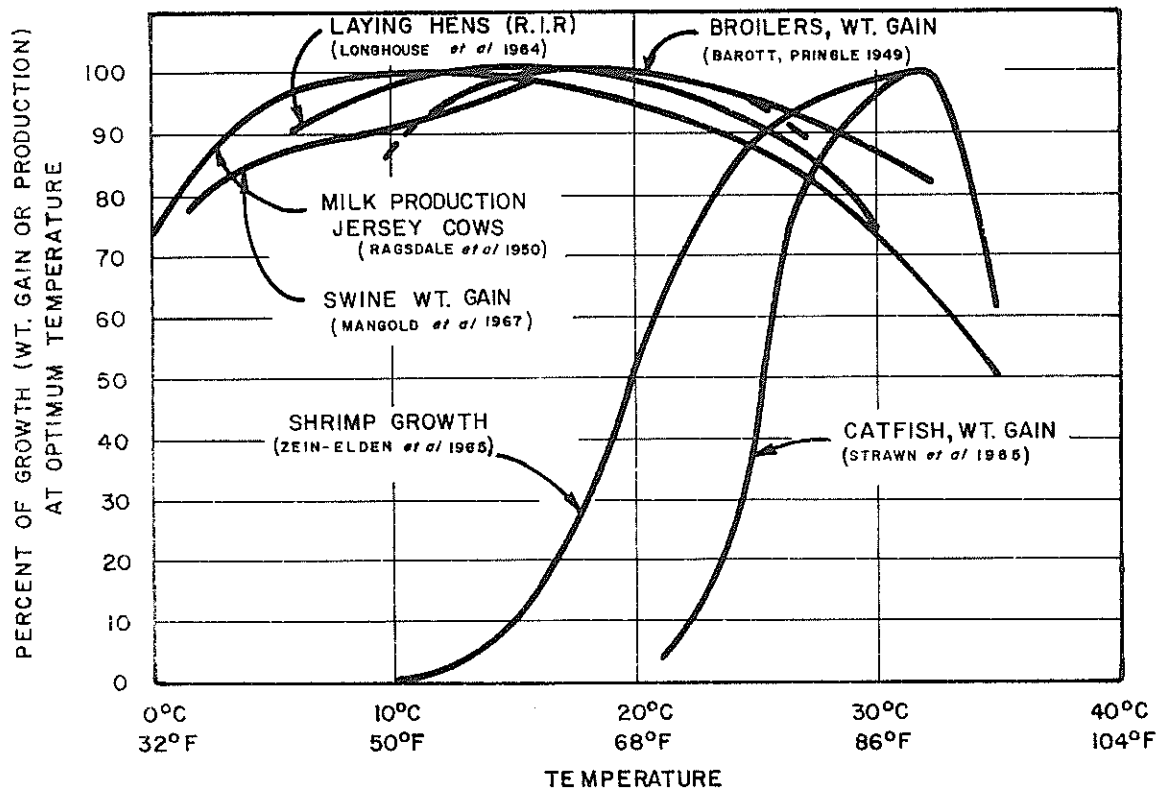


FIGURE 1. Effect of Temperature on Growth or Production of Food Animals.

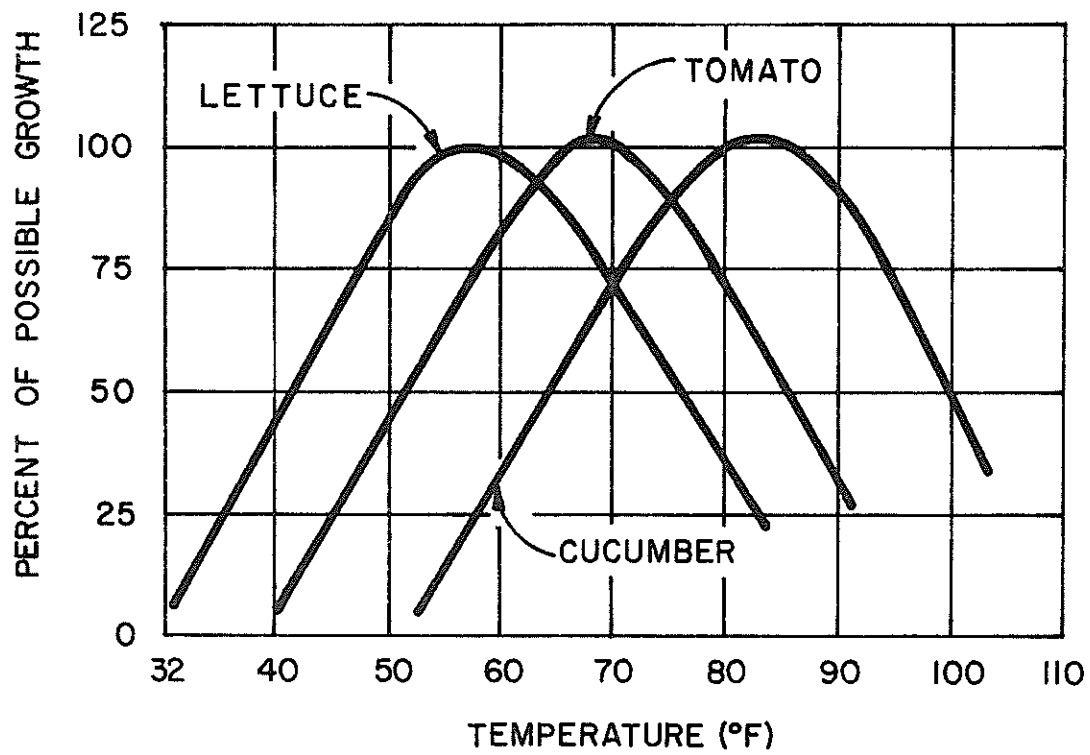


FIGURE 2. Idealized Growth Curves for Several Crops

It has been reported that sub-surface irrigation using as similar 100°F water has resulted in increased crop yield [4].

The results of tests with sprinkler systems for applying the heated water indicated the following:

- (1) Even though waters with temperatures of 135°F were used, that spraying from a height of 8-10 feet did not have any crop damage,
- and (2) that using the thermal water for frost protection had all the benefits of cold water plus the advantage of providing a thermal blanket over the crop or orchard [5]. It was further found that during hot weather the heated water had no adverse effects since it effectively increased the humidity. (Again such a result would depend on the average ambient humidity.)

It is an important coincidence that the outlet temperature range of condenser cooling water from power stations is in the comfort range for most plants and animals as shown previously in Figures 1 and 2. Feed is a very expensive fuel, costing about \$5 per million BTU compared to \$.50 to \$1 per million BTU for natural gas. The pending curtailment of new uses for natural gas dictates that it would not be an acceptable alternative for maintaining the temperature of animal enclosures; yet thermal pollution would be.

Although it is not inconceivable that industry, including the electrical power generating industry would enter into agricultural enterprises to utilize their waste heat before it becomes thermal pollution, it is becoming an acceptable idea to industry that you can afford to pay someone to handle your pollution problems [6,7]. Thus a cooperative effort would solve the thermal pollution problem for the industry and benefit the

agricultural operation in addition.

B. Municipal-Utility Use of Thermal Pollution

The temperature of thermal pollution has been described as being low temperatures which has little use for industrial heating. There exist within a municipality utility complex several areas where such low temperature sources i.e. hot water, can be used. These uses are:

- (1) As a utility for multiple dwelling heating and cooling,
- and (2) As a utility for domestic sewage treatment.

District heating systems are not uncommon in this country. There are some fifty large units, the largest being Consolidated Edison's in New York City. It supplies Manhattan with a peak of about 300 MW of heat. Design engineers have estimated that centralized heating operating under optimum conditions may be competitive with separate heating units up to a distance of ten miles [8]. Such distances solve the sociological problems that arises from "living next to the municipal utilities". Areas of multi-family dwellings and other multistory buildings could be served at costs comparable with conventional separate units.

In order to achieve the type of service described above there needs to be a change in the operating philosophy of the power generating station. The principal change is to operate the turbine discharge as shown in Figure 3. Operated as shown in the third schematic in Figure 3, the power company would have less revenue from primary electrical power, but but selling the higher temperature discharge stream its overall revenue would be greater and its thermal pollution problem would be eliminated.

Regardless of the manner of operating the power generating station it is advisable in future urban planning to locate such units next to the municipal sewage treatment plant or vice versa. One of the major

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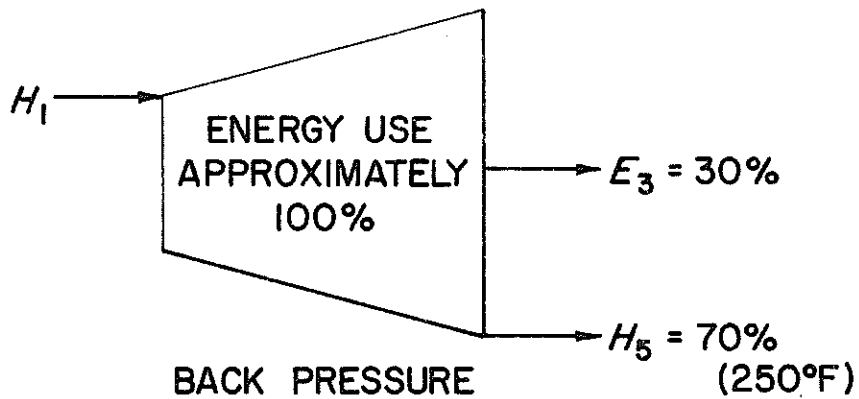
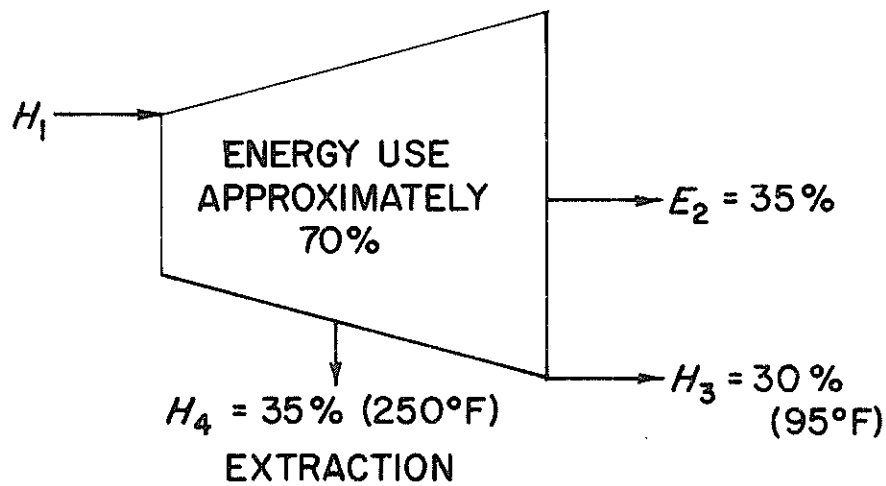
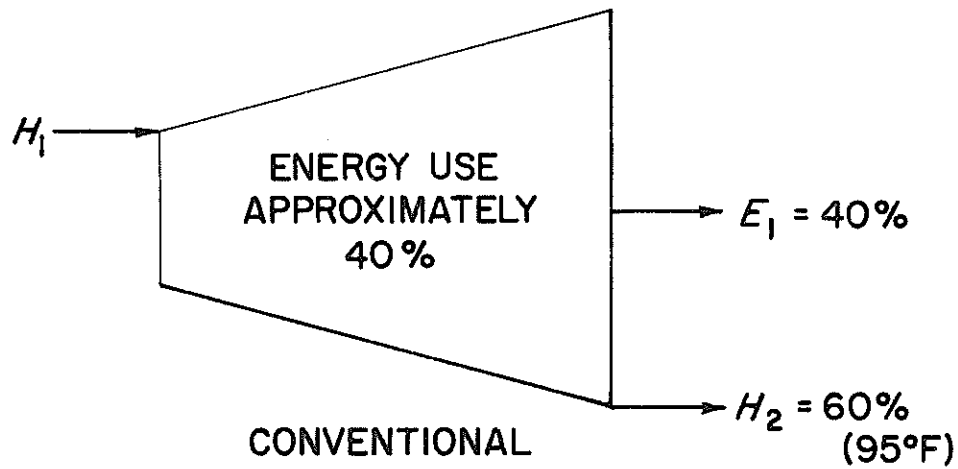


FIGURE 3. Conventional and Dual-Purpose Steam Turbine Performance

problems with water resources is the need to use more sophisticated treatment processes (called advanced waste treatment) and to operate the current processes more efficiently to achieve the necessary "zero-effluent". This requires energy. Steam from the power plant at 32 psig (274°F) can be used efficiently to desalt sewage plant effluent [9]. It has been reported that sewage treatment at elevated temperatures (100°F) shows the following properties: (1) heating results in a dispersion effect on suspended solids, resulting in a homogeneous waste; (2) the solubility of solid material increases; (3) anaerobic digestion improves; (4) the solubility of gases decreases. The solubilization of the suspended solids increases the rate of microbiological processes by giving the population a more uniform environment and reducing mass transfer limitations.

In the discussion of the useful application of the sensible heat of the waste fluid stream it has been assumed that the stream was not polluted with respect to its intended use, i.e. condenser water containing certain salts (chromium) could be used in heating however the water could not be used in direct application for agricultural production. A second example would be a refinery waste containing hydrogen sulfide. Before this waste could be used for heating the H_2S would have to be removed because of its corrosive chemical properties. Further not all existing thermal pollution sources will readily find the previously described uses for the waste energy and these sources will require treatment by physical or chemical processing to reduce the thermal pollution. Adiabatic degassing is such a process.

IV. Description of Simulation Model

A. Physical Separation of Gas-Liquid Streams

Physical separation of dissolved gases from water involves the unit operations of stripping or flashing. In stripping, an inert gas is used as a carrier for the removal of the dissolved component. Mass transfer of the dissolved component from the water to the carrier gas is the controlling mechanism. In flashing, the feed stream is separated into a gas phase and a liquid phase. The controlling mechanism of flashing is phase formation or nucleation. The gas phase from both operations will contain both the dissolved component and water vapor, however in flashing the quantity of water vapor will be much greater on a percentage basis.

There are many industrial or commercial processes in which there is an interest in the separation of a dissolved gas component from water solution. In oil field operations, sour water which is being used for secondary recovery of petroleum must first be purified of hydrogen sulfide to reduce corrosion [10]. The reclamation of refinery waste water involves the removal of both dissolved hydrogen sulfide and ammonia [11,12]. In both processes involving hydrogen sulfide, this material can be chemically reacted to produce sulfur. Although the quantities are usually much smaller, modern sewage treatment processes are being developed for separating both hydrogen sulfide and ammonia from domestic waste. Many fish hatcheries have experienced difficulties with high levels of dissolved nitrogen. These levels are detrimental to the fish [13].

Each of these problems can be approached by either stripping or flashing. Currently, stripping is the more frequently employed unit operation although the design question has not considered the thermal pollution associated with the system. In both unit operations water is vaporized.

If the process is conducted under adiabatic conditions, the latent heat of vaporization of the water must be supplied from the sensible heat of the solution. The net result is a reduction in the temperature of the liquid stream. (In addition to the latent heat of vaporization of the water, there will be a heat of solution associated with the dissolved component, however in most design calculations this is neglected.) If the operation is conducted under reduced pressure (vacuum) operations such as would be associated with most water sources, a critical parameter is the quantity of the gas stream which must be handled. Flashing would produce less volume than stripping. Further the capital investment in equipment for flashing is less than that for stripping. Stripping, however, usually produces a greater reduction in the quantity of gas remaining in the water. Since in a thermal pollution abatement program, the critical criterion is the temperature reduction, this report considers adiabatic degassing of water sources using a flashing process.

Specifically, the report considers the feasibility of thermal pollution reduction through adiabatic degassing for three water systems. These are:

- (1) Water which has been used to absorb SO_2 from power plant stack gas,
- (2) Sour (H_2S) water which has been generated either in normal refinery operations or has been produced from natural sources,
- and (3) Sewage effluent containing ammonia.

B. Model Equations

The primary requirement of a simulation model is that the results are consistent with the experimental observations, although the model

itself is a mathematical abstract not necessarily describing the physical or chemical mechanism. A convenient model for flashing employs the concept of an ideal stage. The basic descriptive equations for the analysis of an ideal stage are a combined component balance and an energy (enthalpy) balance. Steady state operation is assumed. Figure 4 is a schematic flow diagram for the unit operation of flashing. The equations for this process are

$$F_1(\psi, p) = \sum_{i=1}^c \frac{z_i(K_i(p) - 1)}{\psi(K_i(p) - 1) + 1.0} = 0 \quad (1)$$

$$\text{and } F_2(\psi, p) = (1 - \psi) \sum_{i=1}^c \frac{z_i(\lambda_i - Q_i)}{1 - \psi(1 - K_i(p))} + \bar{h}_o - \sum_{i=1}^c H_F^i z_i = 0 \quad (2)$$

The function $F_1(\psi, p)$ is the basic combined component (or material) balance and the function $F_2(\psi, p)$ is the energy balance. The definition of each of the terms is given in the list of Nomenclature and the derivation of the basic equations are given in Appendix A. A corollary problem in the development of any simulation or mathematical model is that of determining the number of independent and dependent variables. This problem is usually classified as determining "the degrees of freedom" [14,15]. Table 1 shows the degree of freedom of the system as zero. Thus, there is a unique solution. This agrees with the mathematical description which shows the system is modelled by two equations in two unknowns, ψ and p . As written the balances assume that the composition and enthalpy of the feed stream is known and that the temperature of the flash is specified. With the appropriate thermodynamic equilibrium data, solution of the balance equations give the equilibrium pressure of the flash and the quantity of the dissolved gas released and water vapor formed. Table 2

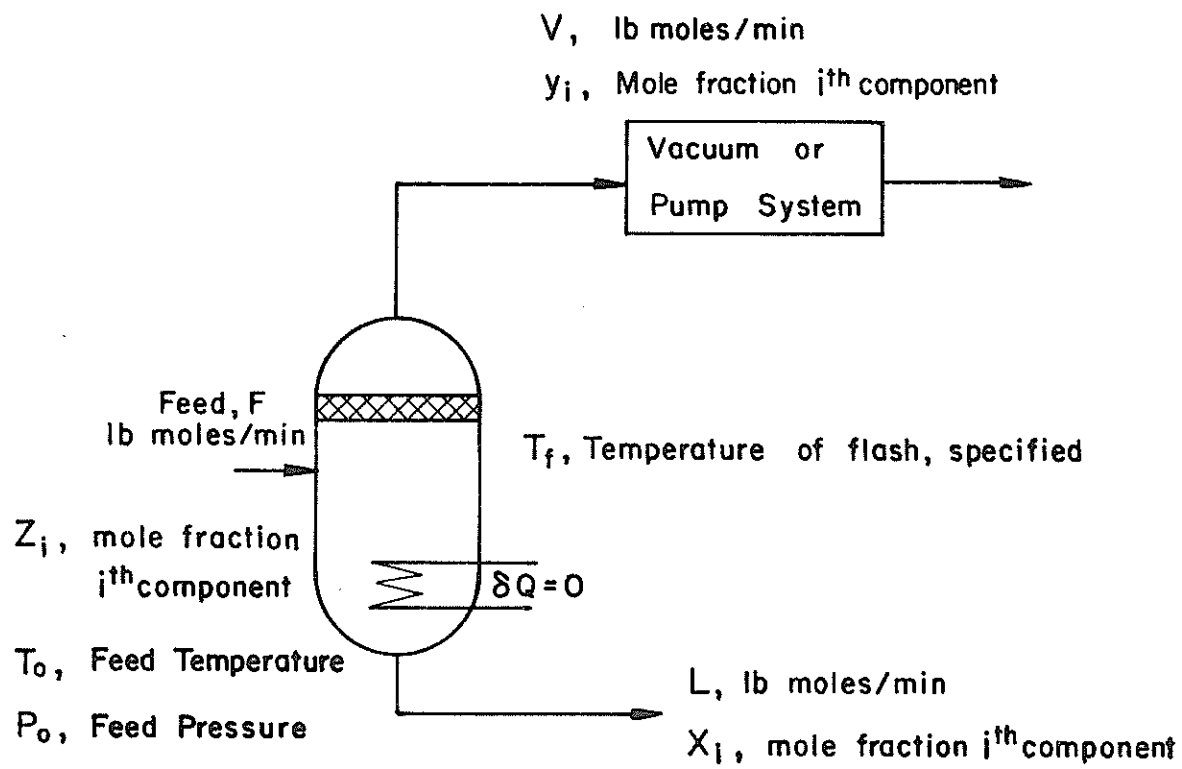


FIGURE 4. Flow Schematic

Table 1. Degrees of Freedom Analysis

Number of 1 Phase Streams	1	
Number of 2 Phase Streams	1	
(NOTE: The vapor and liquid streams are shown as separate streams, however, in the sense of Gibbs Phase Rule, they are a single two phase stream)		
Number of Variables for 1 Phase Stream		C + 2
Number of Variables for 2 Phase Stream		C + 2
Energy Variable		<u>1</u>
Total, N_v		2C + 5
Number of Relations		
Material Balances		C
Energy Balance		<u>1</u>
Total, N_R		C + 1
Number of Variables Fixed by the Environment		
Feed Composition and Quantity		C + 2
Temperature of Flash		1
Adiabatic Operation		<u>1</u>
Total, N_f		C + 4

$$\text{Degrees of Freedom} = N_v - N_R - N_f = 0$$

Table 2. Example Calculations

Feed stream: Sour water containing 200 ppm H_2S $F = 462.8$ lb moles/hr

Pressure of Feed Stream - 1 atm

Temperature of Feed Stream = $32.4^\circ C$

Temperature of Flash - specified as $27^\circ C$ ($5.4^\circ C$ drop)

Volume of Vapor: $V = 3.93 \times 10^6$ cubic feet

composition of vapor: $H_2S = .005296$

$H_2O = .994$

Volume of Liquid: $L = 800$ lbs/min

composition of liquid: $H_2S = 7.845 \times 10^{-8}$

$H_2O = .9999$

Pressure of Flash Vessel: .138 psia

is a sample calculation. As mentioned, the computation can only be made if appropriate thermodynamic data is available. The data needed is vapor-liquid equilibrium values as functions of temperature and enthalpy data.

V. Discussion of Thermodynamic Data

The thermodynamic data required for the solution of the model equations are values of the equilibrium constant between a gas-vapor phase and a liquid phase, and enthalpy data for all the components in the system. In all three cases to be examined the system is treated as a binary system of one gas component and water. As mentioned many of the systems will have more than two components; however the experimental data for the appropriate multicomponent systems is not available and as will be discussed, estimation techniques are not sufficiently accurate to warrant their use. This is not true in general but is the case for water systems.

A. Vapor-Liquid Equilibrium

At constant temperature and constant pressure, the thermodynamic statement for defining a two-phase equilibrium is that the chemical potential of each component in each phase is equal, or as shown in Equation 3:

$$\mu_i^v = \mu_i^L. \quad (3)$$

It has been shown [16] that an equivalent statement is equality of the fugacities

$$f_i^V = f_i^L. \quad (4)$$

It can be shown that the fugacity can be calculated from the following equation

$$RT \ln \frac{f_i}{y_i P} = \int_0^P \left[\bar{v}_i - \frac{RT}{P} \right] dP. \quad (5)$$

To solve the integral term, an equation of state for each component is required. For the gaseous fugacities these equations are available for hydrogen sulfide, ammonia, and sulfur dioxide; however this information is not available for water vapor. There is a further complication in that in aqueous solution there are no available equations of state for any of the components. Experimental data is therefore required.

The hydrogen sulfide-water system has been extensively studied experimentally in conjunction with the recovery of deuterium from water [17]. This data is given in Appendix B and is used in the simulation. The data is correlated in terms of x_i , mole fraction of hydrogen sulfide in water (liquid) and y_i , mole fraction of water in hydrogen sulfide (gas). It is necessary to relate these to the equilibrium constant, K_i , of Equation 1.

The usual definition of the vapor-liquid equilibrium constant is

$$K_i = y_i/x_i \quad (6)$$

For hydrogen sulfide-water the experimental data is readily calculatable as equilibrium data. For the other systems being examined an idealization of Equation 5 must be used. If the vapor-gas state is considered as having the properties of an ideal gas, Equation 5 reduces to $f_i^V = y_i P$ for the vapor, and to $f_i^L = x_i H_i$ for the liquid phase components. Substituting into Equation 4 gives

$$P_i = y_i P = x_i \tilde{H}_i \quad (7)$$

which is Henry's Law. The appropriate equilibrium constant, K_i , is calculated by \tilde{H}_i/P . The problem of calculating K is now a problem of obtaining values for Henry's Law constants.

All thermodynamic data for computing the appropriate vapor-liquid equilibrium values are given in Appendix B.

B. Calculation of Enthalpy

Equation 2 of the simulation model is an enthalpy balance. For the process of adiabatic degassing of the design systems the total energy required to vaporize a portion of the water and to separate the dissolved gas component is supplied by reducing the sensible heat of the feed liquid. Subsequently, the gas-vapor phase and the liquid phase leave the process at the lower temperature. It is this effect that is sought as the solution for thermal pollution.

The following thermodynamic data are required for calculation of the energy balance:

- (1) Caloric equation of each component
 - (2) Latent heat of vaporization of water as a function of temperature
 - (3) Heat of solution of gas components in aqueous solutions
- and (4) Excess enthalpy of mixing.

Caloric equations evaluate the heat capacity of a component as a function of temperature. These equations are empirically developed and usually presented as polynomials of temperature. Latent heat is also obtained from experimental data as is the heat of solution. The excess enthalpy is calculated by

$$\Delta h^E = -RT \sum_{i=1}^c x_i \left(\frac{\partial \ln \gamma_i}{\partial \ln T} \right)_{P_i, x} \quad (8)$$

This assumes that there are available relationships evaluating the activity coefficient, γ_i . This data is not readily available for the systems that we are studying.

These systems are important industrially and extensive enthalpy data has been developed. This may seem like a contradiction to the statement on the availability of activity coefficient data. It is not, for this information is not separated out of the enthalpy data. The data is presented in graphical form as relative enthalpy versus mass fraction of the gaseous component. The data is equilibrium data giving the relationship between saturated liquid and saturated vapor. Data of this type is given for the ammonia-water system in Appendix B.

For other systems where neither graphical or activity coefficient data is available the assumption is made that the system is ideal. The enthalpy of mixing is zero.

One additional correction must be considered, this is pressure-volume effect. Enthalpy is an exact differential in variables S and P. Differentiation of the function gives a term $(\partial H/\partial P)_S dP$. This term is equivalent to the product VdP . For the conditions of the adiabatic degassing process, this term may be neglected.

VI. Description of Process Equipment

The equipment chain exclusive of control equipment consists of a closed vessel in which the flash takes place accompanied by phase separation and a means for removing the gas-vapor phase, e.g. the vacuum system. The closed vessel would be insulated to achieve adiabatic operation. Both the vessel and vacuum equipment would require a corrosion resistant material. For the three systems of interest, two are acidic, e.g. hydrogen sulfide and sulfur dioxide, and one is basic, e.g. ammonia. Stainless steel would be used.

A. Flash Vessel

The flash chamber is generally constructed as a vertical drum. For such drums the diameter is set to provide the necessary cross section for the volumetric flow rate of the gas-vapor phase. A satisfactory criteria to prevent excessive entrainment would be to restrict the linear velocity of the gas-vapor phase to less than 2 ft/sec. A more rigorous calculation of the limiting linear velocity is available [19]. Under normal operating conditions a vertical flash drum would have the relative dimensions as shown in Figure 5. All feed and exit lines are designed for a head loss of 0.4 psi per 100 ft. of pipe (or tubing). The design temperature is set at 50°F above the operating temperature. The design pressure is specified as 10% above the operating pressure, but at least 25 psig unless the drum is operating in a vacuum in which case a design pressure of 100 psig is used [20].

B. Vacuum Equipment

Industrial operations for adiabatic degassing normal operate at positive pressures, however the specific systems that are considered in this report would originate at near atmospheric pressure and would require

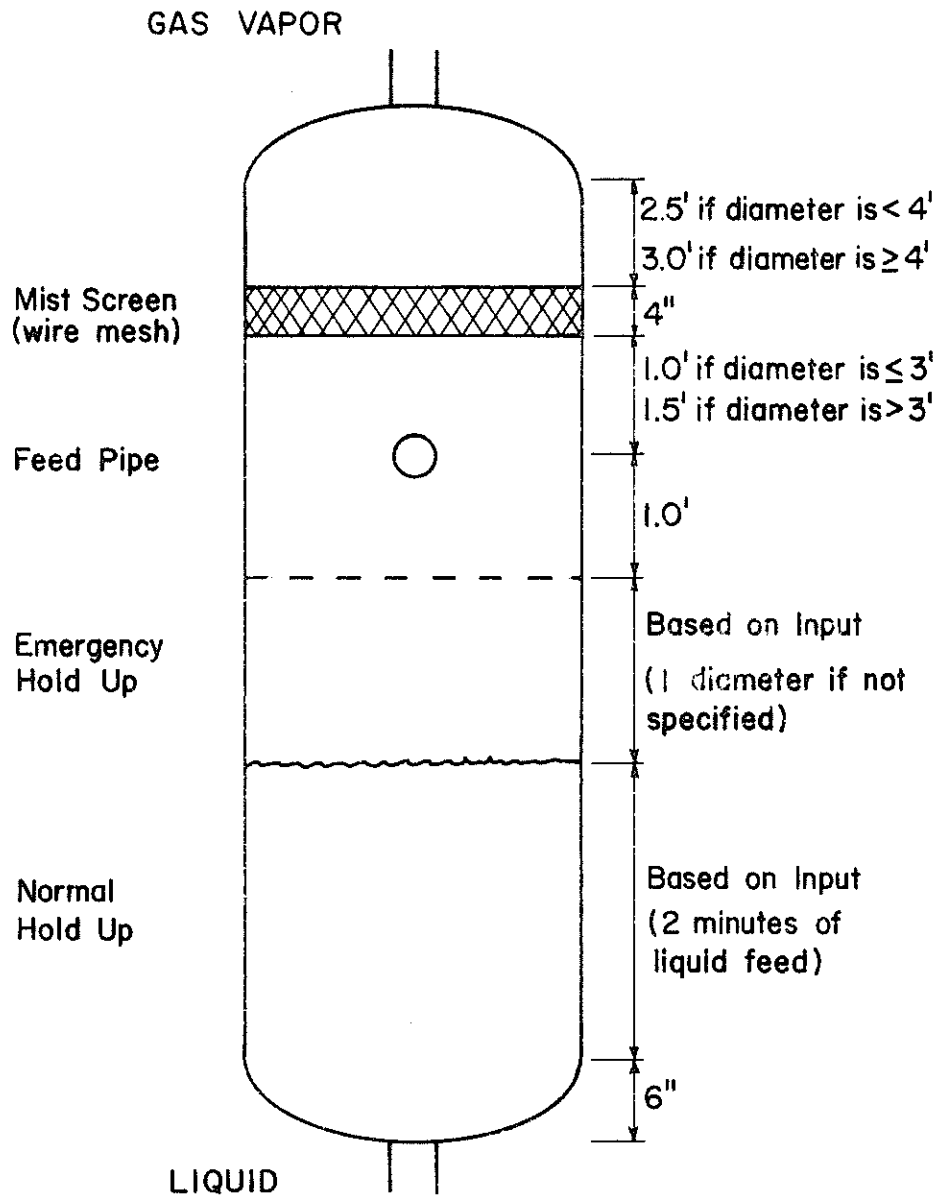


FIGURE 5. Flash Vessel Design

vacuum operation of the flash chamber for the desired separation. The two most common vacuum systems consist of steam-jet ejectors or mechanical vacuum pumps. Figure 6 is a schematic of the application of vacuum equipment [21].

Ejectors are important in industrial operations for creating and holding a vacuum in a system. They have no moving parts and can be constructed in a wide range of materials. They operate by the action of one high pressure stream upon a second of lower pressure. The steam ejector is the unit most frequently used in vacuum processing. It has the following features which makes it a good choice [22]:

- (1) handles wet, dry or corrosive vapor mixtures,
 - (2) develops any reasonable vacuum needed for industrial operations,
 - (3) available in all sizes to match any volume and vacuum requirements,
 - (4) efficiencies are reasonable-to-good,
 - (5) having no moving parts, they require minimum maintenance, and operate at a reasonable steady state when corrosion is not a problem,
 - (6) quiet operation,
 - (7) stable operation within design range,
 - (8) installation costs comparatively low with respect to mechanical pumps and ejectors have smaller space requirements,
- and (9) simple operation.

Ejectors may be single or multistage. The extra stages, with or without interstage condensing of steam, allow the system to operate at lower absolute pressures, as shown in Figure 6. It is advisable to use as few ejectors as possible to achieve the necessary vacuum. The motive steam design pressure must be selected as the lowest expected pressure at the ejector

MECHANICAL VACUUM PUMPS

STEAM-JET EJECTORS

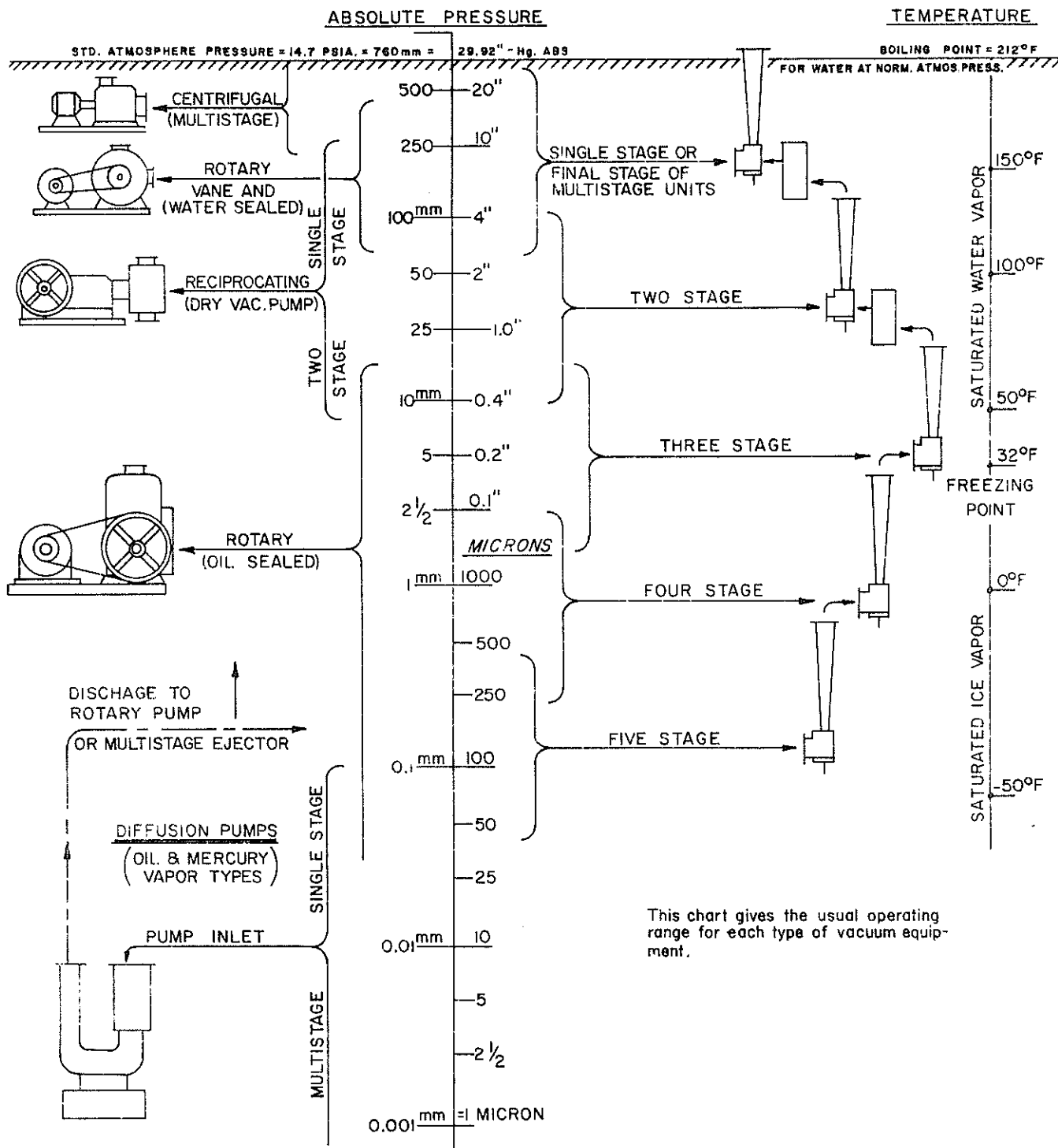


FIGURE 6. Vacuum Equipment

steam nozzle. The unit will not operate stably on steam pressures below the design pressure [23]. Recommended steam design pressure is equal to the minimum expected line pressure at ejector nozzle minus 10 psi. To insure stable operation the steam pressure must be above this minimum value. For ejectors discharging to the atmosphere, steam pressures below 60 psig at the ejector are generally uneconomical. Single-stage ejectors designed for pressures below 200 mm Hg abs. cannot operate efficiently on steam pressures below 25 psig. The relationship between operating pressure e.g. vacuum and the motive steam consumption is not linear. If there is a large change in the requirements (greater vacuum) it would be more economical to change the ejector rather than to increase the steam consumption.

Figure 6 shows the many types of mechanical vacuum pumps that can be considered. This report considers only one type - the Nash Hytor wet vacuum pump [24]. It is a rotary vane and water sealed capable of operating down to an absolute pressure of 60 mm Hg or if jet boosters are added it can operate at absolute pressures in the range of 5-10 mm of mercury.

The Nash pump design is ideally suited to the handling of wet, saturated gases and to conditions where corrosion or liquid carryover are present. The Nash pump uses no internal lubrication. It can therefore handle systems which would dilute, emulsify or form sludge with the hydrocarbon lubricant. The fact that the pump operates with a liquid seal eliminates the problem of moisture carryover in the gas phase. One further advantage of the Nash-Hytor pump for the adiabatic degassing of water solutions is that the water vapor can be condensed within the pump.

The only moving part of the pump is the rotor. The rotor is positioned eccentrically and revolves freely without metal contact in a cylindrical casing containing water. The water rotates with the rotor but follows

the contour of the casing due to centrifugal force. The water which entirely fills the rotor chamber at the inlet, recedes as the rotor advances and then the converging casing forces the water back into the chamber. The replacement of the water by air or gas and its subsequent expulsion cause the pumping (vacuum) action.

In small size units the pumps are directly coupled to electric motors.

VII. Simulation and Results

The availability of the computer has provided the necessary tool for enabling an engineer to perform a sufficiently detailed analysis that the usual procedure of several stages of experimental scale-up can be eliminated. There are limitations in computer simulations but if these are explicitly stated as in any analysis the results can be evaluated accordingly. The previous sections of this report have considered these limitations and discussed how they will be included. This section describes the specific cases evaluated, the mathematical algorithm of the simulation model and the simulation results and evaluation.

A. Problem Statement

The reduction of thermal pollution by adiabatic degassing is studied by computer simulation for three gas-water systems.

1. System Hydrogen Sulfide-Water

Sour water (H_2S) is found in nature, is generated in petroleum refining operations, is produced in petroleum production operations, and is generated in domestic sewage treatment processes. In the past, hydrogen sulfide has been considered the pollutant and the purpose of treating the sour water has been to eliminate it. However with thermal pollution of water courses increasing each source must be examined and measures evaluated for reducing the sensible heat discharged. Concentrations in the entire range from negligible to saturation have been reported.

2. System Ammonia-Water

The two primary sources of ammonia-water as a thermal pollution potential are in petroleum refining operations and in domestic sewage

treatment processes. In both cases the ammonia is a pollutant as well as is any excess sensible heat in the solution. There would still be treatment required for the ammonia but the concentration in the stream to be treated would have increased and the total volume of the stream would have decreased. Ammonia usually is in concentrations somewhere between 5-12 mg/liter in domestic sewage (at that point in the system where treatment is effected). In refinery's it can be much greater, the system being under pressure.

3. System Sulfur Dioxide-Water

A recent news release described the use of sea water to scrub SO_2 from power plant flue gas [25]. The article mentioned that the concentration of SO_2 in the water was between 0.3% and 1.0% (by weight). The article did not discuss the sensible heat that the sea water would gain in the scrubbing operation.

Most power plant stack discharges would be between 100°F and 250°F with a corresponding temperature in the sea water leaving the process at temperatures between 95°F and 105°F . These would also be conditions similar to inland power plants except the solution would not be saline.

These three systems are simulated for the following set of conditions:

Feed Rate - 1000 lb moles per minute (roughly 1.3×10^5 gallons/hour)

Inlet Gas Temperature - 90°F or 100°F

Temperature Drop - 5°F

Gas Concentration in Inlet - 0.01 mole fraction

In addition to these runs, the effect of approximate thermodynamic data on the simulation was studied for the hydrogen sulfide-water system.

B. Algorithm for Solving the Simulation Model

The algorithm for solving the simulation model is a combination of the Newton-Raphson method and Kramer's method. The model equations are

$$F_1(\psi, p) = \sum_{i=1}^c \frac{z_i(K_i - 1)}{\psi(K_i - 1) + 1.0} = 0 \quad (1)$$

$$\text{and } F_2(\psi, p) = \bar{h}_o + (1 - \psi) \sum_{i=1}^c \frac{z_i(\lambda_i - Q_i)}{1 - \psi(1 - K_i)} - \sum_{i=1}^c z_i H_F^i \quad (2)$$

The Newton-Raphson method is a linearization of the Taylor series expansion of the functions $F_1(\psi, p)$ and $F_2(\psi, p)$ and the subsequent solving for the values of ΔP and $\Delta\psi$. The values are obtained by Kramer's method. The initial values of ψ and p are corrected by the ΔP and $\Delta\psi$. The algorithm is executed iteratively until the correct roots e.g. physically realistic, are found. The correct roots are found by the fact that ψ must be between 0 and 1.0 and P must be positive and less than the inlet pressure. The algorithm equations are

$$0 = F_1(\psi_n, P_n) + \frac{\partial F_1(\psi_n, P_n)}{\partial P} \Delta P + \frac{\partial F_1(\psi_n, P_n)}{\partial \psi} \Delta\psi \quad (9)$$

$$0 = F_2(\psi_n, P_n) + \frac{\partial F_2(\psi_n, P_n)}{\partial P} \Delta P + \frac{\partial F_2(\psi_n, P_n)}{\partial \psi} \Delta\psi \quad (10)$$

Kramer's method gives

$$\Delta P = \frac{\begin{vmatrix} -F_1(\psi_n, P_n) & \frac{\partial F_1(\psi_n, P_n)}{\partial \psi} \\ -F_2(\psi_n, P_n) & \frac{\partial F_2(\psi_n, P_n)}{\partial \psi} \end{vmatrix}}{\begin{vmatrix} \frac{\partial F_1(\psi_n, P_n)}{\partial P} & \frac{\partial F_1(\psi_n, P_n)}{\partial \psi} \\ \frac{\partial F_2(\psi_n, P_n)}{\partial P} & \frac{\partial F_2(\psi_n, P_n)}{\partial \psi} \end{vmatrix}} \quad (11)$$

and

$$\Delta\psi = \frac{\begin{array}{|c|c|} \hline \frac{\partial F_1(\psi_n, P_n)}{\partial P} & -F_1(\psi_n, P_n) \\ \hline \frac{\partial F_2(\psi_n, P_n)}{\partial P} & -F_2(\psi_n, P_n) \\ \hline \end{array}}{\begin{array}{|c|c|} \hline \frac{\partial F_1(\psi_n, P_n)}{\partial P} & \frac{\partial F_1(\psi_n, P_n)}{\partial \psi} \\ \hline \frac{\partial F_2(\psi_n, P_n)}{\partial P} & \frac{\partial F_2(\psi_n, P_n)}{\partial \psi} \\ \hline \end{array}} \quad (12)$$

New values of ψ and P are computed by

$$\psi_{n+1} = \psi_n + \Delta\psi \quad (13)$$

$$\text{and } P_{n+1} = P_n + \Delta P$$

The differentiation of the functions is given in Appendix A.

In the algorithm it is necessary to access the thermodynamic data. The data for hydrogen sulfide-water are in functional form and are readily entered into the computer program. The data for the ammonia-water and sulfur dioxide-water systems are entered in tabular form as shown in Appendix B. These data are accessed through a table-lookup routine which utilizes linear interpolation (two-dimensional) for intermediate values of the data.

C. Results

Table 3 is a sample of the computer output for the H_2S -water system simulation. The table shows that the temperature has been reduced $1.3^\circ K$ (or $2.3^\circ F$) and the concentration of H_2S in the liquid has been reduced by 57.5%. Although this example is not within the problem specifications of considering at least a 5° temperature drop it will be used to illustrate

Table 3. Sample Computer Output

Feed Quantity	FEED = 1.31×10^5 gallons/hour
Feed Temperature	TFEED = 305.2°K
H ₂ S Concentration	XFI = 0.01 (mole fraction)
Pressure Inlet	PTOTAL = atmospheric 760 mm Hg.
Temperature Out	T = 303.9°K
H ₂ S Concentration in Liquid	X1 = 0.00425 (mole fraction)
Water Vapor Concentration in Gas	Y2 = 0.0914 (mole fraction)
Vapor-to-Feed Ratio	SAI = 0.00629
Pressure of Flash	PMM = 491.156
Volume Gas Phase	V = 40.792 (liters measured at flash conditions)

the economic evaluation of the process. Table 4 is a summary of the calculations for this case. The calculations as well as the cost data are shown in Appendix D. At the low vacuum shown the ejector is not efficient. The operating costs do not include pumping costs on the liquid phase.

Table 4. Economic Evaluation

	Equipment Cost Only
1. Vessel: vertical construction, 6.4 ft diameter, 31 ft high, 316 Stainless Steel, 100 psig	\$ 53,000
2. Ejector: 316 Stainless Steel, Single Stage	
a. Operating cost \$13.56/hour	6,000
3. Vacuum pump: 316 Stainless Steel	
a. Operating cost \$3.60/hour	37,000

A second case is shown in Table 5. This simulation included a 5°F temperature drop. The corresponding economic evaluation is shown in Table 6.

Table 5. Simulation Example 2

Feed Quantity	1.31 x 10 ⁵ gallons/hour
Feed Temperature	305.2°K
H ₂ S Concentration	0.01 (mole fraction)
Pressure	760 mm Hg
Temperature Out	302.5°K (4.96°F)
H ₂ S Concentration in Liquid	0.00406 (mole fraction)
Water Vapor Concentration in Gas	0.37676 (mole fraction)
Vapor-to-feed Ratio	0.00954
Pressure of Flash	155.101 mm Hg

Table 6. Economic Evaluation, Example 2

	Equipment Cost Only
1. Vessel: vertical construction, 7.85 ft. diameter, 32.25 ft. high; 316 Stainless Steel, 100 psig	\$ 66,400
2. Ejector: 316 Stainless Steel, Single Stage	
a. Operating cost \$75/hour	6,000
3. Ejector: 316 Stainless Steel, 2 Stage with Intercondenser	
a. Operating cost \$25/hour	15,000
4. Vacuum Pump: 316 Stainless Steel	
a. Operating Cost \$13.75/hour	51,200

Only the data for H₂S has been recorded here. The output for the other systems indicated the same order of magnitude for the economic evaluation. Two variations from the above results are significant. These are

- (1) if the feed temperature is 100°F instead of 90°F the operating costs are reduced to achieve a 5° temperature drop. This is consistent with thermodynamics

and (2) for 10° or 15° temperature drops, the ejector system becomes competitive with the vacuum pump as far as operating costs are concerned. In fact the vacuum pump will not operate efficiently at the absolute pressures of the 15° drop.

There is one final consideration and this is the effect of the thermodynamic data on the analysis. The data in Table 5 were obtained with the good experimental correlations of Appendix B. The simulation was run using a simple Henry's law data for the solubility of H₂S in water. Table 7 is a comparison of these two sources of thermodynamic data.

Table 7. Comparison of ψ

	ψ
Appendix B. Experimental Data	0.00954
Henry's Law Estimate Data	0.01250

Table 7 shows that the estimated ψ is in error by 31%. It is important to use good experimental data, and the more complicated calculations which result are required.

VIII. Glossary and Nomenclature

1. **Adiabatic:** The system is thermally isolated from the surroundings; according to thermodynamics no quantity of heat is exchanged between the system and the surroundings during the process.
2. **Advanced Waste Treatment:** Those waste water treatment processes that follow the conventional primary and secondary treatment, e.g. the operations of reverse osmosis, ultrafiltration, dialysis, distillation, etc.
3. **Chemical Potential:** According to thermodynamics the partial molar Gibbs free energy, i.e. the change in Gibbs free energy when one mole of a component is added to an infinite solution.
4. **Degrees of Freedom:** Computed as the difference between the number of variables and the number of relationships (or equations) between the variables. Associated with the idea that in engineering design problems there are going to be opportunities for optimization i.e., at least one degree of freedom. This means that at least one variable can have its value assigned by the engineer.
5. **Entrainment:** In a flashing solution droplets of the liquid are carried along with the vapor-gas phase. High entrainment lowers the separation that is achieved in the equipment.
6. **Equilibrium:** That thermodynamic state in which there is no change in the macroscopic properties of the system.
7. **Excess Enthalpy:** The enthalpy of mixing of nonideal systems. Calculated as the difference between the enthalpy of the mixture and the corresponding enthalpy if the mixture were ideal.

8. Fugacity: For an ideal gas it is equal to the equilibrium partial pressure. A property of real gases calculated from thermodynamics. Related to the chemical potential by $d\mu = RT d \ln (\text{fugacity})$.
9. Ideal Stage: A concept used in the design and analysis of equipment for the physical separation of components. A unit in which there is complete mixing of all feed streams and the exiting streams are in thermodynamic equilibrium.
10. Newton's Method (Newton-Raphson) a root finding technique. Newton-Raphson is for multidimensional problems.
11. Sensible Heat: That portion of the total enthalpy change for a process which is associated with only a temperature change, i.e. there are no phase transitions or no heats of reaction (solution) are included in this step of the process.
12. Simulation: The practice of mathematically modeling a given process for the purposes of studying its behavior when the real process is not available. The mathematical model does not necessarily represent the true mechanism of the process, but the model response should be as similar as possible to the real system response. A simulation is run not solved.
13. Thermal Pollution: Thermal energy that is released to the environment as the result of an energy generating process, chemical or petroleum process, and domestic utility processes. Much of the release is due to current operating efficiencies being relatively low and demand high. Present emphasis is on those systems in which the thermal pollution is associated with an aqueous waste.

14. Unit operation: A system of classification of a single step of a process sequence. The concept is organized around the functioning of equipment rather than the physico-chemical mechanism.

Nomenclature

System Variable	Definition
F	Feed Rate, lb moles/min
f	Fugacity, mm Hg
$F_1(,P)$	Material Balance Function
$F_2(,P)$	Energy Balance Function
\tilde{H}	Enthalpy, Gas-Vapor Phase, BTU/lb mole
h	Enthalpy, Liquid Phase, BTU/lb mole
H	Henry's Law Constant, mm Hg/mole fraction
K	Equilibrium Constant
L	Liquid Rate, lb moles/min
N	Number (in degrees of Freedom)
P	Pressure, mm Hg
Q	Heat of Solution, BTU/lb mole
R	Ideal Gas Law Constant, BTU/lb mole °R
S	Entropy, BTU/°R
T	Temperature, °R
V	Vapor-Gas Rate, lb moles/min
v	Partial Molar Volume, ft ³ /lb mole
x	Mole Fraction, Liquid Phase
y	Mole Fraction, Vapor-Gas Phase
z	Mole Fraction, Feed

System Variable	Definition
μ	Chemical Potential, BTU/lb mole
λ	Latent Heat, BTU/lb mole
ψ	Vapor-to-Feed Ratio
γ	Activity Coefficient

Subscripts
and
Superscripts

c	Total number of components
ϵ	Excess property
F	Refers to Flash temperature and Pressure
f	Fixed Variables (Degrees of Freedom)
i	i^{th} Component
L	Liquid Phase
n	n^{th} Step in Iteration
O	Refers to Feed Property
R	Restrictions (Degrees of Freedom)
V	Vapor-Gas Phase
v	Variables (Degrees of Freedom)

Special Nomenclature for H_2S -Water Thermodynamic Data

P' = pressure, atm ($P_0 = 1 \text{ atm}$)

(P) = pressure, lb/sq. in. abs

V = volume, liters/g. mole ($V_0 = V \text{ at } P_0, T_0$)

(T) = temperature, $^{\circ}\text{K}$ ($T_0 = 218.2^{\circ}\text{K}$)

X = mole fraction hydrogen sulfide in water liquid

Y = mole fraction water in hydrogen sulfide gas

ΣH = enthalpy of $\text{H}_2\text{S}(\text{g})$, cal/mole

h_w = enthalpy of pure water (liquid), cal/mole

λ = heat of vaporization of water, cal/mole

Q = enthalpy of mixing, cal/mole

S_{soln} = enthalpy of H_2S (dissolved) - water (liquid), cal/mole

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X. Appendix A. Derivation of Mathematical Model

A. Material Balance

All model equations are for the process system shown in Figure 1 in the text. The nomenclature is as given in the list of Nomenclature. Three model equations are shown for the combined material balance since all three appear in the literature. The advantages of the CHSS equation are demonstrated.

$$\text{Overall Material Balance: } F = L + V \quad (\text{A1})$$

Material Balance for *i*th Component:

$$z_i F = x_i L + y_i V \quad (\text{A2})$$

Thermodynamic Vapor-Liquid Equilibrium

$$K_i = y_i / x_i \quad (\text{A3})$$

(1) Model Equation, HLLD [25]

Substitution of A1 and A3 into A2 gives

$$z_i F = x_i (F - V) + x_i K_i V \quad (\text{A4})$$

$$z_i = x_i \{ (1. - V/F) + K_i V/F \}$$

$$x_i = \frac{z_i}{\{ 1. - \psi + \psi K_i \}} \quad (\text{A5})$$

From the definition of mole fraction

$$\sum_{i=1}^c x_i = 1. \quad (\text{A6})$$

$$\sum_{i=1}^c \frac{z_i}{1 + \psi(K_i - 1)} - 1.0 = 0 \quad (\text{A7})$$

(2) Model Equation, CHEV [27]

Equation A3 is rewritten as

$$L x_i = L / V K_i V y_i. \quad (\text{A8})$$

Equation A1 is rewritten as

$$\frac{L}{V} = \frac{F - V}{V} = \frac{1 - \psi}{\psi} \quad (\text{A9})$$

Equation A2 therefore becomes

$$y_i \left\{ 1 + \left(\frac{1 - \psi}{\psi} \right) \left(\frac{1}{K_i} \right) \right\} = \frac{1}{\psi} z_i \quad (\text{A10})$$

$$y_i = \frac{K_i z_i}{1 + (K_i - 1)\psi} \quad (\text{A11})$$

Since y_i is also a mole fraction

$$\sum_{i=1}^c y_i = \sum_{i=1}^c \frac{K_i z_i}{1 + (K_i - 1)\psi} = 1.0 \quad (\text{A12})$$

(3) Model Equation, CHSS [28]

From Equations A1, A2 and A3

$$z_i F = K_i x_i (F - L) + x_i L \quad (\text{A13})$$

$$z_i F = x_i \{V(K_i - 1) + F\} \quad (\text{A14})$$

$$x_i = \frac{z_i F}{V(K_i - 1) + F} \quad (\text{A15})$$

$$\sum_{i=1}^c x_i = \sum_{i=1}^c \frac{z_i}{\psi(K_i - 1) + 1} = 1.0 \quad (\text{A16})$$

Likewise, from Equations A1, A2 and A3

$$z_i F = y_i V + \frac{y_i}{K_i} (F - V) \quad (\text{A17})$$

$$z_i F = y_i \left\{ V \left(1 - \frac{1}{K_i} \right) + \frac{F}{K_i} \right\} \quad (\text{A18})$$

$$y_i = \frac{z_i K_i}{\psi(K_i - 1) + 1} \quad (\text{A19})$$

$$\sum_{i=1}^c y_i = \sum_{i=1}^c \frac{z_i K_i}{\psi(K_i - 1) + 1} = 1.0 \quad (\text{A20})$$

Combining Equations A16 and A20 gives

$$\sum_{i=1}^c \frac{z_i K_i}{\psi(K_i - 1) + 1} - \sum_{i=1}^c \frac{z_i}{\psi(K_i - 1) + 1} = 0 \quad (\text{A21})$$

and finally

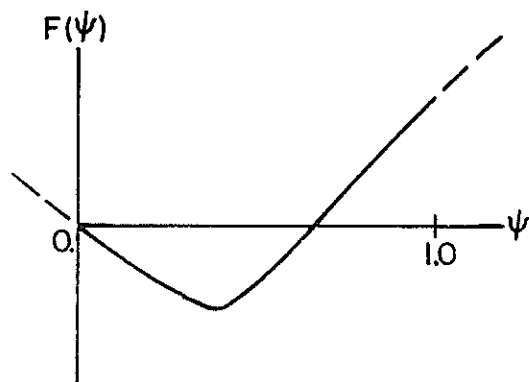
$$\sum_{i=1}^c \frac{z_i (K_i - 1)}{\psi(K_i - 1) + 1} = 0 \quad (\text{A22})$$

Each of the model equations, e.g. A7, A12 and A22 are a combined material balance for an ideal stage or flash chamber. Each model equation is an implicit function of ψ , the vapor-to-feed ratio. Newton's method for finding the root is used in computing the material balance. The selection of the model equation, CHSS, to be used in the simulation is based upon its convergence properties in the application of Newton's Method. Figure A-1 shows each of the material balance model equations plotted as an implicit function, $F(\psi) = 0$, versus ψ . Model Equation CHSS is used. As shown in part (c) of the figure, the root can be found by iteration regardless of the starting point, whereas for the other two model equations convergence is a function of the starting point.

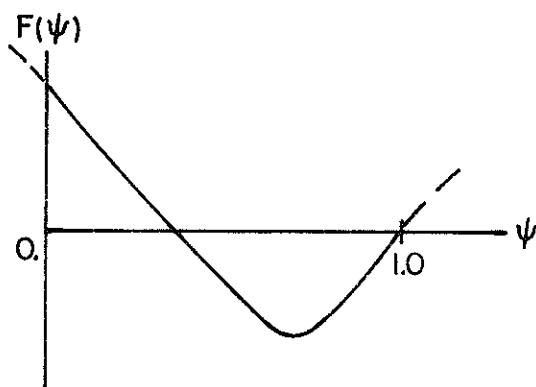
B. Enthalpy Balance

The enthalpy balanced is derived for the process as shown in Figure 1. The flash chamber is operated adiabatically. The contributions to the enthalpy are as discussed in the text. Although the complete definition of all symbols are given in the list of Nomenclature, the following explanation is to clarify the derivation:

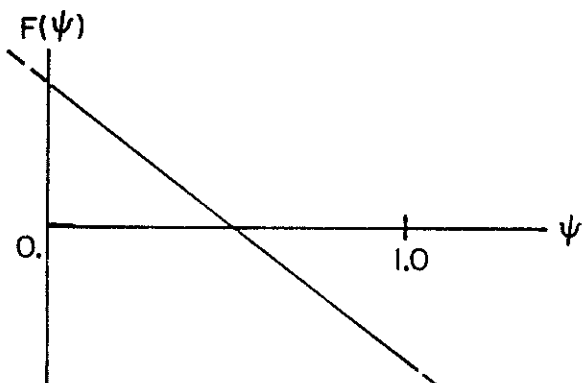
- (1) All values of enthalpy are referenced to a standard state which is the stable phase of the component at 25°C and 1 atm. The values are all specific enthalpy, BTU/lb mole.



(a) Model Equation, HLLD



(b) Model Equation, CHEV



(c) Model Equation, CHSS

FIGURE A-1. Graphical Representation of Material Balance, $F(\Psi)$

- (2) The overbar refers to the total enthalpy of an individual stream.
Capital H is usually gas phase while lower case h is liquid phase.

Enthalpy of the feed (as liquid)

$$\bar{h}_o = \sum_{i=1}^c z_i (h_o^i + Q_o^i) \quad (\text{A23})$$

Enthalpy of the vapor-gas phase

$$\bar{H}_F = \sum_{i=1}^c y_i H_F^i = \sum_{i=1}^c y_i (h_F^i + \lambda_F^i) \quad (\text{A24})$$

Enthalpy of the liquid phase

$$\bar{h}_F = \sum_{i=1}^c x_i (h_F^i + Q_F^i) \quad (\text{A25})$$

The enthalpy balance is

$$\bar{h}_o = \psi \bar{H}_F + (1 - \psi) \bar{h}_F \quad (\text{A26})$$

It is necessary to eliminate y_i and x_i from Equation A26, e.g. from Equations A24 and A25. From Equation A2

$$\psi \bar{H}_F = \sum_{i=1}^c H_F^i z_i - (1 - \psi) \sum_{i=1}^c H_F^i x_i \quad (\text{A27})$$

Substituting from Equation A26

$$\bar{h}_o - (1 - \psi) \bar{h}_F = \sum_{i=1}^c H_F^i z_i - (1 - \psi) \sum_{i=1}^c H_F^i x_i \quad (\text{A28})$$

From the definition of \bar{h}_F

$$\bar{h}_o = \sum_{i=1}^c H_F^i z_i + (1 - \psi) \left\{ \sum_{i=1}^c x_i (h_F^i + Q_F^i - H_F^i) \right\} \quad (\text{A29})$$

From the definition of H_F^i and x_i

$$\bar{h}_o = \sum_{i=1}^c H_F^i z_i + (1 - \psi) \left\{ \sum_{i=1}^c \frac{z_i (Q_i - \lambda_i)}{1 - \psi(1 - K_i)} \right\} \quad (\text{A30})$$

C. Differentiation of $F_1(\psi, P)$ and $F_2(\psi, P)$

The functions $F_1(\psi, P)$ and $F_2(\psi, P)$ are Equations A22 and A30 respectively, written in implicit form.

$$\frac{\partial F_1(\psi, P)}{\partial P} = \sum_{i=1}^c \frac{z_i \psi \left(\frac{\partial K_i}{\partial P} \right) \psi}{[1 - \psi(1 - K_i)]^2} \quad (\text{A31})$$

$$\frac{\partial F_1(\psi, P)}{\partial \psi} = \sum_{i=1}^c \frac{z_i (1 - K_i)}{[1 - \psi(1 - K_i)]^2} \quad (\text{A32})$$

$$\frac{\partial F_2(\psi, P)}{\partial P} = -(1 - \psi) \sum_{i=1}^c \frac{(\lambda_i - Q_i) z_i \psi \left(\frac{\partial K_i}{\partial P} \right) \psi}{[1 - \psi(1 - K_i)]^2} \quad (\text{A33})$$

$$\begin{aligned} \frac{\partial F_2(\psi, P)}{\partial \psi} &= (1 - \psi) \sum_{i=1}^c \frac{z_i (\lambda_i - Q_i) (1 - K_i)}{[1 - \psi(1 - K_i)]^2} \\ &\quad - \sum_{i=1}^c \frac{z_i (\lambda_i - Q_i)}{1 - \psi(1 - K_i)} \end{aligned} \quad (\text{A34})$$

X. Appendix B. Thermodynamic Data

A. Vapor-Liquid Equilibrium

1. Hydrogen Sulfide-Water [17]

The following are empirical correlations given data for the systems

H₂S-water.

$$\text{Hydrate Temperature } ^\circ\text{C} = 9.3987 \ln P - 24.85$$

(a) Humidity

Temperature Range: hydrate point to 171°X

Pressure Range: 100 to 400 lb/sq. in. abs.

$$\begin{aligned} \ln Y = & 9.6689 - 9.1243(\ln P) + 0.85231 (\ln P)^2 \\ & - 0.028290(\ln P)^3 + 0.056442(T) - 6.8678 \times 10^{-5}(T)^2 \\ & + 1.8741 \times 10^{-8}(T)^3 + 0.023154(T)(\ln P) \\ & - 7.6273 \times 10^{-6}(T)^2(\ln P)^2 + 9.5097 \times 10^{-10}(T)^3(\ln P)^3 \end{aligned} \quad (\text{B1})$$

(b) Solubility: Low Temperatures

Temperature Range: hydrate point to 100°C

Pressure Range: 100 to 400 lb/sq. in. abs.

$$\begin{aligned} \ln X = & 5.0375 + 0.011270(P) - 2.0071 \times 10^{-5}(P)^2 \\ & + 1.5586 \times 10^{-8}(P)^3 - 0.044033(T) \\ & + 5.7530 \times 10^{-6}(T)^2 + 8.0270 \times 10^{-8}(T)^3 \end{aligned} \quad (\text{B2})$$

(c) Solubility: High Temperatures

Temperature Range: 100 to 171°C

Pressure Range: 100 to 400 lbs/sq. in. abs.

$$\begin{aligned} X = & -0.066875 + 1.4866 \times 10^{-4}(P) - 6.1119 \times 10^{-8}(P)^2 \\ & + 3.4556 \times 10^{-4}(T) - 4.5473 \times 10^{-7}(T)^2 \\ & - 2.6892 \times 10^{-7}(P)(T) + 3.3587 \times 10^{-13}(P)^2(T)^2 \end{aligned} \quad (\text{B3})$$

2. Hydrogen Sulfide-Water [29]

The following are Henry's Law constants for H₂S-water as a function of temperature:

Table B-1. Henry's Law Data

T, °C	H ₂ S*10 ⁻⁴ , atm/mole fraction
0	0.0268
10	0.0367
20	0.0483
30	0.0609
40	0.0745
50	0.0884
60	0.1030
70	0.1190
80	0.1350
90	0.1440
100	0.1480

Equilibrium Constant from above data

$$K_{\text{H}_2\text{S}} = (-3.333265 * 10^3 + 13.09089 * T)/P \quad (\text{B4})$$

3. Ammonia-Water System [30]

Table B-2. Vapor pressure of Aqueous Ammonia Solution

This author collected the available data on the partial vapor pressure of ammonia in water and plotted the results on logarithmic paper to reduce the curvature and obtain constant percentage errors. The results of Raoult, Carius, Perman, Watts, Sims, Roscoe and Ditmar, Gragoe, Myers and Taylor, Mallet, Mollier, Smits and Postma, Doryer and Gaus were used.

Additional data for the vapor pressure of aqueous solutions of ammonia at 0° are given by Klarman, 1924; at 25° by Scheffer and de Wijs, 1925; and Breitenbach, 1925; and at 100° by Calingaert and Huggins, 1923. Other determinations of conductivities and vapor pressures at 0°, 10°, 18°, 25° were made by Morgan and Maas, 1931.

Gms. NH ₃ per 1000 gms. H ₂ O	Partial Pressure of NH ₃ in mm. Hg at						
	0°	10°	20°	30°	40°	50°	60°
1000	947						
900	785						
800	636	987					
700	500	780					
600	380	600	945				
500	275	439	686				
400	190	301	470	719			
300	119	190	298	454	692		
250	89.5	144	227	352	534	825	

(Cont.)

Gms. NH ₃ per 1000 gms. H ₂ O	Partial Pressure of NH ₃ in mm. Hg at						
	0°	10°	20°	30°	40°	50°	60°
200	64	103.5	166	260	395	596	834
150	42.7	70.1	114	179	273	405	583
100	25.1	41.8	69.6	110	167	247	361
75	17.7	29.9	50.0	79.7	120	179	261
50	11.2	19.1	31.7	51	76.5	115	165
40		16.1	24.9	40.1	60.8	91.1	129.2
30		11.3	18.2	29.6	45	67.1	94.3
25			15	24.4	37.6	55.7	77
20			12	19.3	30	44.5	61
16				15.3	24.1	35.5	48.7
12				11.5	18.3	26.7	36.3
10					15.4	22.2	30.2

Table B-3. Solubilities of Ammonia Water [30]

t°	Mole fraction percent ammonia	Partial pressure in mm. of		Density of solution	Percent contraction in volume
		Ammonia	Water		
20° (Cont.)	43.086	1226	8.4	0.854	8.16
	43.731	1281	8.3	0.848	7.37
	48.175	1677	7.05	0.845	8.96
	49.941	1938	6.33	0.835	8.36
	53.940	2655	5.1	0.825	9.47
	55.970	3076	4.45	0.817	9.47
H 40	56.923	3277	4.15	0.815	9.65
	25.011	752	36.5	0.902	6.05
	25.366	774	36.2	0.9005	6.21
	30.690	1134	32.1	0.8833	7.21
	32.686	1335	29.5	0.817	7.68
	33.134	1376	29.0	0.8755	7.74
	36.326	1787	23.9	0.864	8.22
	39.026	2180	20.5	0.856	8.52
	41.133	2460	19.0	0.849	9.05
	42.925	2832	18.42	0.843	10.00
	44.624	3226	18.0	0.837	9.49
	44.557	3214	18.0	0.837	9.42
	46.335	3640	17.6	0.828	9.40

Table B-4. Partial Vapor Pressure of Aqueous Solutions of SO₂ [30]

The author collected the available data on the partial vapor pressure of sulfur dioxide in water and from the plotted results constructed the following table. He assumed that the dissociation is constant at any particular temperature and that Henry's law applies to the undissociated solute. On the basis of this assumption it has been shown (Haslam, Hershey and Keen, Ind. Eng. Chem, 16, 1225, 1924) that

$$S = H_p + \sqrt{KH_p} \quad \text{or} \quad \frac{S}{\sqrt{p}} = H\sqrt{p} + \sqrt{KH}$$

when S = gms. SO₂ dissolved in 1000 gms. H₂O; p = partial pressure of SO₂ in mm. Hg; H = Henry's law constant and K = dissociation constant of the H₂SO₃. The results of Schonfeld, Sims, Roczeboom, Lindner, Freeze, Smith and Parkhurst and Watts, were used.

Gms. SO ₂ per 1000 gms. H ₂ O	Partial pressure of SO ₂ in mm. Hg at							
	0°	7°	10°	15°	20°	30°	40°	50°
0.2	0.25	0.3	0.3	0.3	0.5	0.6	0.8	1.3
0.5	0.6	0.7	0.75	0.8	1.2	1.7	2.8	4.3
1.0	1.2	1.5	1.75	2.2	3.2	4.7	7.5	12.0
1.5	1.9	2.6	3.1	3.8	5.8	8.1	12.9	20.0
2.0	2.8	3.7	4.6	5.7	8.5	11.8	13.3	31.0
3.0	5.1	6.9	7.9	10.0	14.1	19.7	57.0	82.0
5.0	9.9	13.5	15.6	19.3	26.0	36.0	87.0	116.0
7.0	15.2	20.6	23.6	28.0	39.0	52.0	121.0	172.0
10.0	23.3	31.0	37.0	44.0	59.0	79.0	186.0	266.0
15.0	38.0	51.0	59.0	71.0	92.0	125.0	322.0	458.0
25.0	69.0	92.0	105.0	127.0	161.0	216.0	665.0	
50.0	148.0	198.0	226.0	270.0	336.0	452.0		
75.0	228.0	307.0	349.0	419.0	517.0	688.0		
100.0	308.0	417.0	474.0	567.0	698.0			
150.0	474.0	637.0	726.0					
200.0	646.0	857.0						

B. Enthalpy Data

1. H₂S-Water System [17]

(a) Enthalpy of Hydrogen Sulfide-Water Vapor

The Specific Enthalpy of pure water liquid:

$$H_w = (-148.44 + 0.033299(T) + 2.4258 \times 10^{-3}(T)^2 - 1.9610 \times 10^{-6}(T)^3) * 18. \quad (B5)$$

The specific heat of vaporization of water:

$$\lambda_w = (1112.6 - 5.0786(T) + 0.020208(T)^2 - 3.8312 \times 10^{-5}(T)^3 + 2.5753 \times 10^{-8}(T)^4) * 18 \quad (B6)$$

Molar Enthalpy of Hydrogen Sulfide Gas

$$H = 4463 + 7.15(T-T_o) + 0.00166(T^2 - T_o^2) + P'V - P_o V_o - \alpha \left(\frac{1}{V} - \frac{1}{V_o} \right) - \left(\frac{1}{V^2} - \frac{1}{V_o^2} \right) + \left(\frac{1}{V^3} - \frac{1}{V_o^3} \right) \quad (B7)$$

where $\alpha = A + 2RE/(T)^2$

$$= 3REB/2(T)^2 - CA/2$$

$$= RBDE/(T)^2$$

and the volume is found from a Newton-Raphson method solution to

$$P'V^4 - RTV^3 - \beta V^2 - \gamma V - \delta = 0 \quad (B8)$$

using an initial value of V equal to R(T)/(P).

where: $\beta = R(T)B - A - RE/(T)^2$

$$\gamma = -R(T)BD + CA - RBE/(T)^2$$

$$\delta = RBDE/(T)^2$$

Table I lists the values for the constants.

Table I. Constants for Equations

A	4.1497
B	0.0514
C	0.02086
D	0.02890
E	1.79×10^{-6}
K1	24.219
R	0.08206

(b) Enthalpy of Water Vapor - Hydrogen Sulfide gas mixtures:

$$\Sigma H = (1 - Y) * H + Y * (h_w + \lambda) * 18 \quad (B9)$$

(c) Enthalpy of Hydrogen Sulfide-Water Liquid:

$$H_{\text{soln}} = X * H + (1 - X) h_w - XQ \quad (B10)$$

where Q is obtained from

$$\ln Q = -2.5922 + 0.11344(T) - 3.5701 \times 10^{-4}(T)^2 + 3.3231 \times 10^{-7}(T)^3 \quad (B11)$$

2. Enthalpy Ammonia-Water System

Data were taken from the chart on p. 592 of Reference number 31.

3. Enthalpy Sulfur Dioxide-Water System

Table B-5. SO₂-Water [32]

SO ₂ Concentration wt. % SO ₂ / 100 wt. % H ₂ O	Heat of Solution from Rohr. (25) at 21° C. cal./mol SO ₂	Calculated* Heat of Solution, ΔH _{soln} from Rohr cal./mole. mol mixture	Calculated* Heat of Solution from P ^b values of Table II cal./mole. mol mixture	Difference %
0.03	10,040	10,525	10,402	1.18
0.05	9,682	10,467	10,538	1.40
0.06	9,360	10,407	10,281	1.25
0.10	9,210	10,348	10,208	1.37
0.15	8,930	10,179	10,036	1.28
2.50	8,100	9,078	8,733	3.95
1.00	7,735	8,410	8,013	4.45
2.00	7,375	7,781	7,204	6.01
5.00	7,170	7,460	6,825	8.30
6.00	7,030	7,255	6,788	6.88
5.00	6,950	7,143	6,704	6.55
5.00	6,900	7,053	6,601	7.55
7.00	6,800	6,916	6,596	6.37
10.00	6,730	6,826	6,519	4.71

* Latent heat of water at 21°C. = 10,500 cal./mol.

4. Heat Capacity of Ammonia (Gas) and Sulfur Dioxide (Gas) [19]

$$(a) C_{p_{\text{NH}_3}} = 6.70 + 0.0063T \frac{\text{Cal}}{\text{gm mol } ^\circ\text{K}}$$

$$(b) \quad C_{P_{SO_2}} = 7.70 + 0.0053T - 8.3 * 10^{-7} T^2 \frac{\text{Cal}}{\text{gm mol } ^\circ\text{K}}$$

X. Appendix C

1. Computer program for the simulation of an adiabatic degassing process for the system H_2S -water.
2. Computer program for the simulation of an adiabatic degassing process for the system NH_3 -water and the system SO_2 -water.

MAIN

```

16 READ (5,500)PTOTAL,TEFFD,XF1,PL
   WRITE(6,602)PTOTAL,TEFFD,XF1
500 FORMAT (4F10.3)
602 FORMAT('PTOTAL= ',F8.4,'TEFFD= ',F8.3,'XF1= ',F8.5)
   IF (PTOTAL.EQ.0.0) CALL EXIT
11 PTOTAL =PTOTAL/14.7
   XF2 = 1.-XF1
   THD = 9.3987*ALOG(PTOTAL)-24.85
   CALL HDATA(HLF,XF1,TEFFD,0.,0.,TEFFD,PTOTAL)
   T =TEFFD-2.
   I=1
20 CALL DATA(T,PTOTAL,THD,Y2,X1)
   SK =(1.-Y2)/X1
   OK =Y2/(1.-X1)
   CALL HDATA(HL,X1,T,HV,Y2,TEFFD,PTOTAL)
   SAI =(HLF-HL)/(HV-HL)
   F = XF1/(1.-SAI+SK*SAI)+ XF2/(1.-SAI+OK*SAI)-1.
   IF(I.EQ.0)GO TO 10
   F1 =F
   TOLD =T
   T =T+0.01
   I =0
   GO TO 20
10 T =T-F/((F-F1)/0.01)
   I= 1
   IF (ABS(TOLD-T)-0.01 ) 30,30,20
30 WRITE (6,600) (T,X1,Y2)
600 FORMAT (4H T= ,F10.3,4H X1=,F7.5,4H Y2=,F8.5)
   PMM=PTOTAL*760.0
   WRITE(6,607)SAI,PMM
607 FORMAT(5H SAI=,F10.5,6H PMM= ,F10.3)
   PTOTAL = PTOTAL*14.7
   PTOTAL = PTOTAL-0.5
   IF (PTOTAL.LT.PL) GO TO 16
   GO TO 11
END

```

```

SUBROUTINE DATA(T,P1,TH,Y,X)
  P=P1*14.7
  Y=-9.6689-9.1243*ALOG(P)+0.85231*ALOG(P)**2-0.02829*ALOG(P)**3+
  10.056442*T-6.8678E-5*T**2+1.8741E-8*T**3+0.023154*T*ALOG(P)-
  27.6273E-6*T**2*ALOG(P)**2+9.5097E-10*T**3*ALOG(P)**3
  Y =EXP(Y)
  Y =Y/(1.+Y)
  X =5.0375+0.01128*P-2.0071E-5*P**2+1.5586E-8*P**3-0.044033*T+
  15.753E-6*T**2+8.0270E-8*T**3
  X =EXP(X)
  X =X/(1.+X)
  RETURN
END

```

HDATA

```

SUBROUTINE HDATA(HL,X,T,HV,Y,TFFF0,P)
HW = (-148.44+0.33299*T+2.4258E-3*T**2-1.9610E-6*T**3)*18.
AW = (1112.6-5.0786*T+0.02020R*T**2-3.8312E-5*T**3+2.5753E-8*T**4)*
118.
Q = -2.5922+0.11344*T-3.5701E-4*T**2+3.3231E-7*T**3
Q = EXP(Q)
T0=212.8
P0 =1.
TT=T
PP=P
CALL NEWTON(T0,VO,ALFA0,P0)
CALL NEWTON(TT,V,ALFA,PP)
H=4463.+7.15*(T-T0)+0.00166*(T**2-T0**2)+P*V-VO-ALFA*(1./V-1./VO)-
I(1./V**2-1./VO**2)+(1./V**3-1./VO**3)
HV = (1.-Y)*H+Y*(HW+AW)
HL = X*H+(1-X)*HW-X*Q
RETURN
END

```

```

SUBROUTINE NEWTON (T,V,AL,P)
A=4.1497
B=0.0514
C=0.02086
D=0.02890
E=1.79E-6
K=24.219
R=0.08206
AL=(A+3.*R*E/T**2+R*B*D*E/T**2)/2.
BF=R*T*B-A-R*E/T**2
GA=-P*T*B*D+C*A-R*B*E/T**2
DA=R*B*D*E/T**2
V=R*T/P
I=0
20 F =P*V**4-R*T*V**3-BF*V**2-GA*V-DA
SLOP=4*P*V**3-3*R*T*V**2-2*BF*V-GA
VOLD=V
V=V-F/SLOP
IF (ABS(VOLD-V)-0.001) 30,30,20
30 WRITE (6,605) V
605 FORMAT (5H V= ,F10.3)
RETURN
END

```

MAIN

```

DIMENSION XFEED(10),X(10),Y(10),H(10),HL(10),HV(10),Q(10),P(10),
HS(10),HK(10),HH(10),UK(10),
IA1(50,50),A2(50,50),A3(50,50),A4(50,50)
READ (5,500)XFEED(1),XFEED(2),XFEED(3),FQ,TFEED,PTOTAL,PL
READ (5,503) M,N,((A1(I,J),J=1,M),I=1,N)
WRITE(6,611)((A1(I,J),J=1,M),I=1,N)
READ (5,504) M,N,((A2(I,J),I=1,N),J=1,M)
WRITE(6,612)((A2(I,J),J=1,M),I=1,N)
READ (5,504) M,N,((A3(I,J),I=1,N),J=1,M)
WRITE(6,613)((A3(I,J),J=1,M),I=1,N)
READ (5,504) M,N,((A4(I,J),I=1,N),J=1,M)
WRITE(6,614)((A4(I,J),J=1,M),I=1,N)
611 FORMAT(//'A1'/(7F9.4))
612 FORMAT(//'A2'/(8F9.4))
613 FORMAT(//'A3'/(9F9.4))
614 FORMAT(//'A4'/(2F9.4))
READ(5,508) TTR
45 PTOTAL=PTOTAL+ 5.0
500 FORMAT (7F10.3)
503 FORMAT (2I5/(8F10.3))
504 FORMAT (2I2/(5F10.3))
508 FORMAT (F10.3)
C REPEAT THE LOOP AFTER NEXT STATEMENT
T=TFEED
X(1) = XFEED(1)
X(2) = XFEED(2)
X(3) = XFEED(3)
Q(1)=1.0
Q(2) = XFEED(2)/XFEED(1)
Q(3) = XFEED(3)/XFEED(1)
CALL ENTH(HL,HV,Q,T,A1)
HS(2) = Q(2)*375.5
HS(3) = Q(3)*65.0
HH(2)=HL(1)-(HS(2)+HS(3))
HH(2)=HL(2)
HH(3)=HL(3)
T=TTR
5 L=0
3 Q(1)=1
Q(2)=X(2)/X(1)
Q(3)=X(3)/X(1)
CALL DATANH(T,Q(2),P(2),A2)
CALL DATANH(T,Q(3),P(3),A3)
CALL DATAHO(T,X(1),P(1),A4)
Y(1)=P(1)/PTOTAL
Y(2) = P(2)/PTOTAL
Y(3) = P(3)/PTOTAL
WM = (18.0*Y(1)+17.0*Y(2)+64.0*Y(3))/(Y(1)+Y(2)+Y(3))
Y(1) =18.0*Y(1)/WM
Y(2) =17.0*Y(2)/WM
Y(3) =64.0*Y(3)/WM
IF (X(2).GT.0.0.AND.X(3).GT.0.0) GO TO 26
19 IF (X(2).EQ.0.0) GO TO 22
UK(3) =0.0
UK(2)=Y(2)/X(2)
GO TO 25
22 UK(2)=0.0
JK(3)=Y(3)/X(3)

```

MAIN

```

25 UK(1)=Y(1)/X(1)
   GO TO 27
26 UK(1)=Y(1)/X(1)
   UK(2)=Y(2)/X(2)
   UK(3)=Y(3)/X(3)
27 CONTINUE
   REMAIN=-1.0
   CALL ENTH(HL,HV,Q,T,A1)
   HS(2) = Q(2)*375.5
   HS(3) = Q(3)*65.0
   HL(1)=HL(1)-(HS(2)+HS(3))
   SAI=0.0
   SUM=0.0
   DO 105 I=1,3
   DO 102 J=1,3
   DO 100 K=1,3
100 SUM=SUM+(UK(K)*HV(K)-HL(K))*X(K)
102 SAI=SAI+(XFEEED(J)*HH(J)-HL(J)*X(J))/SUM
105 REMAIN=REMAIN+UK(I)*XFEEED(I)/(1.0-SAI+UK(I)*SAI)
   IF(L.EQ.1) GO TO 30
   R1=REMAIN
   L=L+1
   TOLD=T
   T=T+0.001
   GO TO 3
30 R2=REMAIN
   SLOP=(R2-R1)/0.001
C   BY NEWTON RAMPHUNSON METHOD
   T=T-R2/SLOP
   DT=ABS(TOLD-T)
   IF(DT.LT.0.001) GO TO 9
   DO 10 I=1,3
10 X(I)=XFEEED(I)/(1.0-SAI+UK(I)*SAI)
   GO TO 5
9   DO 32 I=1,3
   X(I)=XFEEED(I)/(1.0-SAI+UK(I)*SAI)
   Y(I)=UK(I)*XFEEED(I)/(1.0-SAI+UK(I)*SAI)
32 CONTINUE
C   PRINT ALL VARIABLES NEEDED
60 WRITE (6,600)(XFEEED(I),I=1,3),T,SAI,(X(I),I=1,3),(Y(I),I=1,3)
600 FORMAT (68H FEED COMPOSITIONS   TEMPERATURE FEED RATIO COMPOSITION
1   X AND Y /3F6.4,2F10.4,5X,6F6.4)
   WRITE (6,601) REMAIN,(X(I),I=1,3)
601 FORMAT (12H REMAIN   X/1H ,F10.5,2X,F10.4,2X,F10.4,2X,F10.4)
   IF (PTOTAL.GT.PL )GO TO 46
   GO TO 45
46 READ(5,500) (XFEEED(I),I=1,3),TFEED,PTOTAL,PL
   IF (XFEEED(1).EQ.0.0) CALL EXIT
   WRITE (6,605)
605 FORMAT(//' NEW FEED OUTPUT'//)
   GO TO 45
   END

```


ENTH

```
      SUBROUTINE ENTH(HL,HV,Q,T,A)
      DIMENSION HL(10),HV(10),Q(10),A(50,50)
      I=2
20  IF (T-A(I,1)) 41,30,30
30  I=I+1
      GO TO 20
41  CONTINUE
      DO 50 J=2,4
40  HL(J-1)=A(I,J)*(T-A(I-1,1))/(A(I,1)-A(I-1,1))+A(I-1,J)*(A(I,1)-T)/
      1 (A(I,1)-A(I-1,1))
50  CONTINUE
      DO 100 J=5,7
10  HV(J-4)=A(I,J)*(T-A(I-1,1))/(A(I,1)-A(I-1,1))+A(I-1,J)*(A(I,1)-T)/
      1 (A(I,1)-A(I-1,1))
100 CONTINUE
      RETURN
      END
```

DATANH

```

SUBROUTINE DATANH(T,Q,P,A)
DIMENSION A(50,50)
J=2
3  IF (1-A(1,J)) 10,15,20
20 J=J+1
GO TO 3
10 J1=J-1
J2=J
I=2
2  IF (Q-A(I,1)) 30,35,40
30 I=I+1
GO TO 2
40 I1=I-1
I2=I
IF (A(I1,J2)-0.0) 66,66,77
66 P=0.0
GO TO 6
77 IF (A(I2,J1)-0.0) 88,88,70
88 P=0.0
GO TO 7
85 IF (A(I,J1)-0.0) 99,99,33
99 P=0.0
GO TO 9
93 IF (A(I,J2)-0.0) 55,55,70
55 P=0.0
GO TO 9
15 I=2
18 IF (Q-A(I,1)) 12,16,17
12 I=I+1
GO TO 18
16 P=A(1,J)
GO TO 9
17 IF (A(1,J)-0.0) 101,101,102
101 P=0.0
GO TO 9
102 IF (A(I-1,J)-0.0) 201,201,70
201 P=0.0
GO TO 9
70 J1=J-1
J2=J
I1=I-1
I2=I
DQ = A(I1,1)-A(I2,1)
DT = A(1,J2)-A(1,J1)
DQL = Q-A(I2,1)
DQH = A(I1,1)-Q
P1 = (DQL/DQ)*A(I1,J1)+(DQH/DQ)*A(I2,J1)
P2 = (DQL/DQ)*A(I1,J2)+(DQH/DQ)*A(I2,J2)
100 DTL = T-A(1,J1)
DTR = A(1,J2)-T
P = (DTL/DT)*P2+(P1*DTR)/DT
9 CONTINUE
RETURN
END

```

DATAHO

```
SUBROUTINE DATAHO(T,Q,P,A)
DIMENSION A(50,50)
I=2
20 IF (T-A(I,1)) 40,30,30
30 I=I+1
   GC TO 20
40 CONTINUE
   DT=A(I,2)-A(I-1,1)
   DH=A(I,1)-T
   DL=T-A(I-1,1)
   P1=(A(I,2)*DL+A(I-1,2)*DH)/DT
   P=P1*Q
   RETURN
END
```


3

0.0	32.0000	42.6000	50.0000	59.0000	68.0000	96.0000	134.0000	172.0000
0.7000	64.0000	85.7000	0.0	0.0	0.0	0.0	0.0	0.0
0.1500	47.4000	63.7000	72.0000	0.0	0.0	0.0	0.0	0.0
0.1000	30.0000	41.7000	47.4000	56.7000	69.8000	0.0	0.0	0.0
0.0700	22.8000	30.7000	34.9000	41.9000	51.7000	68.8000	0.0	0.0
0.0500	14.8000	19.8000	22.6000	27.0000	33.6000	45.2000	14.0000	0.0
0.0200	6.9000	9.2000	10.5000	12.7000	16.1000	21.6000	6.6500	0.0
0.0100	3.8000	5.1000	5.9000	7.1000	9.2000	12.5000	32.2000	45.8000
0.0100	23.3000	31.0000	37.0000	44.0000	59.0000	79.0000	186.0000	266.0000
0.0070	15.2000	20.6000	23.6000	28.0000	39.0000	52.0000	121.0000	172.0000
0.0050	9.9000	13.5000	15.6000	19.3000	26.0000	36.0000	87.0000	116.0000
0.0030	5.1000	6.9000	7.9000	10.0000	14.1000	19.7000	57.0000	82.0000
0.0020	2.8000	3.7000	4.6000	5.7000	8.5000	11.9000	13.3000	21.0000
0.0010	1.9000	2.6000	3.1000	3.8000	5.8000	8.1000	12.9000	20.0000
0.0005	1.2000	1.5000	1.7500	2.2000	3.2000	4.7000	7.5000	12.0000
0.0001	0.6000	0.7000	0.7500	0.8000	1.2000	1.7000	2.8000	4.0000
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

4

0.0	1.0000
32.0000	4.5872
42.0000	6.7596
50.0000	9.2050
60.0000	13.2436
68.0000	17.5209
80.0000	31.8262
104.0000	59.2704
122.0000	92.4560

FEED COMPOSITIONS

TEMPERATURE FEED RATIO COMPOSITION X AND Y

.76100.21800.0	43.4313	0.0587	0.8260.17430.0	0.06000.91880.0
REMAIN X				

0.0000+	0.8260	0.1743	0.0	
FEED COMPOSITIONS	TEMPERATURE	FEED RATIO	COMPOSITION	X AND Y

.78100.21800.0	44.7658	0.0570	0.82460.17560.0	0.06040.91900.0
REMAIN X				

0.00001	0.8246	0.1756	0.0	
FEED COMPOSITIONS	TEMPERATURE	FEED RATIO	COMPOSITION	X AND Y

.78100.21800.0	46.1170	0.0555	0.82320.17690.0	0.06070.91930.0
REMAIN X				

0.00000	0.8232	0.1769	0.0	
FEED COMPOSITIONS	TEMPERATURE	FEED RATIO	COMPOSITION	X AND Y

.78100.21800.0	47.4294	0.0537	0.82190.17820.0	0.06090.91970.0
REMAIN X				

0.00002	0.8219	0.1782	0.0	
FEED COMPOSITIONS	TEMPERATURE	FEED RATIO	COMPOSITION	X AND Y

.78100.21800.0	48.7221	0.0521	0.82050.17940.0	0.06110.92020.0
REMAIN X				

0.00005	0.8205	0.1794	0.0	
FEED COMPOSITIONS	TEMPERATURE	FEED RATIO	COMPOSITION	X AND Y

.78100.21800.0	49.9959	0.0505	0.81930.18070.0	0.06120.92060.0
REMAIN X				

0.00001	0.8193	0.1807	0.0	
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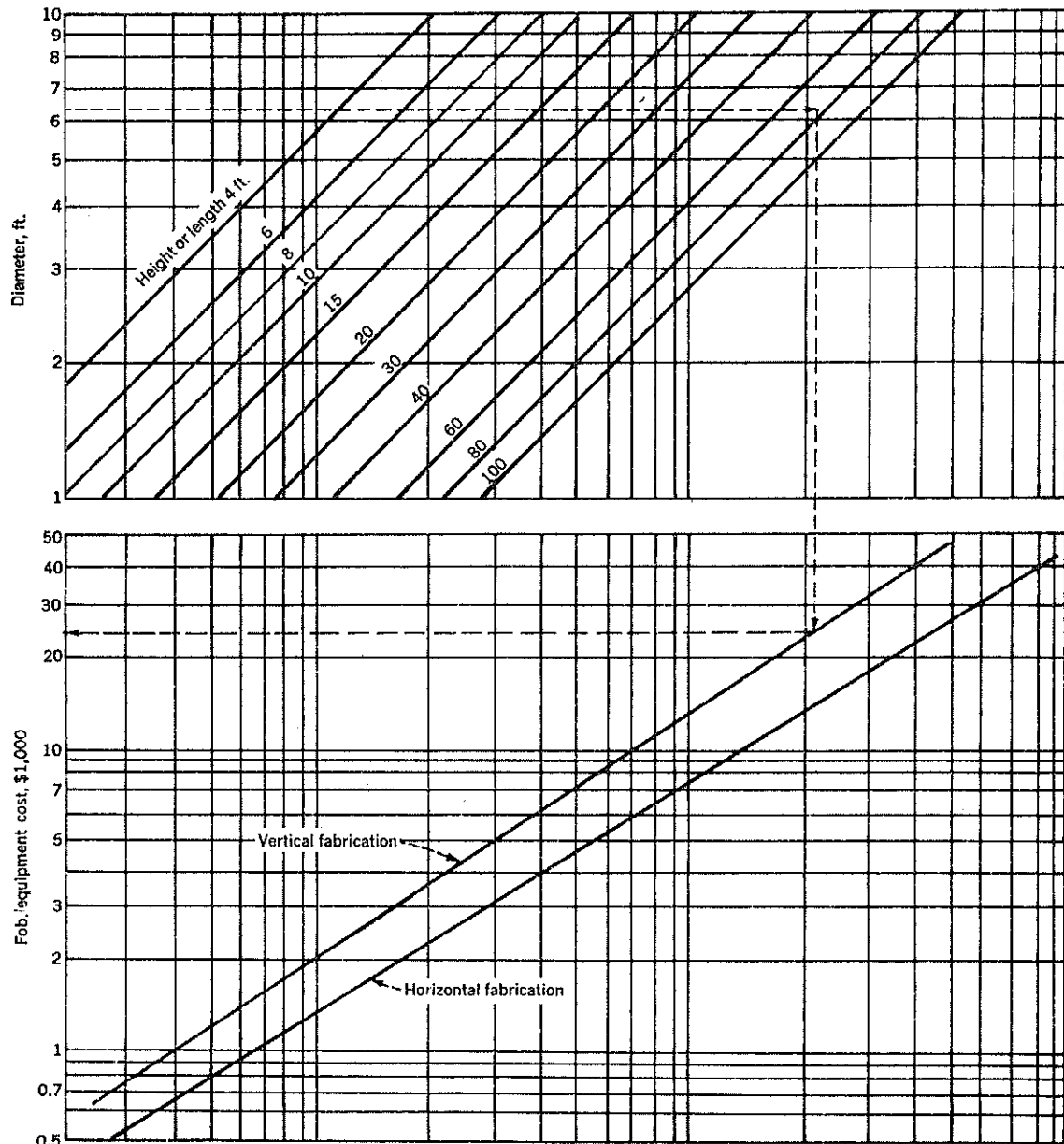
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.78100.21800.0 REMAIN X 0.00000	50.9072	0.0493	0.81830.18150.0	0.06120.92110.0
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.78100.21800.0 REMAIN X 0.00000	51.0087	0.0482	0.81740.18240.0	0.06120.92150.0
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.78100.21800.0 REMAIN X 0.00004	52.7014	0.0471	0.81660.18320.0	0.06120.92190.0
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.78100.21800.0 REMAIN X 0.00001	53.5876	0.0460	0.81570.18410.0	0.06110.92240.0
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.78100.21800.0 REMAIN X 0.00003	54.4618	0.0449	0.81480.18490.0	0.06110.92280.0

NEW FEED OUTPUT

FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.99330.0 REMAIN X 0.00000	0.0057	66.0758	0.0226	0.99920.0 0.0007
FED COMPOSITIONS	TEMPERATURE	FED RATIO	COMPOSITION	X AND Y
.99330.0 REMAIN X 0.00000	0.0067	66.9146	0.0189	0.99910.0 0.0009

X. Appendix D. Cost Data

A. Flash Chamber [33]



Required
 Diameter, ft.
 Length, ft.
 Design pressure, psig
 Shell material
 Fabrication (horiz. or vert.)

Time base
 Mid-1968
Exponent
 Size exponent vertical 0.65
 horizontal 0.60

Included
Vertical:
 Shell and 2 heads
 Nozzles and manways
 Skirt, base ring and lugs
 Tray supports

Basis of chart
 Carbon steel material
 50-psig. design pressure
 Average nozzles and manways
 ASME code construction
 Shop fabrication

Horizontal:
 Shell and 2 heads
 Nozzles and manways
 Saddles, 2

Flash Chamber (cont'd)

Process Vessel Cost, \$ = [Base cost × F_m × F_p]/Index

Adjustment factors

Shell Material	F_m		Pressure Factor	
	Clad	Solid	Psi.	F_p
Carbon steel	1.00	1.00	Up to 50	1.00
Stainless 316	2.25	3.67	100	1.05
Niocl	3.89	6.34	200	1.15
Titanium	4.23	7.89	300	1.20
			400	1.35
			500	1.45
			600	1.60
			700	1.80
			800	1.90
			900	2.30
			1,000	2.50

Field installation modules

Vertical fabrication

Module	5A (V)	5B (V)	5C (V)	5D (V)	5E (V)
Base dollar magnitude, \$100,000	Up to 2	2 to 4	4 to 6	6 to 8	8 to 10
Equipment fab. cost, E	100.0	100.0	100.0	100.0	100.0
Piping	60.0	59.6	59.5	59.4	59.3
Concrete	10.0	9.9	9.8	9.8	9.8
Steel	8.0	7.9	7.8	7.8	7.8
Instruments	11.5	11.5	11.4	11.3	11.3
Electrical	5.0	4.9	4.9	4.9	4.9
Insulation	8.0	8.0	8.0	8.0	8.0
Paint	1.3	1.3	1.3	1.3	1.3
Field materials, m	103.8	103.1	102.7	102.5	102.4
Direct material, E + m = M	203.8	203.1	202.7	202.5	202.4
Material erection	84.0	83.5	83.2	83.0	82.9
Equipment setting	15.2	14.9	14.0	13.5	13.2
Direct field labor, L	99.2	98.5	97.2	96.5	96.1
Direct M & L cost	303.0	301.6	299.9	299.0	298.5
Freight, insurance, taxes	8.0	8.0	8.0	8.0	8.0
Indirect cost	112.0	102.5	98.9	98.7	95.5
Base module cost	423.0	412.1	406.8	405.7	402.0
L/M ratios	0.48	0.47	0.47	0.47	0.46
Material factor, E + m	2.04	2.03	2.03	2.02	2.02
Direct cost factor, M & L	3.03	3.02	3.00	2.99	2.98
Indirect factor	0.37	0.34	0.33	0.33	0.32
Module factor (norm)	4.23	4.12	4.07	4.06	4.02

Note: All data are based on 100 for equipment, E.
Dollar magnitudes are based on carbon steel.

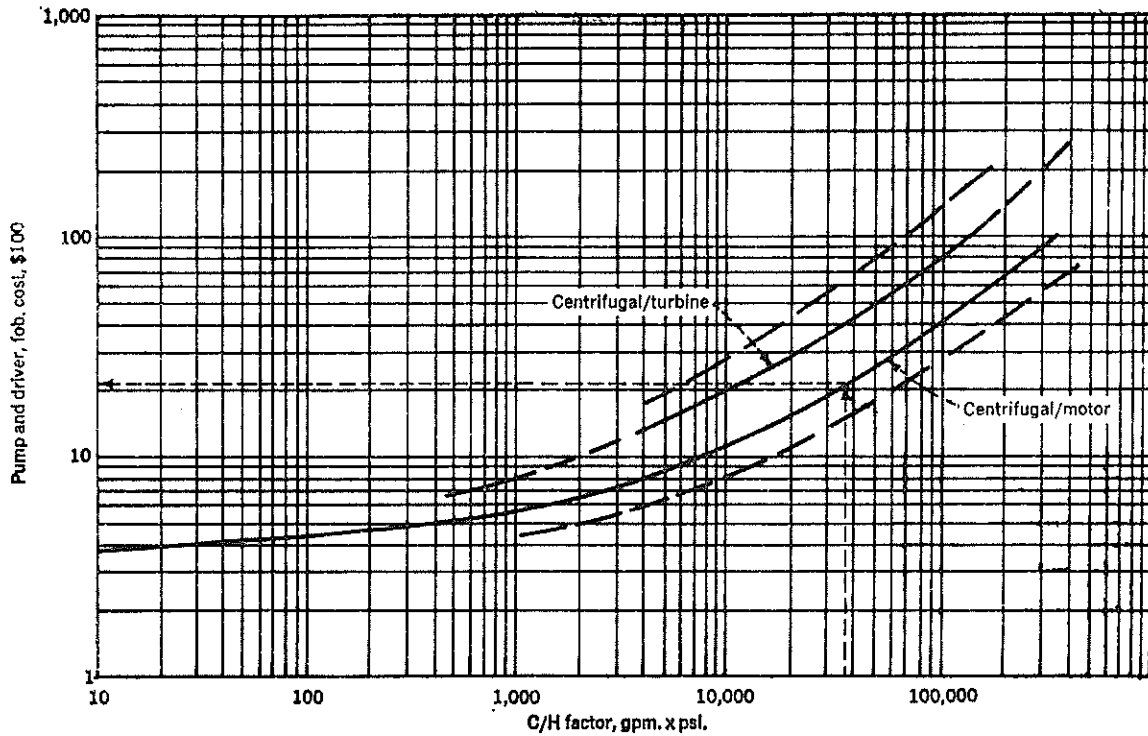
Field installation modules

Horizontal fabrication

Module	5A (H)	5B (H)	5C (H)	5D (H)	5E (H)
Base dollar magnitude, \$100,000	Up to 2	2 to 4	4 to 6	6 to 8	8 to 10
Equipment fab. cost, E	100.0	100.0	100.0	100.0	100.0
Piping	41.1	40.1	39.7	39.4	39.2
Concrete	6.2	6.1	6.0	5.9	5.9
Steel	—	—	—	—	—
Instruments	6.2	6.1	6.0	5.9	5.9
Electrical	5.2	5.1	5.0	5.0	5.0
Insulation	5.2	5.1	5.0	5.0	5.0
Paint	0.5	0.5	0.5	0.5	0.5
Field materials, m	64.5	63.0	62.2	61.7	61.5
Direct material, E + m = M	164.5	163.0	162.2	161.7	161.5
Material erection	52.2	51.0	50.4	50.0	49.8
Equipment setting	9.3	8.3	7.7	7.2	7.0
Direct field labor, L	61.5	59.3	58.1	57.2	56.8
Direct M & L cost	226.0	222.3	220.3	219.0	218.3
Freight, insurance, taxes	8.0	8.0	8.0	8.0	8.0
Indirect cost	83.6	75.6	72.7	72.3	69.8
Base module cost	317.6	305.9	301.0	299.3	296.1
L/M ratios	0.37	0.36	0.35	0.35	0.35
Material factor, E + m	1.64	1.63	1.62	1.62	1.61
Direct cost factor, M & L	2.26	2.22	2.20	2.19	2.18
Indirect factor	0.37	0.34	0.33	0.33	0.32
Module factor (norm)	3.18	3.06	3.01	2.99	2.96

Note: All data are based on 100 for equipment, E.
Dollar magnitudes are based on carbon steel.

B. Vacuum Pump



Required
Capacity, gpm.
Differential pressure, psi.
Suction pressure, psig.
System temp., °F.
Casing material

Time base
Mid-1968

Exponent
Average exponent 0.52

Included
Pumping unit
Driver and coupling
Base plate

Centrifugal Pump Cost, \$ = [Base cost × F_m × F_o]/index

Adjustment factors

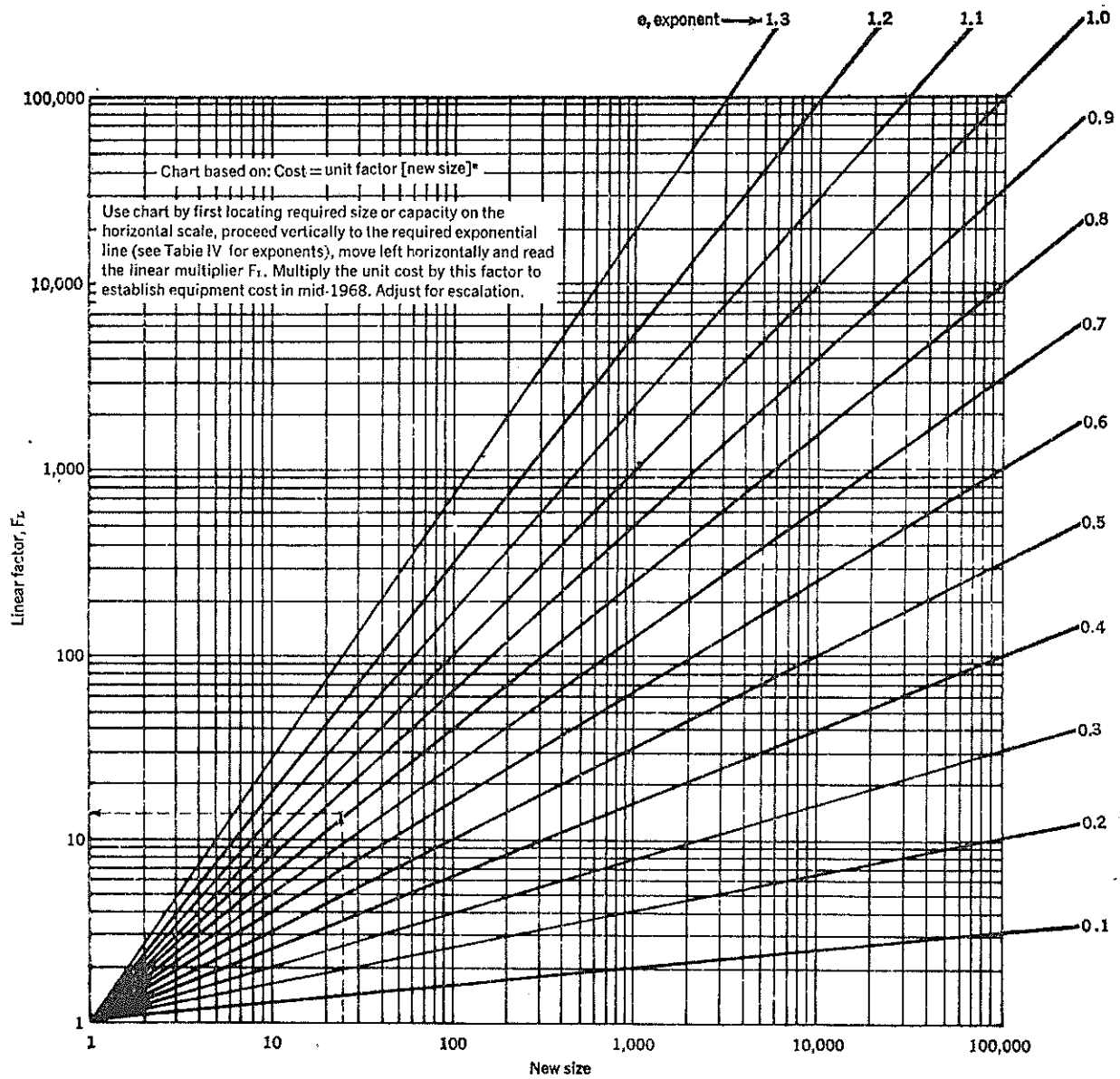
Material	F_m	Operating Limits			Max. value
		Suction pressure, psig.	250	500	
Cast iron	1.00				
Bronze	1.28				
Cast steel	1.32				
Stainless	1.93				
Carpenter 20	2.10				
Worthite	2.44				
Hastelloy C	2.89				
Monel	3.23				
Nickel	3.40				
Titanium	8.98				
		System temperature, °F.	250	350	850
		Factor F_o	1.0	1.5	1.9

Field installation modules

Module	Field installation modules				
	GA	6B	GC	GD	GE
Base dollar magnitude, \$100,000	Up to 2	2 to 4	4 to 6	6 to 8	8 to 10
Equipment fob. cost, E	100.0	100.0	100.0	100.0	100.0
Piping	30.2	29.8	29.6	29.5	29.4
Concrete	4.0	3.9	3.9	3.9	3.9
Steel	—	—	—	—	—
Instruments	3.0	2.9	2.9	2.9	2.9
Electrical	31.0	30.5	30.3	30.3	30.2
Insulation	2.5	2.5	2.5	2.4	2.4
Paint	0.8	0.8	0.8	0.8	0.8
Field materials, m	71.5	70.4	70.0	69.8	69.6
Direct material, $E + m + M$	171.5	170.4	170.0	169.8	169.6
Material erection	60.0	59.2	59.0	58.6	58.5
Equipment setting	9.7	9.7	8.9	8.7	8.6
Direct field labor, L	69.7	68.4	67.9	67.3	67.1
Direct M & L cost	241.2	238.8	237.9	237.1	236.7
Freight, insurance, taxes*	8.0	8.0	8.0	8.0	8.0
Indirect cost	89.2	81.2	78.5	78.2	75.7
Base module cost	338.4	328.0	324.4	323.3	320.4
L/M ratios	6.41	0.40	0.40	0.40	0.40
Material factor, $E + m$	1.72	1.70	1.70	1.70	1.69
Direct cost factor, M & L	2.41	2.39	2.38	2.37	2.36
Indirect factor	0.37	0.34	0.33	0.33	0.32
Module factor (norm)	3.38	3.28	3.24	3.23	3.20

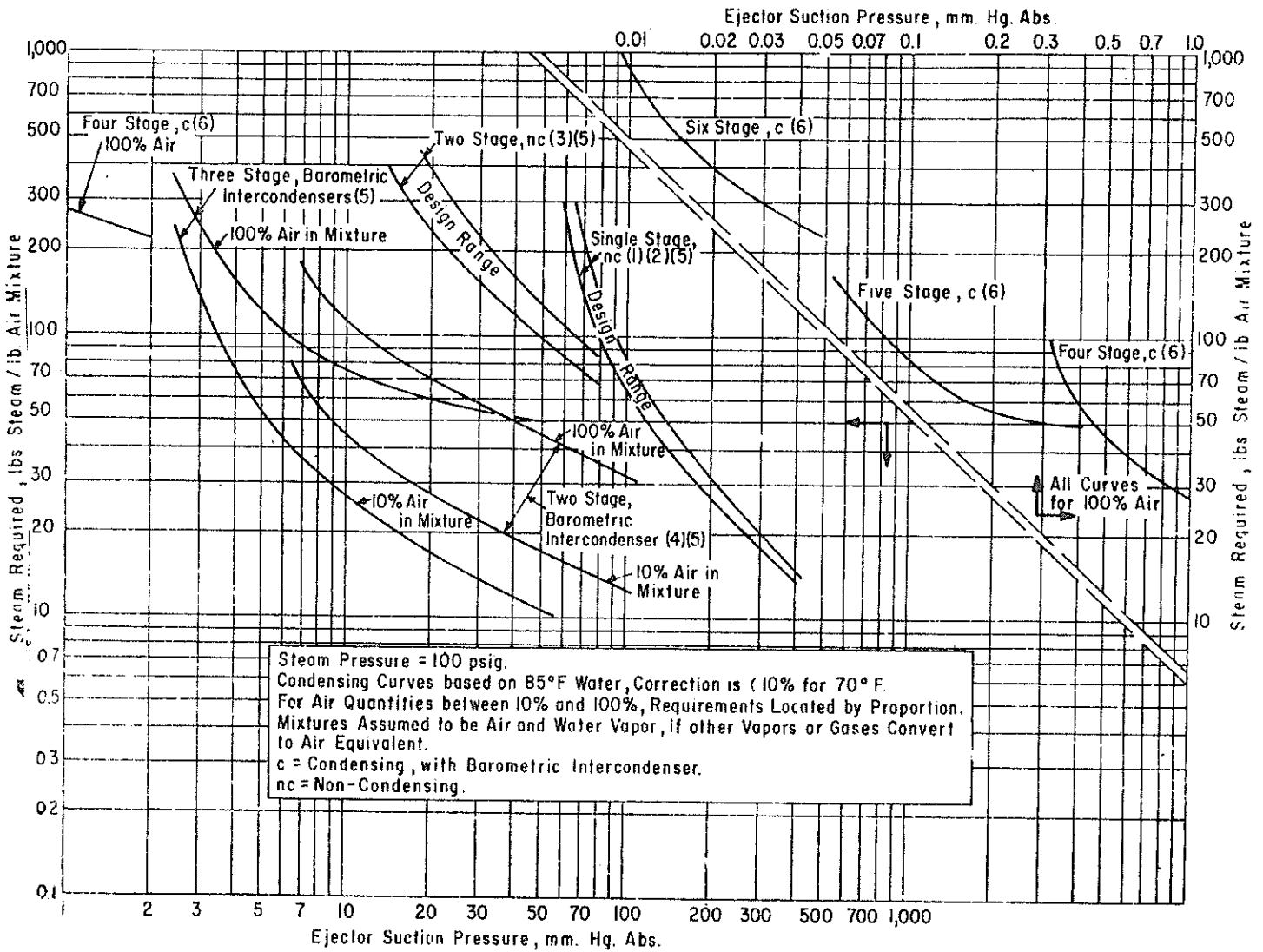
Note: All data are based on 100 for equipment, E .
Dollar magnitudes are based on carbon steel.

C. Ejector



	Unit	Unit Cost \$	Size Exponent	Field Installation Factor	L/M Ratio
Ejectors (cap.)					
4 in. Hg suction.....	Lb./hr.	2,000	0.79	1.10	0.10
6.....	Lb./hr.	200	0.67	1.10	0.10
10.....	Lb./hr.	200	0.55	1.10	0.10
4-stage barometric					
2.5 mm. Hg suction.....	Lb./hr.	2,500	0.45	1.12	0.12
5.0.....	Lb./hr.	1,400	0.48	1.12	0.12
10.0.....	Lb./hr.	900	0.53	1.12	0.12
20.0.....	Lb./hr.	700	0.54	1.12	0.12
5-stage barometric					
0.5-mm. Hg suction.....	Lb./hr.	4,200	0.50	1.15	0.15
0.8.....	Lb./hr.	3,200	0.50	1.15	0.15
1.0.....	Lb./hr.	2,800	0.48	1.15	0.15
1.4.....	Lb./hr.	2,500	0.49	1.15	0.15

F. Ejector Steam Usage



D. Utilities Prices (Self-generated)

1. Steam (100 psig) \$1.00/1000 lbs
2. Electricity \$0.02/KWH

E. Sample Calculations

Data: Table 3 in text

1. Steam usage for ejector 1.1 lbs steam/lb mixture
Ref. Figure 6-25, Vol. I, Reference #22.
2. Total lbs mixture based on 1000 lbs moles
Feed/unit time = 205 lbs
3. Total steam required = 226 lbs
4. Cost of steam = 22.6¢ or \$.226/min
5. Equivalent cost of electricity

$$a. \text{ Work} = - \int_{P_1}^{P_2} V dP = \int_{P_1}^{P_2} \frac{nRT}{P} dP$$

Assume discharge pressure $P_2 = 5 \text{ psig} = 1018 \text{ mm Hg}$

$$W = 6.29 \times 2 \frac{\text{BTU}}{\text{lb mole } ^\circ\text{R}} * 545^\circ\text{R} * \ln \frac{1018}{491}$$

$$W = -4990 \text{ BTU} = 1.47 \text{ KWH}$$

Assume Efficiency = 50%

$$b. \text{ Total KWH} = 3.0$$

$$\text{Cost of Electricity} = \$0.06$$

$$\text{Average molecular weight of feed} = .01 * 34 + .99 * 18 = .34 + 17.82$$

$$= 18.16 \text{ lbs/lb mole}$$

$$\text{Weight of feed} = 18.16 * 10^3 \text{ lbs/unit time} = 2180 \text{ gallons/unit time (min)}$$

6. Flash Chamber Size

$$\text{Vapor Volume} = 6.29 \text{ lb mole} * \left(\frac{359 \text{ ft}^3}{\text{lb mole}} \right) \left(\frac{545^\circ\text{R}}{492^\circ\text{R}} \right) \left(\frac{760}{491} \right) = 3870 \text{ ft}^3/\text{min}$$

$$= 64.5 \text{ ft}^3/\text{sec}$$

Linear Velocity < 2 ft/sec

$$\text{Vessel Diameter} = \left(\frac{4 * 64.5 \text{ ft}^3/\text{sec}}{3.1416 * 2 \text{ ft}/\text{sec}} \right)^{1/2} = 6.4 \text{ ft diameter}$$

Vessel Height = 30.65 ft (based on Figure 2 text)

Vessel Cost = \$53,000 (Stainless 316 (100 psig rating))