PERFORMANCE AND ECONOMICS OF AIR STRIPPING TOWER WITH OFF-GAS CONTROL BY EITHER GAS-PHASE CARBON ADSORPTION OR PLASMA REACTOR IN COMPARISON TO LIQUID-PHASE

CARBON ADSORPTION

BY

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CHAPTER I

INTRODUCTION

The concern about groundwater quality has increased as a result of the numerous times that various organic pollutants have been discovered in groundwater in the United States. Since groundwater constitutes a large portion of water used, 63% of total water used in Oklahoma and 39% of United States as a whole (1), the potential health threat to the public is expected. The sources of contamination are diverse, such as underground storage-tanks and pipe line leakages, fertilizers and pesticides applied to land area, land application of municipal and industrial wastes, and oil field brines. The best way to protect groundwater quality will be the prevention of contamination before it occurs. Once groundwater is contaminated, treatment requires a great deal of time and effort.

The Environmental Protection Agency (EPA) reported that the three most frequently detected volatile organic chemicals (VOCs) in groundwater were trichloroethylene (TCE), tetrachloroethylene (PCE), and 1,1,1 trichloroethene (2). This study used TCE as a target contaminant, while many other VOCs were also studied.

There are several technologies commonly used to treat

groundwater contaminated with VOCs. Following are the most common technologies:

Activated Carbon Adsorption: Contaminated groundwater, pumped up through an extraction well, can be subjected to contact with granular or powdered activated carbon. The large surface area of activated carbon intercepts the hazardous constituents from water. Activated carbon is generally known as an effective and reliable means of removing low solubility organics.

Air Stripping: Air stripping is a physical process in which a countercurrent air-water interface causes volatile materials to partition into the gas-phase. An air stripping tower (AST) is packed with various inert material to increase turbulence and surface area.

There are some more alternatives such as biological treatment and membrane processes. Yet, any single method hardly gives a perfect solution which is economically sound and technically feasible for all pollutants. Conventional water treatment consisting of coagulation, sedimentation, and filtration has been reported to be ineffective for reducing VOCs (3, 4).

The studies of Hand *et al.* (5) showed that two methods, granular activated carbon (GAC) adsorption and packed tower air stripping (AST), are the most viable methods for VOC removal. In the GAC system, however, the adsorbent must be regenerated and the regenerant must be processed to isolate the original adsorbates. This process increases the total

cost of the system. Adsorption is generally a more expensive process than an AST, depending on the contaminant (6, 7).

Therefore, ASTs are often the least cost and most popular method to remove VOCs provided the pollutants are volatile. TCE is a very good candidate for air stripping in this sense. Additional reasons to choose the ASTs are:

- * Easy to operate with minimum skill
- * Less operation and management (O & M) cost than carbon adsorption
- * Aerating to remove one specific contaminant also reduces concentrations of other VOCs.

There are several types of aerators available to treat contaminated water: packed tower, tray, and spray aeration. Approximately two-thirds of the aerators installed within the United States for VOC control are packed towers (8). Therefore, only packed tower air stripping (AST) was considered in this study.

With all the advantages listed above, however, air stripping does not permanently remove the VOCs from the environment. It removes the VOCs from the liquid-phase and places it in the vapor-phase. So, water pollution is just transferred to air pollution. Regulations concerning the air pollution have become more stringent. Due to the additional cost of off-gas control, it is not clear which process, AST+off-gas control or liquid-phase GAC, is most economical. There is a need for an engineered procedure to determine the best available technology, or for other innovative off-gas control technology.

There were two objectives in this study:

Objective 1 (First part of the study): Cost is an important consideration in the evaluation of choices among various types of technologies. The first objective of this study was to present a method which allowed preliminary cost estimations of ASTs with off-gas control, and liquid-phase GAC system. The method presented also finds the optimum design and operating condition of the AST systems (AST+offgas control, or AST alone). The optimum, here, means that the combined treatment cost of the air stripping and the off-gas treatment is the minimum.

Gas-phase adsorption onto activated carbon is assumed to be used as the off-gas control because it is currently considered the standard technology. The rationale behind using a gas-phase GAC contactor is that the GAC usage rate is much less than liquid-phase and adsorption kinetics are much faster, thus the required bed volume is smaller than liquid-phase (9). The first part of this study shows the domain of operating conditions and system configuration of AST+gas-phase GAC in which the process is more cost efficient than liquid-phase GAC system. In order to accomplish this task, a computer program was developed by employing or modifying currently accepted models for each process.

Objective 2 (Second part of the study):

It would be ideal if there is a method that incinerates and ultimately disposes of the toxic wastes in an air stream rather than gas-phase adsorption. Recently, plasma reactors (discharge reactors) were tested using electrical energy at the School of Chemical Engineering, Oklahoma State University (OSU) (10). The study was not intended to treat the off-gases from ASTs. The second part of this study investigated the possibility of using a plasma reactor as the off-gas control technology for an AST.

CHAPTER II

LITERATURE REVIEW

Previous Studies on the Cost Estimations of the AST and GAC Systems

No study has been conducted to develop a method for total system design that allows the optimum design of an AST with off-gas control and a comparison to a liquid-phase GAC system on a cost basis. A few preliminary attempts are seen in the literature. Adams and Clark (11, 12, 13, 14) conducted a series of cost evaluation studies. They (11) presented a cost estimating equation and the parameters for liquid-phase GAC system. Using the cost data of liquidphase GAC systems and a GAC adsorption model, they showed various cost estimates for liquid-phase GAC treatment systems (12). They (13, 14) also estimated the cost of ASTs with GAC off-gas treatment, and compared it to a liquidphase GAC system. However, they did not provide a tool to do the estimation in one model. They treated the system as two separate unconnected units. Without such a tool, optimization of the design and operating conditions of the systems (AST+off-gas control, or AST alone) is almost impossible because of the large number of simulations required. The previous studies also did not investigate the

designs and costs of multicomponent systems. The first objective of this study was to develop a method to optimize the AST+gas-phase GAC processes and to investigate multicomponent systems. In order to accomplish this task, a computer program was developed by employing or modifying currently accepted models for each process. Important aspects of the AST and GAC units (gas and liquid-phase) are discussed below:

AST Design Model

The mass transfer rate of the air stripping process has been successfully predicted by the Onda correlation (15, 16). Using this relationship, David Hand developed a program to design an AST (17). The program (PTAD) was originally written in BASIC language and required the user to input values during program operation. In this study, the design procedure was rewritten in FORTRAN to be consistent with other programs in this study. An input file was prepared for a convenience. Also, the program was modified for multicomponent stripping. The A/W ratios and mass transfer coefficients for all compounds were examined, and the largest values were used for the design of multicomponent system.

Major Operating Variables of AST and Optimization

In order to optimize the AST system, the key operating

variables of the AST should be identified. There are three operating variables that are controllable or can be manipulated in ASTs, air-to-water (A/W) ratio, gas pressure drop, and water loading rate. These three variables are correlated with each other. If any two of the three variables are arbitrarily selected, the remaining one variable is determined automatically. For example, any combination of A/W ratio and pressure drop produces a specific water loading rate as shown in the generalized pressure drop correlation generated by Eckert (18).

In this study, the A/W ratio and the pressure drop were varied over a wide range of possible designs to find the optimum combination of the three major variables of the AST. At the same time, water flow rate was also varied such that the new combination of the all variables (the major variables of AST and water flow rate) is made. The optimum combination of the variables was determined by considering the total cost which included both capital and operating costs.

As the A/W ratio increases, the tower volume decreases. Then, the operating cost of the tower will increase due to increased blower power requirements while the capital cost will decrease. The volume of the off-gas will increase resulting in an increased capital cost for off-gas treatment. The increase in off-gas volume and decrease in contaminant concentration will decrease VOC loading per unit carbon and increase the carbon usage rate of the gas-phase GAC contactor.

As the gas pressure drop increases, the tower volume decreases also. The operating cost of the tower will increase as the capital cost will decrease.

Any variable or parameter that has an effect on the design of an AST also affects the gas-phase GAC in this study, and vice versa, because the optimum design of each process is determined from the total cost of the two processes. For example, variation in the Henry's constant (parameter) seems to have nothing to do with the design of gas-phase GAC. However, it perturbs the configuration and cost of air-stripping, thus yielding a new set of design parameters for both processes. That is, because the combined system of AST and gas-phase GAC unit is designed as a package, best design is whatever yields lowest total cost for whole system.

The model used in this study describes an integrated system (AST+gas-phase GAC). Because of many processes and input variables involved, the total system is not easily expressed as a mathematical equation. In other words, the cost could not be written in equation form as a function of each variable. Therefore, many formal optimization techniques may not be applicable in this system. So, the optimization of the system was conducted using the enumeration technique which entails running the key operating variables independently in small increments and determining the least total cost in the range examined. The range for each variable examined (A/W ratio and pressure drop) was bounded by values considered to be in the normal range. The exact values of these bound are set out in the method section.

There should be an optimum combination of the operating variables that minimize the over all costs of the ASTs and off-gas treatment system. This study tried to find the optimum condition under a given treatment objective.

> Theories Regarding Adsorption onto GAC: Polanyi Adsorption Theory, Dubinin-Radushkevich Isotherm, and Freundlich Isotherm

The first part of this study uses some existing models for GAC adsorption. The adsorption in the models was described by the Dubinin-Radushkevich (D-R) isotherm in gasphase GAC (9, 19, 20, 21), and by the Freundlich isotherm in liquid-phase GAC. The D-R isotherm was based on the Polanyi theory. Also, the Freundlich isotherm can be explained by the Polanyi theory.

Polanyi theory is described by Manes (22). Polanyi theory assumes a fixed-pore volume within a GAC. The fixed volume (W_0) is the maximum space available for adsorption. The force of attraction depends on the component's proximity to the surface of the GAC. The adsorption potential (E) is defined as the free energy that is needed to remove any adsorbate from the adsorption site to the solvent. The

correlation curve between the space volume adsorbed (W) and adsorption potential per molar volume (E/V) for a specific GAC is known as the Polanyi plot. The corresponding equation is:

 $\ln W = A(E/V)^{B} + \ln C$ in which; A, B, C = constants

$$C = W_{o}$$

Dubinin and Radushkevich developed an equation (D-R equation) to describe single-component gas-phase adsorption equilibria which was based on the Polanyi potential theory (23). The Freundlich isotherm is a special case of the Polanyi theory where B = 1 so that a straight line is plotted, whereas the D-R equation predicts a slight curvature. The D-R equation was used to correlate the gasphase isotherms of several VOCs in the following form (9, 19, 20, 21):

Rasmuson determined the values of 0.46 and 3.37E-8 for W_0 and B using toluene and the Calgon's BPL carbon (20, 21). With the values of W_0 and B for the carbon, and R known, the equation becomes:

 $q = (0.46E6*\rho/MW)exp(-1.33E-7*(T/\beta*ln(Ps/PP))^{2})$

No significant differences in GAC capacity for VOCs were expected for the commercially available GACs with the highest VOC capacity (9). The Calgon's BPL GAC has been the industrial standard gas-phase GAC for several years (24) and used in this simulation. Table I shows the properties of the BPL carbon (24).

TABLE I

PROPERTIES OF BPL GAC

Average Diameter; 0.3715 cm Apparent Density; 0.85 g/cm³ Density of Carbon; 2.1 g/cm³ Particle Void Fraction; 0.595

Temperature and Humidity Effect on Gas-Phase Adsorption

At a high relative humidity, many of the small pores of GAC will be filled with condensed water, thus decreasing the effective dry surface. By heating the air to lower the relative humidity, more dry surface will be available for gas-phase adsorption. However, the D-R equation also shows that heating will have an adverse effect on adsorption capacity by increasing the temperature and vapor pressure. A study shows that the opposite effects of relative humidity and temperature balance out at 40 - 50 % relative humidity (9, 24); thus maximum capacity is determined. In this study, off-gas from the AST was assumed to be heated to obtain 40 % relative humidity (RH) for maximum capacity.

Multicomponent Adsorption Theory

It is unlikely that any natural waters are contaminated by single-solute organics. The Ideal Adsorbed Solution Theory (IAST) has been used successfully in predicting multicomponent system behavior (25, 26, 27). The IAST model assumes thermodynamic equivalence of the spreading pressure (π) of each solute at equilibrium. The spreading pressure, π , is defined as the difference between the interfacial tension of the pure solvent-solid interface and that of the solution-solid interface at the same temperature (25). The IAST provides a convenient way for predicting multicomponent equilibrium because it only requires single-solute equilibrium data for each compound. With the Freundlich isotherm equation to describe single-solute adsorption, the solution to the IAST becomes simplified. Crittenden et al. (26) discuss the derivation of the solution. Using the IAST, Crittenden et al. (28) developed an equilibrium column model (ECM) to evaluate multicomponent competition in a fixed-bed adsorption column rather than assuming additive adsorption. This model did a reasonable job in finding the most poorly adsorbing solute, and calculating the overshoot concentration of the solute (28). The overshoot concentration is caused by competitive adsorption in an activated carbon particle. A higher effluent concentration of the weaker adsorbing solute, than the inlet concentration, may be observed when the stronger adsorbing solute deprives the weaker adsorbing solute of a site for adsorption in an initially saturated zone. The highest possible effluent concentration, attained by weaker adsorbing solutes, is generally referred to as the overshoot concentration. The computer program for ECM is presented in Association of Environmental Engineering Professors (AEEP) computer software manual (17) and was used in this study (Subroutine ET).

Plasma Reactor

In general, plasmas can be thought of as an ionized gas mixture. Gases are normally good electrical insulators. Under the influence of an applied electric field of sufficient strength, however, gas molecules can be ionized. Electric conduction then takes place and an electrical discharge occurs.

The plasma reactor utilizes electrical energy to create a relatively low temperature plasma (electric discharge) in

a reactor cavity. The ionized species and electrons are accelerated to high speed by electromagnetic energy. When organic materials flow into the plasma, their chemical bonds are broken by collision with electrons, causing dissociation to occur. The resulting fragments then recombine along the pathways to form simple reaction products.

The use of a plasma reactor to destroy volatile organic compounds has been tried. Some studies (29, 30, 31) were done to investigate the destruction of methane in a plasma Sheinson et al., (29) showed increasing methane reactor. destruction with increasing power input in a plasma reactor. They also found the existence of an optimum frequency for the alternating current that yields maximum power input. Robert et al., (32) studied the reactions of chlorinated hydrocarbons including TCE with water vapor or molecular hydrogen in a low-pressure microwave plasma. Tsai (10) reported a high destruction efficiency of TCE using the identical plasma reactors to those used in this study. All the previous studies have not been intended to treat the off-gases from an air stripping system. This study investigated the possibility of using a plasma reactor as the off-gas control technology for an AST.

CHAPTER III

METHODS

The AST was assumed to be equipped with either of the following two off-gas control devices:

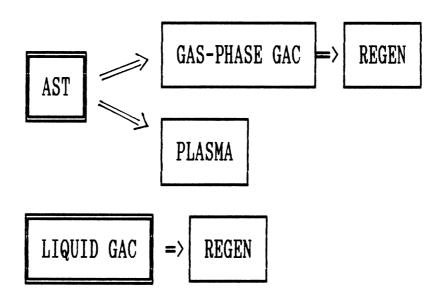
- * Gas-phase adsorption onto activated carbon
- * Plasma reactor

Figure 1 shows the treatment flow diagram which was considered in this study. The methods used in the modeling study, for all systems except the plasma reactor, were explained first. The method regarding the plasma reactor will follow.

Modeling Study

In order to accomplish the first objective, a computer program was developed by adopting many existing models which were then modified and used as subroutines to a main program. The program consisted of seven preexisting subroutines (MPTAD, ONDA, DIFL, DIFG, ET, SPEQ, and USER), five new subroutines (GACBED, GACBEDG, DENVIS, GACCOST, GACCOSTG, and TWCOST), and a new main program. The new subroutines and main program were developed for this study.

The program includes design models of an AST and a gasphase GAC unit in one model such that two of the major



REGEN = Regeneration of the saturated GAC bed

Figure 1. Treatment Flow Diagram

operating variables of the AST, A/W ratio and gas pressure drop, vary automatically until the least total cost of the AST and gas-phase GAC system is determined. The configuration and operating condition at the point where the least cost occurs is considered the optimum. Then, an AST with off-gas control is ready for a fair comparison to a liquid-phase GAC system. The design model of the liquidphase GAC unit is also included in the program so that one run of the program calculates the designs and costs of all unit processes.

The design of gas or liquid-phase GAC unit was not fully optimized in the program due to limited data. The major limitation is the lack of knowledge on the relationship between cost and the regeneration cycle of the GAC bed (time required to saturate a fresh GAC bed). Current cost data are just simply correlated with the GAC bed volume such that a large bed costs more and a small bed costs less. The GAC bed volume is a linear function of the empty bed contact time (EBCT) at a predetermined superficial velocity. Ideally, EBCT is an arbitrary variable that may be varied to find the optimum value. With the current cost data, the cost of a GAC contactor simply decreases by decreasing EBCT, thus making a shallower contactor. As the EBCT decreases, however, regeneration must be done more frequently, which will increase the costs due to the carbon loss and increased handling costs (GAC loss is not varied by the frequency of regeneration in this study because a fixed

percentage of spent carbon is always assumed to be lost in regeneration).

In this study, the depth of the GAC beds (gas and liquid-phase) was predetermined as the product of superficial fluid velocity and EBCT that are to be selected by the program user. The user-defined depth was checked against the minimum depth for the treatment objectives to avoid an immediate breakthrough. Accordingly, optimization of ASTs is based on the predetermined depth of gas-phase GAC bed. For this reason, the EBCT was fixed to 15 minutes for liquid-phase and 1.5 sec for gas-phase GAC unit throughout this study. A practical EBCT for liquid-phase GAC is one that ranges from 7.5 to 30 minutes (33). For gas-phase GAC, EBCT of 1.5 sec produces a bed depth of 1.5 ft at a superficial velocity of 60 ft/minute (fpm). Adams and Clark (13) used a bed depth for gas-phase GAC ranging from 0.5 to 4 ft. Superficial velocity of gas-phase GAC contactors are recommended not to exceed 100 fpm, and preferably be around 60 fpm (30.48 cm/sec) (34). In this study, a value of 30.48 cm/sec was used.

The cross-sectional bed area of gas-phase GAC is varied according to the superficial fluid velocity, A/W ratio of the AST, and the design water flow rate to the AST. In liquid-phase GAC, the bed area is determined by the superficial fluid velocity and the design water flow rate. The gas or liquid-phase GAC system was only partially optimized, again limited by the cost vs regeneration cycle data, by selecting the most economical type of GAC contactor and regeneration method from various types that will be explained later.

The individual parts of the program are explained below:

Main Program

Figure 2 shows the flow chart of the main program.

Data input and parameter estimation: The main program reads in all input data from the data file or estimates necessary parameters such as vapor pressure and the Henry's constant, if user does not have values for these terms. The Henry's constant can be estimated using vapor pressure and solubility of a compound. Density of the gas was estimated using the ideal gas law. Viscosity of the gas was expressed as a function of temperature. Density and viscosity of water were estimated in a subroutine. Diffusivities of gas and liquid were estimated in a subroutine also. All calculations regarding air were based on pure air because a target compound constituted a negligible portion of the total mass or volume of the off-gas from AST.

Simulation: The main program also manipulates subroutine programs as often as needed. The main program varied A/W ratio and air pressure drop for the ASTs, and water flow rate for all processes. The A/W ratio and air pressure drop are two of the three major operating variables of AST as explained in Chapter II. Water flow rate is not a

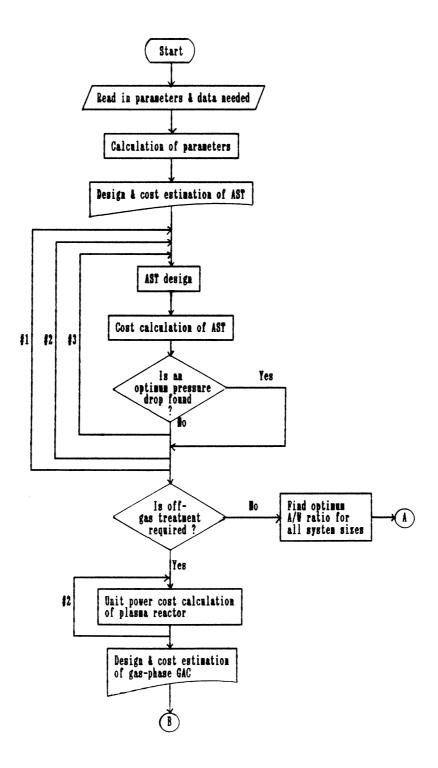


Figure 2. Flow Chart of Main Program

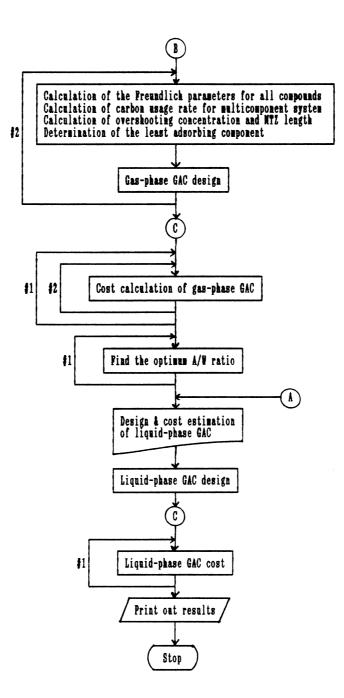
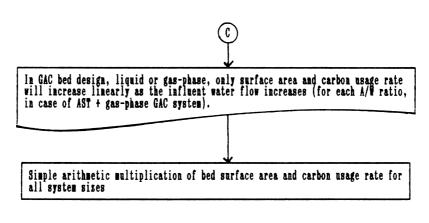


Figure 2. (Continued)



\$1: iteration for 10 different system sizes (10 water flow rates)
\$2: iteration for 50 different A/W ratios
\$3: iteration for 150 different air pressure drops of AST

Figure 2. (Continued)

major variable and can be selected arbitrarily because it is one of the predetermined design variables. In this simulation, the water flow rates were varied to see the effect on the cost. From now on, three variables in simulation refer to the two major operating variables and water flow rate.

The main program can use 10 water flow rates, 50 A/W ratios, and 150 pressure drops, which will cover all ranges commonly used in design. That means that the program may be executed as many as 75,000 times internally for each run. Generally, air pressure drop should be selected between 50 and 200 N/m²/m (35). The pressure drop was varied from 50 to 200 N/m²/m in step size of 1 (actually 151 pressure drops). The A/W ratio was varied from 1.1 to 6.0 times the minimum A/W ratio in step size of 0.1. The air pressure drop and the A/W ratio are selected by the model while flow rate can be user specified.

This study varied one variable and stopped at the optimum point (least cost), then, varied another variable. Finally, the main program determined the best combination of the three variables, A/W ratio, pressure drop, and water flow rate, resulting in the least total cost of the system (AST+off-gas control, or AST alone).

Each iteration of the program segments will be explained.

[1] Design and cost calculation of the AST.The dimensions of the tower were calculated in the

subroutine MPTAD. The cost was estimated in the subroutine TWCOST. Three variables were varied in this part, which were water flow rate, A/W ratio, and pressure drop.

Any combination of the A/W ratio and pressure drop produces a specific water loading rate from the generalized pressure drop correlation (18). Under a specific water loading rate, cross-sectional area is a linear function of the water flow rate. Accordingly, flow rate (million gal /day, mgd) determines only the cross-sectional area when A/W ratio and pressure drop are predetermined. If the flow rate doubles, the area will increase two times. Therefore, it seems that the air stripping design subroutine does not have to be iterated for varying water flow rate (keep the tower height constant and vary the cross-sectional area and tower volume linearly). However, the simulation should find the optimum pressure drop for each A/W ratio. The optimum value should be such that the total cost, including capital and O & M, of the tower is the minimum. The total cost of stripping is not a linear function of the tower volume or cross-sectional area. The pressure drop has effects not only on the cross-sectional area but also on the break power of the blower. As a result, the optimum pressure drop is not a constant value for varying water flow rates. Therefore, tower design should be iterated for all water flow rates. For any combination of these variables, the cost was estimated in the subroutine TWCOST, and the results were stored for later use.

There is no effect of varying pressure drop on the offgas composition or volume. Therefore, this parameter was not used in the program to optimize the gas-phase GAC unit. It affects only the design of the AST. The cost of an AST at each water flow rate and A/W ratio was determined at its own optimum pressure drop.

The water flow rate and A/W ratio of the AST affect the cost of both processes, AST and gas-phase GAC. In any case, the cost of the AST can not be settled until the cost of the off-gas treatment is determined unless the off-gas control is not required. So, the costs of the AST for all A/W ratios were calculated and stored for the later determination.

[2] Preparation for design and cost estimation of the off-gas treatment device

In the first part of this study, only a GAC contactor was designed as the off-gas treatment device. The plasma reactor was just evaluated based on the power cost determined from the experiments.

Under a specific superficial velocity, the crosssectional area of gas-phase GAC contactor is a linear function of gas flow rate which is a linear function of water flow rate to the AST at given A/W ratio. Accordingly, water flow rate to the AST determines only the crosssectional area of the gas-phase GAC contactors. Therefore, the design subroutines for the gas-phase GAC contactors do not have to be iterated for varying water flow rate (keep the tower height constant and vary the cross-sectional area and tower volume linearly). The total cost of the GAC contactor is, however, not a linear function of the tower volume or cross-sectional area. Accordingly, the cost subroutines of the gas-phase GAC contactors were iterated for all water flow rates.

The effluent gas-phase concentration from the stripping tower was calculated in terms of $\mu g/l$. This unit can be converted to ppm (volume/volume) by the following relationship that was derived from the ideal gas law:

1 ppm in air = (1/0.08205)*MW*(P/T) μg/l in air 1 μg/l in air = (0.08205/MW)*(T/P) ppm in air

in which; MW = molecular weight
 P = pressure of the mixture in atm
 T = temperature of the mixture in [°]K

The concentration and volumetric flow rate were adjusted with temperature for the gas-phase GAC contactor. For power cost estimation of the plasma reactor, the effluent concentration and volumetric flow rate from the AST was assumed to be directed to the plasma reactor without any adjustment.

[3] Power cost of the plasma reactor

Only the A/W ratio, among three variables used in the simulation (A/W ratio, air pressure drop, and water flow rate), had an effect on the unit power cost of the plasma reactor. So, the A/W ratio was varied.

[4] Preparation for the gas-phase GAC bed design

The subroutine SPEQ estimates the Freundlich isotherm parameters for the gas-phase GAC. The subroutine ET determines the most poorly adsorbing solute, and calculates the overshoot concentration of the solute for a multicomponent system. Carbon usage rate was calculated in this subroutine.

[5] Determination of mass transfer zone (MTZ) length of the gas-phase GAC unit

This part of the main program makes sure that design bed depth fully covers the MTZ lengths of the gas-phase GAC designs. The overshoot concentration from the subroutine ET was the inlet concentration to this part. There is only one MTZ length for all flow rates under a predetermined inlet concentration and superficial velocity. The inlet concentration was varied by varying the A/W ratio. So, each A/W ratio had its own MTZ length.

The MTZ length was usually shorter than calculated design length of the GAC bed in this study. Otherwise, the program prompts the user to increase the EBCT. MTZ length was determined in the subroutine USER.

[6] Design of the gas-phase GAC contactor

The bed dimensions (length and width) for the GAC contactor were calculated by using the subroutine GACBEDG. The bed length is determined as the product of superficial fluid velocity and EBCT that are to be selected by program user. The system A/W ratio has an effect on the design of the GAC unit and was varied. As the water flow rate increases, the bed cross-sectional area and the GAC usage rate increase linearly at given A/W ratio. Therefore, simple arithmetic calculations were done for the varying water flow rate.

[7] Gas-phase GAC contactor cost

Cost is not a linear function of water flow rate. Two variables were varied. These were water flow rate and the A/W ratio. All costs determined from all combinations of variables were stored. The costs of the AST and the gasphase GAC contactor were summed and stored.

[8] Finding the least cost of the combined system (AST+gas-phase GAC unit) for varying A/W ratio.

For all water flow rates, an optimum A/W ratio was determined. The optimum ratio was such that the combined (AST+gas-phase GAC unit) cost was the minimum.

[9] Design of liquid-phase GAC contactor and determination of mass_transfer zone (MTZ) length

The main program also estimates the design and cost of liquid-phase GAC system in order to determine the best choice between the liquid-phase GAC and AST+gas-phase GAC.

In the liquid-phase GAC contactor, the inlet concentration is not varied, which is not necessarily the case for the gas-phase GAC. So, there is only one MTZ length for all flow rates under a predetermined inlet concentration and superficial velocity. Accordingly, the MTZ length was calculated once. The subroutine ET was used to handle multicomponent system.

The bed dimensions (length and width) were calculated by using the subroutine GACBED. The bed length was determined as the product of superficial fluid velocity and EBCT that are to be selected by program user. As water flow rate increases, the bed cross-sectional area and GAC usage rate increase linearly as explained in the gas-phase GAC part. Therefore, simple arithmetic calculations were done for varying water flow rate.

[10] Liquid-phase GAC contactor cost

Since cost is not a linear function of water flow rate, the water flow rate was varied. All calculated costs were stored.

[11] Print out of results

Results from the process design and cost calculations were stored in an output file and printed as needed.

Subroutine MPTAD

This program was originally developed by David Hand to design an AST (17) and modified in this study as explained in Chapter II. This subroutine calculates the minimum A/W ratio. The A/W ratio is examined for all compounds in the influent water. To meet the treatment objective, the largest A/W ratio required by any compound was used to design the tower. The tower diameter is determined for the largest ratio. This subroutine calls the subroutine ONDA to calculate the mass transfer coefficient, K_La . The tower height is determined using the calculated K_La value. The tower height is also examined for all compounds. The highest one is selected for the tower design. Power consumptions of the blower and pump are calculated in terms of kilowatt hours (KWH). Brake power was calculated for the blower using the equation presented by Reynolds (36) and Metcalf & Eddy, Inc. (37). Break power calculation for the pump accounts for raising the total water flow to the top of the packing.

Tower dimensions reported are the tower height and total (effective) surface area of single tower. For an actual design, the total surface area can be divided by number of towers desired in parallel with due consideration given to the appropriate length/diameter ratio.

Subroutine ONDA

This subroutine calculates the overall mass transfer coefficient and wetted surface area for the subroutine MPTAD. This subroutine was a part of the program, PTAD, developed by David Hand (17).

Subroutine DIFL

Liquid diffusivity was calculated by this subroutine by using either molecular weight (MW), or viscosity of liquid and molal volume of a target compound. If the MW of the compound is greater than 1000, the liquid diffusivity is calculated using the Polson correlation (38). If MW is less than 1000, the Hayduk and Laudie correlation is used (39). This subroutine was a part of the program, PTAD, developed by David Hand (17).

Subroutine DIFG

Gas diffusivity was calculated by this subroutine using the Wilke-Lee modification of the Hirschfelder-Bird-Spotz method. The equation was taken from Treybal (40; p31). This subroutine was a part of the program, PTAD, developed by David Hand (17).

Subroutine GACBED, GACBEDG

These subroutines calculate the dimensions of the carbon bed, and the regeneration cycle. The dimensions are reported as unit height and total (effective) surface area of all beds combined. For actual design, the total surface area should be divided by number of beds in parallel desired with due consideration given to appropriate length/diameter ratio.

Subroutine ET

This subroutine determines the most poorly adsorbing solute, and calculates the overshoot concentration of the solute for the multicomponent system. Carbon usage rate was calculated in this subroutine. The IAST was used to describe multicomponent equilibria. For single component raw water, this model returns back to simple Freundlich isotherm. The original program was obtained from the AEEP manual (17).

Subroutine SPEQ

This subroutine was obtained from Crittenden *et al.* (24). This program uses the Dubinin-Radushkevich (D-R) equation to estimate the Freundlich isotherm parameters for the gas-phase because the subroutines ET and USER use the Freundlich isotherm parameters to describe the adsorption equilibrium.

Subroutine USER

This subroutine calculates the length of MTZ to make sure that the GAC contactor fully contains the MTZ. This subroutine works for both liquid and gas-phase GAC contactors. This subroutine is a simplified version of the Homogeneous Surface Diffusion Model for carbon adsorption. The original program was obtained from the AEEP manual (17) and slightly modified for this study. The modification includes the calculation of the length of MTZ which was considered a function of the target concentration. This subroutine uses the Freundlich isotherm parameters to describe the adsorption equilibrium. The Freundlich isotherm parameters are not readily available for gas-phase components and are not constant with varying component concentration. Therefore, the parameters required for the gas-phase were estimated using the subroutine SPEQ. Normally, the MTZ length was very short in gas-phase adsorption such that normal GAC bed depth covers the MTZ.

Therefore, possible errors involved in the estimation of the Freundlich parameters are insignificant.

Subroutine DENVIS

This subroutine calculates the density and viscosity of water for the desired operating temperature. The equations from the CRC Handbook (41) were used for the density (41; pg. F-5) and for the viscosity (41; pg. F-37).

Subroutine GACCOST

The Drinking Water Research Division (DWRD) of US Environmental Protection Agency (EPA) has collected a vast amount of cost data for GAC treatment systems. Using this data, DWRD developed the following cost estimating equation (11):

 $Y = a + (b)(VAR)^{c}(d^{z})$

in which; Y = the base construction cost or specified O & M requirement.

> VAR = process design or operating variable. a,b,c,d = parameters determined from nonlinear

> > regression.

z = 0 or 1 used to adjust the cost function for a range of VAR values.

The values of a,b,c,d,and z have been developed for several technologies used in GAC treatment such as various types of contactors and regeneration systems. The equation parameters are tabulated in the paper presented by Adams and Clark (11). Using these data, subroutine GACCOST was written for this study.

Construction costs (CC) in the Adams and Clark equation were expressed in 1983 dollars. The Engineering News Record (ENR) Construction Cost Index (CCI) was used (CC*current CCI/380) to update to January 1990 in this simulation. The base year is 1967. Annual capital costs were estimated by multiplying CC by the capital recovery factor (CRF) (11):

 $CRF = I(1+I)^{N} / [(1+I)^{N} - 1]$

in which; I = interest rate, 10%

N = payback period, 20 years.

Maintenance material costs (MM) were expressed in terms of 1983 dollars per year in the estimates presented by Adams and Clark (11). Major cost of the MM will be caused by replacement of equipment. The Marshall and Swift equipment cost index (ECI) was used to update the MM to January 1990 in this simulation (MM * current ECI/761).

Three types of contactors and four types of regeneration systems were available for cost estimates. Cost estimations were done for all types of contactors and regeneration systems, and the least-cost processes were selected for each different case and sent to the main program. The alternative types of contactor were:

[1] Package pressure GAC contactor

[2] Conventional steel pressure GAC contactor

[3] Conventional concrete gravity GAC contactor The alternatives for regeneration were:

- [1] Infrared reactivation
- [2] Fluidized bed reactivation
- [3] Multihearth reactivation

[4] Disposal and Replacement with virgin carbon In option [4], disposal of used carbon is done by incineration. Since Adams and Clark (11) did not give a formula for the replacement option (they just presented a graph), an equation was developed for interpolating the graph as shown in the source program in Appendix C.

All units were designed with extra capacity (30 %) to accommodate a surge flow. The CC of all types of contactors and GAC storage units were based on the total effective design volume of the GAC contactor while the MM was determined using the actual utilized portion of the volume. GAC was assumed to be 95% saturated before each regeneration. This saturation may be achieved through serial or parallel operation.

Table II shows the cost parameters used in this study. These parameters were used by Adams and Clark (11) except the natural gas price. The cost estimating methods and parameters for the GAC systems are well explained by Adams and Clark (11), and are consistent with those used in this study unless otherwise specified.

Subroutine GACCOSTG

The study of the Drinking Water Research Division (DWRD) of USEPA did not include data for gas-phase

TABLE II

COST PARAMETERS

System Operation of GAC Contactor = 70 % Reactivator Uptime = 75 % GAC Loss per Regeneration = 12 % Liquid-phase GAC Price = \$0.9/1b at 100,000 1b Gas-phase BPL Carbon Price, Calgon Co. = \$2.0/1b at 20,000 1b Labor Rate = \$15/hr Electric Rate = \$0.08/Kwh Natural Gas Price[‡] = \$0.003/std.cu.ft. Process Water Price = \$0.35/1000gal

*: Peters and Timmerhaus (1990)

adsorption and regeneration (11). So, the cost model of the liquid-phase GAC contactor was modified for gas-phase. The modifications included the following:

- * Pumping energy requirement was dropped in the gas-phase. Instead, the energy requirement for an air blower was added. Brake power calculation for the blower was based on the equation presented by Reynolds (36) and Metcalf & Eddy, Inc. (37).
- * The gas-phase GAC contactor did not include the construction and energy cost of the backwash pumping system.
- * An air heating cost was included to decrease the relative humidity to 40%.
- * The conventional concrete gravity contactor was not included as a gas-phase contactor.
- * The initial GAC cost was included in the package contactor. However, the GAC price was based on a liquid-phase GAC. So, the price difference between a liquid-phase and gas-phase carbon was added for the gas -phase contactor.
- * In the virgin carbon replacement option, the GAC price was based on a liquid-phase GAC. So, the price

difference was added for the gas-phase contactor. In order to calculate the blower power requirement, pressure drop through the GAC bed should be calculated. A pressure drop correlation is available only for packed tower air stripping (18). Such a correlation has not been developed for the gas-phase GAC contactor, and the packed tower correlation cannot be applied to a GAC contactor because the correlation was developed for counter current flow of water and air. The Ergun equation was used in this study. The Ergun equation calculates the pressure drop using various parameters of the bed and fluid (42). The fluid parameters such as viscosity and density will be constant throughout bed, in case of a non-compressible fluid like water. There would be a little compression of air at the inlet of a bed. However, the effect on the viscosity and density of gas is ignored here and the constant operating pressure is assumed throughout the bed.

In order to obtain the optimum condition for adsorption, off-gas from the AST was assumed to be heated to obtain 40 % relative humidity (RH). The off-gas was assumed to be 100 % saturated and isothermal at the top of AST with the influent water due to the large contact area between the air and water. This assumption gave a slightly conservative estimation of heating cost because the maximum heat requirement was used to lower the RH (100% -> 40%). A natural gas-fired heater was assumed to be used.

The following parameters were also adjusted for the elevated temperature in the main program.

- * Operating temperature of the gas-phase GAC contactor
- * Vapor pressure of the compound
- * Density and viscosity of the off-gas from the AST
- * Off-gas flow rate from the AST
- * Influent gas-phase concentration to the GAC contactor
- * Gas-phase diffusivity of the compound

Heat capacity (Cp) of the air was estimated from the

ideal gas law (43; p3.122): Cp of $N^2 = 6.50 + 0.001 \text{ T}$ Cp of $O^2 = 8.27 + 0.000258 \text{ T} - 187700/\text{T}^2$ Cp of air = 0.79(Cp of N²) + 0.21(Cp of O²) in which; T = 'K Cp = cal/deg-mol 1 mole of air = 29 g

The middle point of the temperature range, from initial temperature to temperature required to obtain 40 % RH, was used for the T to estimate the Cp of N^2 and O^2 .

Example: $T = 17^{\circ}C$ (300°K), for 10°C -> 24°C. Heating cost of the air was estimated using the following informations.

> 1 cal = 0.00397 Btu Typical heating value of natural gas = 1050 btu/cuft (43; p9.12)

Steam regeneration may be another alternative for the gas-phase GAC. Steam regeneration was not included in this study because the performance of the process and the disposal method of the spent steam have not been well established. The regenerated bed should be dried to remove condensed water. The drying gas should be treated also.

The estimated cost of the gas-phase adsorption system may be a little conservative because a lower cost is expected for the contactor and regeneration system of the gas-phase GAC. For example, dewatering and drying of a saturated bed for regeneration is not required for gas-phase GAC.

This subroutine calculates the various costs of the ASTs. A specific formula is not readily available for this Therefore, the following equations were developed purpose. for the curves given in Gumerman's report (44): For packed tower (44; p460, 466, 467); CC = 10.**(2.480708+0.699403*LOG(TV*100./PTOP))MM = 10.**(3.71184 - .951171 * LOG(TV))+.20046*(LOG(TV))**2.) LABOR = 10.**(1.84073 - .399972*LOG(TV))+.121128*(LOG(TV))**2.) For administration, laboratory, and maintenance building (44; p469, 472, 473); CC = 10.**(4.3617+.633898*LOG(FLOWL*100./PTOP))-.0380989*(LOG(FLOWL*100./PTOP))**2.) MM = 10.**(3.29564+.293344*LOG(FLOWL))+.0639727*(LOG(FLOWL))**2.) Labor = 10.**(3.17059+.68173*LOG(FLOWL)-.105693*(LOG(FLOWL))**2.) BE = 10.**(4.7412+.638106*LOG(FLOWL))-.0357398*(LOG(FLOWL))**2.) in which; CC = construction cost, \$/year MM = maintenance material, \$/year Labor = hr/yearBE = Building energy, KWH/year TV = Tower Volume; ft PTOP = Percent operation of packed tower, % FLOWL = Plant capacity, MGD The construction cost (CC) of tower did not include pump cost. So, the following equation was developed for the

curves presented by Peters and Timmerhaus (45; p527, Figure 14.41):

PUMP = 10.**(5.42915-1.46769*LOG(2298.25*BPW*100. /PTOP) +.237617*(LOG(2298.25*BPW*100. /PTOP))**2.)

in which; BPW = pump break power requirement, KW.

Costs for contractor profit, 5 %, and engineering and legal fees, 10 %, were added to the construction cost reported in Gumerman's report (44), in order to keep an equal basis with the other processes in this study. These additions produced a 15 % higher construction cost than the cost reported. Construction contingencies factor and special site work were included in the original report. Tower volume was designed such that 70 % of the design capacity was utilized for average water flow. Gumerman's report was based on the cost of October 1978 dollars. So, the CC was adjusted to January 1990 using the CCI, and the MM was adjusted using the ECI. Annual capital costs were estimated by multiplying the CC by the capital recovery factor (CRF).

Parameter Estimation

The following parameters should be estimated externally by the program user. The value of the affinity coefficient, β , is determined from the ratio of a specific physical property to that of the reference compound. The ratio of polarizability can be used to calculate β (21).

 $\beta = a/a_{ref}$ $a = (n^2-1)MW/((n^2+2)\rho) \qquad (Lorentz-Lorenz Equation)$ n = refractive index

Values for refractive index, n, were taken from the Handbook of Organic Chemistry (46). If the value was not available, it was evaluated by the summation of the atomic and structural contributions (43; p3.240).

Henry's constants of many of the compounds are reported in the literature as a function of temperature (47, 48, 49, 50). The reported values will be more realistic than those estimated using vapor pressure and solubility. The Henry's constants used in this work were adjusted to the water temperature.

Vapor pressure was estimated using the Antoine equation (51): Vapor pressure in mmHg = $10.0**(A - B/(T^C + C))$ The constants, A, B and C were not readily available for many compounds. In order to determine the three unknowns, three pairs of temperature-vapor pressure points were selected from Perry's Handbook (43) so that the three temperatures cover the temperature range of interest. By solving the three simultaneous equations, the constants for the Antoine equation were determined.

Molal volumes of the target compounds were determined using Le Bas method (52).

PSDFR (pore to surface diffusion flux ratio) was reported in previous studies (12, 53) to be 3.72 for many compounds (aliphatic hydrocarbons). Therefore, 3.72 was used as the PSDFR for liquid-phase adsorption. In the gasphase, a value of 16.0 was used as the PSDFR. This value was taken from the example data in the AEEP manual (17).

Off-gas from the AST was assumed to be heated to obtain 40 % relative humidity. The required temperature increase, listed in Table III, was read from a psychrometric chart. Table IV shows the examples of the parameters estimated.

Methods for Plasma Reactor Study

In order to investigate the possibility of using a plasma reactor as the off-gas control technology for an AST, laboratory experiments were conducted.

First, TCE destructive tests were done on a bench scale. These tests were designed to determine the destruction efficiency of the plasma reactor. A saturation device (Figure 3) similar to that employed by the EPA (54) was used to prepare TCE-contaminated air. In the initial tests, highly contaminated air with TCE (9000 ppm) was created and used as a feed stream to the plasma reactor. Grab samples of the feed and effluent were taken during test runs and analyzed on an electron capture gas chromatograph in the School of Civil Engineering, OSU. Destruction efficiencies of TCE based on peak area were 92.0 % and 93.8 % for the two tests with only a trace of by-products showing up on the chromatograms. In the initial destruction tests, the GC method given in Table V was used.

After taking those two data points, TCE destructive tests were not continued as part of this study. Later, TCE destructive tests were conducted in the School of Chemical Engineering, OSU, and high destruction efficiencies (>95%)

TABLE III

REQUIRED TEMPERATURE INCREASE TO OBTAIN 40 % RH FROM SATURATION

Sat. Temp.	Temp. of 40 % RH	Required Increase
(°C)	(°C)	(°C)
		······································
0	12.9	12.9
2	15.3	13.3
4	17.4	13.4
6	20.0	14.0
8	22.2	14.2
10	24.4	14.4
12	26.4	14.4
14	28.9	14.9
16	31.2	15.2
18	33.5	15.5
20	35.6	15.6
22	37.7	15.7
24	40.0	16.0
26	42.2	16.3

TABLE IV

EXAMPLES OF THE PARAMETERS ESTI	IMATED
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Compound	Å	B	C	Hc	₩.V.	₿	K	1/n
Trichloroethylene	5.3976	631.94	154.59	0.190748	0.1071	0.816	196.626	0.4163
Tetrachloroethylene	7.5406	1694.6	245.29	0.3569**	0.1280	0.976	650.6 ²⁶	0.4579
Toluene	6.7624	1254.5	211.31	0.1190 49	0.1182	1.000	348.012	0.365
Chlorobenzene	5.9570	1004.3	180.41	0.08977 43	0.1169	1.059	381.0 ¹²	0.31
Bromoform	4.9134	657.45	134.0	0.009944	0.0995	0.963	161.0,61	0.5629
Chloroform	5.7000	647.54	164.61	0.07594 48	0.0923	0.694	30.461	0.5325
1,1,1-trichloroethane	13.08	5926.8	514.91	0.3516	0.1145	0.841	29.714	0.495
Bthylbenzene	11.612	4616.7	409.12	0.1332^{49}	0.1404	1.15	507.0 ¹²	0.53
1,2-dichlorobenzene	6.886	1584.8	210.14	0.06015	0.1378	1.157	865.012	0.38
Cis-1,2-dichloroethylene	6.9264	1143.0	222.51	0.0764650	0.0862	0.651	30.5 ¹²	0.59
Trans-1,2-dichloroethylene	6.967	1116.3	224.95	0.1876 20	0.0862	0.662	12	0.39
Carbon tetrachloride	8.4565	2079.7	299.1	0.605848	0.1132	0.694	50.114	0.594

K = liquid-phase Freundlich isotherm parameters for F-400 type GAC, (µmol/g)(l/µmol)^(1/h)
1/n = liquid-phase Freundlich isotherm parameters for F-400 type GAC, dimensionless
A, B, C = Constants for Antoine equation, dimensionless, determined from temperature -vapor pressure relationships
Hc (at 10°C) = Henry's constant, dimensionless
β = affinity coefficient, dimensionless
M.V. = molal volume, m'/kg-mol
* = Estimated refractive index is very close to that of chloroform. So, the reported data of chloroform was used to estimate the β.

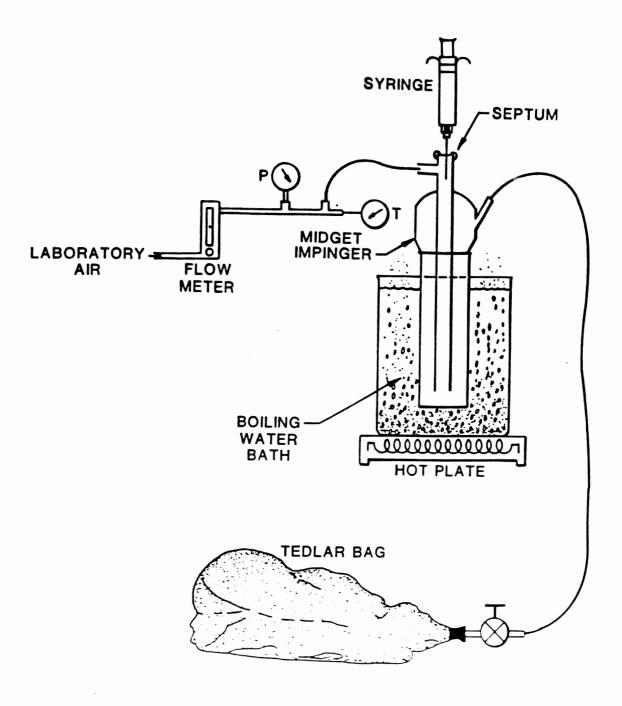


Figure 3. Train for TCE Saturation

TABLE V

GC METHOD USED IN DESTRUCTION TEST

GC Column; 3 % SP-1000 on 100/120 Supelcoport Detector; Electron Capture Detector Oven Temp.; 75°C Run Time; 3 min Injector Temp.; 100°C Detector Temp.; 275°C Carrier Gas (5 % Methane + 95 % Argon); 60 cc/min were obtained (10). The results from the tests (10) were used in this study for the cost calculations of the plasma reactors.

Second, electrical characteristics and power requirements of plasma reactor were estimated. In the second phase, feed gas to the plasma reactor was supplied from a pilot scale AST. In this stage, TCE was not added to the feed water of the AST. Therefore, a TCE-free off-gas was fed to the plasma reactor. The only reason for using pilot-scale AST was to generate large quantities of off-gas with the appropriate temperature and humidity.

The plasma reactor part of the experimental apparatus is shown in Figure 4. The apparatus includes a power source (California Instruments Model 161T oscillator with a range of 0 to 120 volts and frequency generation of 40 to 5000 Hz), transformer (Jefferson Electric with a maximum secondary voltage of 7500 V), high voltage test probe, and the reactor. The reactors were constructed using pyrex glass and consisted of coaxial glass tubes (Figure 5). The inside of the inner tube and outside of the outer tube were coated with inorganic silver paint that acted as an electrode. The geometries of the various reactors are given in Table VI. The length of all the reactors was 37.5 cm with a 20.2 cm long effective discharge zone. For the measurement of the secondary voltage, a Simpson AC high voltage probe was used in conjunction with a Simpson 620 multimeter. The primary power input (total power input to

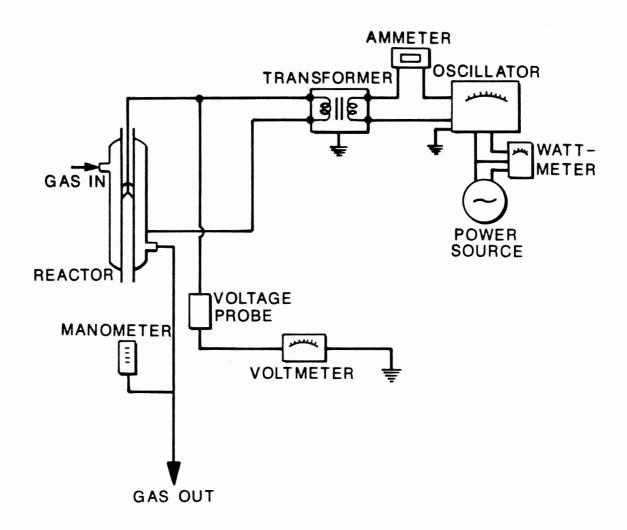


Figure 4. Schematic of Plasma Reactor System

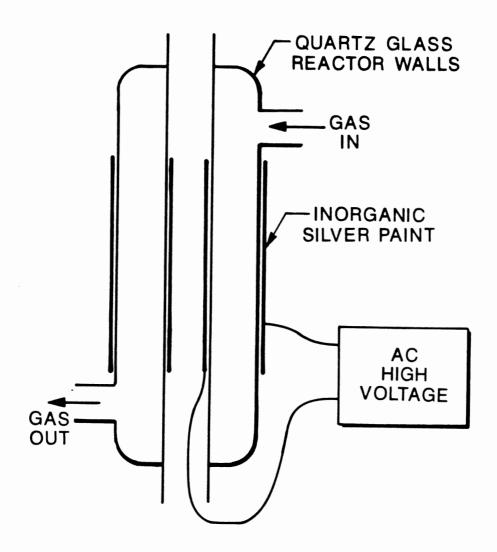


Figure 5. Alternating Current Plasma Reactor

TABLE VI

Reactor		Diam	eter	Gap	Di am eter		
	Inner	Tube	Outer	Tube		Ratio	
	D1 (cm)	D2 (cm)	D3 (cm)	D4 (cm)	(D3-D2)/2 (cm)	(D3/D2)	
#1	1.27	1.50	2.19	2.50	0.345	1.460	
#2	1.55	1.80	2.19	2.50	0.195	1.217	
#3	1.77	2.00	2.64	3.00	0.320	1.320	

GEOMETRIES OF THE PLASMA REACTORS

plasma reactor) was measured by General Electric wattmeter. Gas flow rate to the reactor was measured using a calibrated rotameter.

The pilot scale air stripping column was connected to the plasma reactor. A schematic of the air stripping system is shown in Figure 6. The air stripping tower was composed of a glass column with an inside diameter of 7.52 cm (3 in) and a length of 1.83 m (6 ft). The tower consists of three sections, a 1.4 m (4 ft) high center piece, open at both ends, and two 0.35 m (1 ft) long end pieces each sealed at The inlet and outlet ports for the gas and liquid one end. streams and the manometer ports were placed in the end pieces. The three pieces were connected with two 88 mm (3 in) diameter stainless steel clamps containing Teflon gaskets. The column was packed with a ceramic packing material. The packing height was 1 m. Information on the packing material (40) is given in Table VII. Operating condition of AST is given in Table VIII.

The experimental procedures for the non-destructive tests was:

- The AST was turned on and the water and air flow rates were set to 1 l/min and 30 l/min respectively. These flow rates were kept constant throughout the experiment.
- 2. A small portion of the off-gas flow from the AST was separated from the main flow using a T-connection. The amount of the slip stream (2 l/min) was adjusted by using a control valve to obtain the desired flow rate.

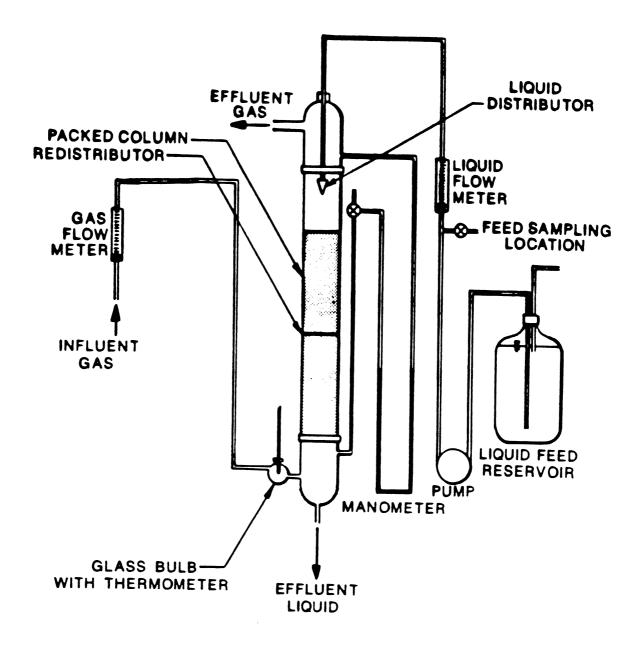


Figure 6. Schematic of Air Stripping System

TABLE VII

PACKING MATERIAL USED IN EXPERIMENTS

Name: Intalox Saddles Size: 0.25 inch Packing Factor: 725 Porosity: 0.75 Specific Surface: 984 m²/m³ or 300 ft²/ft³

TABLE VIII

OPERATING CONDITION OF AST

Water (TCE-free) Flow Rate: 1 1/min Water Temperature: 22°C Air Flow Rate: 30 1/min Air Temperature: 24°C Pressure Drop across the Tower: 80 N/m²/m The branch stream was directed to the top port of the reactor and exited from the bottom. The off-gas from the reactor and AST was vented to a hood.

- The supply power was turned on and the primary voltage was set.
- 4. The frequency was varied from 60 Hz to 1000 Hz with a 100 Hz increment. The secondary voltage and primary power input (watts) were recorded for each frequency. There were some fluctuations in all the gage-readings at the frequency that is nearest to breakdown (optimum frequency). About 10 minutes was allowed to pass to establish steady state conditions.
- 5. With the same reactor, the steps 3 and 4 were repeated for three different primary voltages.
- 6. Tests were continued for other reactors.
- For reactor #3, tests were repeated for the different flow rates (1 to 12 l/min) to the reactor.

CHAPTER IV

RESULTS AND DISCUSSION

The results of modeling study are explained first. The results regarding the plasma reactor will follow. All tables and figures are appended at the end of this chapter. The results reported in this study are in the form of a limited sensitivity analysis of the model. The sensitivity analysis was considered to be limited in that most of the results reported on the integrated model used TCE as a representative compound.

> Effect of Air Pressure Drop on the Cost of AST

Air pressure drop of the AST was varied, while all other variables were held constant, to see the effect on the cost of AST. Figure 7 shows the results for TCE. This figure is typical of those generated using other contaminants. The pressure drop had a minor effect on the cost. The cost variation was minimal (0.3 cents between the minimum and the maximum values in the range of 40-200 N/m²/m pressure drop). The treatment option in Figure 7 is the AST without off-gas treatment because the varying pressure drop has no effect on the off-gas composition or volume, but has

effect on the design of the AST. The A/W ratio was fixed at 1.5 times the minimum which was close to the determined optimum value. The procedure for determining the optimum value of the multiplier (i.e. 1.5) for the minimum A/W ratio will be explained in the next section. The lowest range of the pressure drop was extended to 40 N/m²/m to see the curve more clearly. All other simulations were conducted with the lowest bound of 50 N/m²/m because the original pressure drop correlation generated by Eckert (18) was valid from 50 N/m²/m.

The optimum pressure drops determined for the optimum A/W ratio in the combined systems are shown in Table IX. The least cost appears in the range of 50-62 N/sq.m/m. The raw water temperature was fixed at 10°C unless otherwise specified. Groundwater temperature ranges from 3°C to 19°C at a depth of about 100 ft in the United States (55).

> Effect of A/W Ratio on the Cost of AST with Gas-Phase GAC

The operating A/W ratio is calculated as a multiple of the minimum A/W ratio, below which the treatment objective will not be achievable. The minimum A/W ratio is expressed as follows (56):

Minimum A/W ratio = (Ci - Ce)/(Hc*Ci) in which; Ci = influent concentration Ce = effluent concentration Hc = dimensionless Henry's constant

The minimum value is multiplied by a certain constant that produces the most economical tower design. It has been suggested that about 3.5 times the minimum A/W ratio gives the least cost design for the AST process (56). Figure 8 illustrates the effect of the A/W ratio on the cost. However, if off-gas control is considered, the least cost occurs at about 1.7 times the minimum A/W ratio. The cost of an AST alone decreases continuously until the A/W ratio reaches 3 to 4 times the minimum because the tower volume is inversely proportional to the A/W ratio; thus capital cost of the AST decreases. Beyond 3 to 4 times the minimum, operating costs will offset the decreasing capital cost. As the A/W ratio increases, off-gas volume increases. The increase in off-gas volume and decrease in contaminant concentration will increases carbon consumption and the frequency of regeneration. Therefore, as the ratio increases, the cost of gas-phase GAC contactor increases constantly. The balance point is about 1.7 times the minimum as seen in the Figure 8. At the ratio of 1.7, the total cost is 22.5 cents/1000 gal. At the ratio of 3.5, the total cost increases 8.4 % resulting in 24.4 cents/1000 gal. This difference exists in the total cost of AST + gas-phase GAC system designed by the integrated model versus the two processes designed independently and coupled together. The cost differences determined for various compounds are shown in Table X. Without considering the system to be designed as a package, an AST with off-gas control is not in a proper

design and is not ready for a fair comparison to liquidphase GAC. All simulation in this study used the optimum A/W ratios that were determined for each different case. The optimum A/W ratios determined for various compounds are shown in Table IX. A range of 1.2 to 2.1 times the minimum A/W ratio resulted in the least cost AST with gas-phase GAC Figures 7 and 8 demonstrate the individual effect system. of the two variables, air pressure drop and A/W ratio, on the cost. In these figures only, the named variable was changed while all the other Figures (9-31) were generated using the optimum combination of the two variables. For instance in figure 9, only the influent concentration of TCE The model then calculated the optimum design was varied. and operating conditions for each system shown in the figure. Each optimum design and operating condition has a total cost that is calculated by the model. This cost, which represents the least total cost for any system, is then plotted against the one variable that was varied. Tn this manner, the effect of the one variable that was varied can be seen on all systems.

In Figures 9-31, the 'AST' means the AST system without off-gas control option, and the AST system was run with 3.5 times the minimum A/W ratio and the optimum air pressure drop. The 'AST in combined system' means the AST part in the AST+gas-phase GAC system, and the system was run with the optimum A/W ratio and the optimum air pressure drop.

Concentration Effect on the Cost and Design of All Processes

The plots similar to Figure 8 were generated to show the effect of higher influent concentrations on the cost of the total system. For instance, at an influent concentration of 500 ppb the optimum A/W ratio was 1.8 times the minimum and the cost at the combined system was 30.8 cents/1000 gal whereas the cost at a multiplier of 3.5 was 33.5 cents/1000 gal. This represents a total cost increase of 8.7 % between the multipliers 1.8 and 3.5. Using an initial concentration of 1000 ppb the optimum A/W ratio was 1.7 times the minimum and the cost of the combined system was 37.3 cents/1000 gal while the cost at a multiple of 3.5 was 40.8 cents/1000 gal; a cost increase of 9.3 %. As illustrated by this example calculation for TCE, along with the data shown in Figure 8, total cost for the combined system increases as the influent concentration to the AST increases. However, this cost increase is not in the form of a linear relationship due to the large number of variables taken into account in developing the best design and least cost option for each particular situation. Also, the total cost differential between the optimum multiple determined by this algorithm and those normally consider the best (i.e. 3.5) increases as the influent concentration to the AST increases. Again, this increase is not linear. Tn order to illustrate the effect of influent concentration on the AST and GAC systems, Figure 9-11 were constructed. The

influent liquid-phase concentration was varied from 10 ppb to 1000 ppb TCE in Figures 9 and 10, and from 100 ppb to 35000 ppb TCE in Figure 11. The 35000 ppb (35 ppm) represents one of extreme groundwater contamination (57). Air stripping without off-gas control was shown to be the least cost option. The effluent concentration, Ce, is the liquid-phase concentration coming out of the AST or liquidphase GAC.

Off-gas control using gas-phase GAC costs more than air stripping itself in the high concentration range as shown in Figure 9 (>500ppb). However, the combined cost of the two processes is less expensive than liquid-phase adsorption using GAC, and this tendency does not change over the concentration range examined.

If off-gas treatment is required, the cost and tower volume of the AST should be increased in order to save more in the off-gas treatment. That is why the cost and tower volume of the AST in a combined system (AST+gas-phase GAC) is higher than the AST without off-gas control as set out in Figures 9-12. The cost of plasma will be discussed at the end of this chapter. The tower volume was largely influenced by the influent concentration as set out in Figure 10.

Effect of Water Temperature on AST and Gas-Phase GAC

Increased water temperature has a positive effect on

the vapor pressure of a solute in water, thus making the solute more volatile. Increased water temperature also has various effects on the coefficients used for design of an AST along with the vapor pressure. It decreases surface tension, viscosity, density of water in the calculation of the specific wetted packing area in the Onda correlation, thus yielding a larger specific interfacial area (a) for mass transfer, and overall mass transfer coefficient ($K_{L}a$). Also, increased temperature has a positive effect on gas and liquid diffusivity thus increasing individual mass transfer coefficients and $K_{L}a$.

Increased temperature effects on Henry's constant have been studied by various researchers. Kavanaugh and Trussell (58) used a Van't Hoff-type equation to model the relationship of Henry's law constant to temperature. This equation showed a two-fold increase in the Henry's law constant for every 10°C rise in water temperature for most of the volatile compounds investigated. Munz and Roberts (48) found the increase of Henry's constant to be a factor of approximately 1.6, for eight VOCs, for each 10°C rise in water temperature between 10 to 30°C.

By increasing the Henry's constant, increased water temperature increases $K_{L}a$ again. The overall increased removal rate of contaminants by air stripping, because of increased water temperature, has been reported many times (59, 60).

In the case of gas-phase GAC, however, the temperature

has the opposite effect. The D-R equation shows that increased temperature and vapor pressure have an adverse effect on adsorption capacity of gas-phase GAC.

Thus, there is a positive effect of increased water temperature on air stripping but a negative effect on removal by gas-phase GAC. There has been no information reported in the literature regarding the gross effect of the temperature on the performance of the coupled system.

Figure 12 shows the results of this phase of the study. Figure 12 shows that the gas-phase GAC cost decreases as the water temperature increases. This is contradictory to the theory. However, the TCE concentration in the off-gas increases as the water temperature increases, due to decreased A/W ratio to achieve same percent removal as at a lower temperature, i.e., due to decreased off-gas volume. Therefore, increased GAC usage rate caused by high temperature is disguised by decreased GAC usage rate caused by decreased off-gas volume. Moreover, as the off-gas volume decreases at high water temperature, the volume of the gas-phase GAC bed decreases, which reduces the capital cost of the gas-phase GAC system. As a whole, the cost of gas-phase GAC part of the combined system decreases 18.1 % as the water temperature increases from 0°C to 26°C. Of course, the AST cost decreased as the water temperature increases, 20.6 % for the AST alone, and 20.2 % for the AST in the combined system. The total cost of the combined system decreased 19.4 % as the water temperature increased.

Effect of Influent Water Flow Rate on the Cost of AST with Off-Gas Control and Liquid-Phase GAC System

Figures 13-24 show the effect of influent water flow rate on the cost of air stripping with off-gas control and liquid-phase GAC for various compounds. In other words, the figures show system-size dependence of treatment costs. Table XI shows the compounds studied. Individual inlet concentrations were set at 100 ppb for all compounds, and the effluent concentrations were set at 5 ppb. As the flow rate to the treatment system increases, that is, as the system capacity increases, the unit cost decreases as set out in Figures 13-24. In all cases except bromoform, the AST was the more economical choice as compared to liquidphase GAC even with AST off-gas control.

Multicomponent Simulation

Figure 25 shows the simulation results of individual and multicomponent systems. All letters and numbers with Figure 25 are identified by compound in Table XI. The X and Y-axis represent the treatment costs if the compound or the multicomponent systems in the figure are treated by the corresponding treatment options: The X-axis is for AST+gasphase GAC and the Y-axis is for liquid-phase GAC. The data for Figure 25 was taken from Figures 13-24 at a flow rate of 1 mgd.

The multicomponent system B is composed of four compounds. These four compounds are positioned in the same area, bottom left, in Figure 25. That is, these compounds can be more easily treated than others in the figure under either treatment option. When compounds #5, #7, and #10 were added to system B, these new combinations became systems D, E, and F respectively. When the cost of these three systems are compared to system B, the cost and design of a multicomponent system is highly dependent on the least strippable or least adsorbable component. Examples of the controlling compound are compound #5 in system D, #7 in system E, #10 in system F.

The multicomponent systems A, B, and C do not include a compound as difficult to remove as ones appearing in the systems D, E, and F. All components in multicomponent systems A, B, and C (1,2,3,4,8,9) are positioned at about the same area in the figure. Even without a controlling compound, an appreciable amount of cost increase is observed in multicomponent systems A, B, and C, probably due to increased GAC usage rate caused by competitive adsorption and desorption among the components.

The diagonal line in the figure divides the range of economical treatment option. Any compound or multicomponent system in the upper left side of the diagonal line may be treated more economically using the AST + gas-phase GAC system. The liquid-phase GAC system will be preferred by the compounds or multicomponent systems in the bottom right

side of the diagonal line. In all cases, except bromoform and multicomponent system D which contains bromoform, the AST + gas-phase GAC system was the more economical choice as compared to liquid-phase GAC.

Figures 26-31 show system-size dependence of the cost of the 6 multicomponent systems (systems A-F).

Results of Plasma Study

The plasma reactor was connected to the AST to investigate the characteristics of the total system with respect to power, frequency, and voltage. A series of breakdown tests with TCE-free air (non-destructive tests) were performed to determine the breakdown voltages and frequencies of the plasma reactors. Here, breakdown means that the flowing gas is ionized so that a plasma status is established in the reactor cavity. Breakdown could be easily identified because of an audible noise from the reactor and because of the sudden increase in power input to the system. In darkness, a blue-colored glow could be seen during breakdown.

The frequency of the current was varied from 60 Hz to 1000 Hz in 100 Hz increments. Figures 32, 33, and 34 show the variations in secondary voltage with frequency at different primary voltages for the various reactors. The voltage remains fairly constant until a noticeable increase of voltage is observed at breakdown frequency followed by a gradual decrease. As the primary voltage increases from 20 V to 60 V, the frequency that draws maximum secondary voltage decreases in all reactors.

The total power input for the reactors is shown in Figures 35, 36, and 37. The word, total, is used here because the net power input to sustain the plasma will be a portion of the total power. The other remaining portion of the total power will be dissipated in other electrical devices such as the frequency generator and transformer. The net power input to the plasma reactor was not measured due to the lack of available measuring devices. The total power input to the plasma reactor is actually what the reactor electrical cost is based on. Total power input reaches a maximum immediately after plasma is established. Total power input to the system is dependent on frequency. As the frequency increases, the power input remains fairly constant until a steep increase up to a maximum is observed followed by a gradual decrease. All three reactors showed the same trend. As the previous study (10) showed in the destructive tests, the maximum power input yielded the maximum conversion of the target contaminant. Therefore, the frequency that draws the maximum power input may be called the optimum frequency. The optimum frequency was dependent on the reactor design and the primary voltage applied (Figures 35, 36, and 37). As the primary voltage increases from 20 V to 60 V, the optimum frequency decreases in all reactors. The optimum frequency roughly coincides with the frequency that draws maximum secondary voltage in

Figures 32, 33, and 34. The system can be tuned by varying the frequency to obtain higher power input. This is in agreement with the previous studies (10, 29, 31). A higher primary voltage increases secondary voltage and total power input for all reactors.

Volumetric flow rate of the feed gas determines the residence time of the gas in the discharge zone. Flow rates were varied from 1 1/min to 12 1/min in reactor #3. Power input did not change as the flow rates changed at each frequency (60-1000 Hz) and at each primary voltage (20 V, 40 Jz)V, and 60 V). That is, the shape of the Figure 37 did not change at varying flow rate. There were some fluctuations in power input at the optimum frequency as the flow rate increased. This power fluctuation over time was a typical phenomenon of the plasma even at constant flow rates. Since it was shown that increased flow rate did not draw more power to the system, increased flow rate reduced the power demand by the reactor per unit volume of carrier gas. This fact explains the decreased conversion efficiency at increased flow rate in the previous study (10).

The power cost of the plasma reactor was calculated and compared to the total cost of other processes. Capital cost, by-products removal cost, and 0 & M cost were not included in the plasma reactor evaluation. A total power input of 130 W and an air flow rate of 7 l/min, the highest flow rate in the destruction tests (10), were used during cost estimation. The previous study (10) showed that the percentage removal was maintained at a high value (>95%) and did not decrease until a very high concentration of TCE (15 kppm) was introduced into the reactor. Even uncontaminated air required the same amount of power to maintain the plasma (10). The gas-phase concentration, ppb or ppm, was expressed on a volume/volume basis and not a weight/weight basis in all figures presented in this study. At an A/W ratio of 20:1 with 100 % removal of TCE, a liquid concentration of 35 mg/l becomes a gas concentration of 1.75 mg/l or 310 ppm (35/20 mg/l = 1.75 mg/l = 1750 µg/l = 310 ppm). The unit conversion between µg/l and ppm in the gasphase was discussed in the main program.

Figure 11 shows that a plasma reactor is an expensive process in spite of the fact that the cost represents only electric power cost. Moreover, this price should be added to that of the air stripping process to obtain a total system cost. The A/W ratio used in the AST+plasma reactor system was 1.5 times the minimum, which was also favorable to the plasma reactor by generating a smaller amount of offgas.

The cost of a gas-phase or liquid-phase GAC contactor was highly dependent on contaminant concentration while that of plasma was not. Therefore, plasma reactors will have an advantage at high contaminant concentrations. The off-gas concentration from an AST, however, will not exceed 500 ppm (volume/volume) when the influent liquid concentration to the tower is 35 ppm (weight/weight). It may be too early, to conclude that the plasma reactor is not suitable as an off-gas control for ASTs. The experiments were not conducted on a fully optimized design. Also, scaling up may increase the power efficiency that is actually transferred to the plasma reactor.

TABLE IX

OPTIMUM GAS PRESSURE DROP AND MULTIPLES OF MINIMUM A/W RATIO FOR COMPOUNDS INVESTIGATED IN COMBINED SYSTEM

Compound Name	Pressure Drop (N/sq.m./m.)	Multiples of Minimum A/W Ratio
Trichloroethylene	60	1.7
Tetrachloroethylene	54	2.1
Toluene	62	1.7
Chlorobenzene	62	1.7
Bromoform	50	1.3
Chloroform	59	1.3
1,1,1-Trichloroethane	50	1.8
Ethylbenzene	62	1.8
1,2-Dichlorobenzene	60	1.7
Cis-1,2-Dichlorobenzen	e 57	1.2
Trans-1,2-Dichlorobenze	ene 50	1.2
Carbon tetrachloride	50	1.6

Individual Ci; 100 ppb Individual Ce; 5 ppb Water flow rate; 1 MGD

TABLE X

TREATMENT COSTS OF COMBINED SYSTEM DETERMINED AT OPTIMUM A/W RATIO AND 3.5 TIMES THE MINIMUM A/W RATIO

Compound Name	At Optimum A/W Ratio	At 3.5 Times Minimum A/W Ratio	Difference
	(cents,	/1000 gal)	(%)
Trichloroethylene	22.5	24.4	8.4
Tetrachloroethylene	18.9	19.4	3.0
Toluene	23.0	24.8	7.8
Chlorobenzene	23.4	25.5	8.7
Bromoform	52.5	69.7	32.8
Chloroform	39.6	54.2	36.9
1,1,1-Trichloroethane	21.0	22.2	6.0
Ethylbenzene	22.0	23.3	6.2
1,2-Dichlorobenzene	25.1	28.1	12.1
Cis-1,2-Dichlorobenzene	50.1	77.8	55.5
Trans-1,2-Dichlorobenze	ne 38.5	54.5	41.6
Carbon tetrachloride	21.8	24.0	9.9

Individual Ci; 100 ppb Individual Ce; 5 ppb Water flow rate; 1 MGD Air pressure drop; optimum for each case

TABLE XI

COMPOUNDS AND COMPOUND COMBINATIONS INVESTIGATED

Compound No.	Compound name	
1	Trichloroethylene	
2	Tetrachloroethylene	
3	Toluene	
4	Chlorobenzene	
5	Bromoform	
6	Chloroform	
7	1,1,1-Trichloroethane	
8	Ethylbenzene	
9	1,2-Dichlorobenzene	
10	Cis-1,2-Dichlorobenzene	
11	Trans-1,2-Dichlorobenzene	
12	Carbon tetrachloride	
Α	Compound 1 + Compound 3	
В	1+2+3+4	
С	1+2+3+4+8+9	
D	1+2+3+4+5	
E	1+2+3+4+7	
F	1+2+3+4+10	

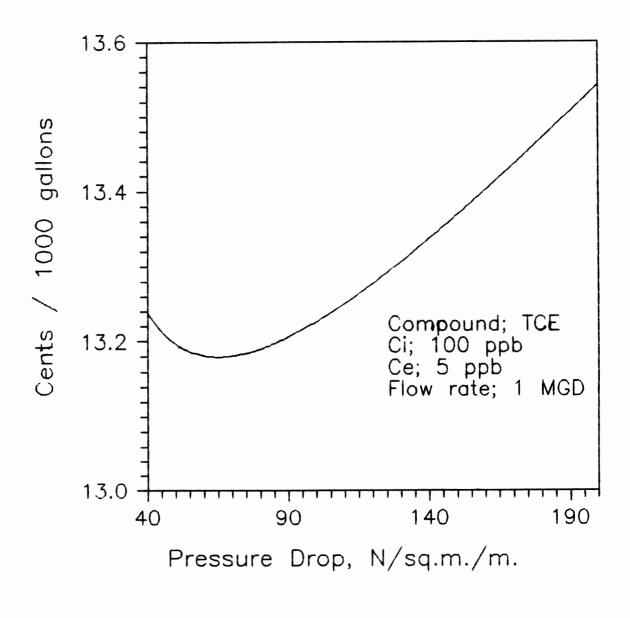


Figure 7. Cost Estimates of AST as a Function of Pressure Drop

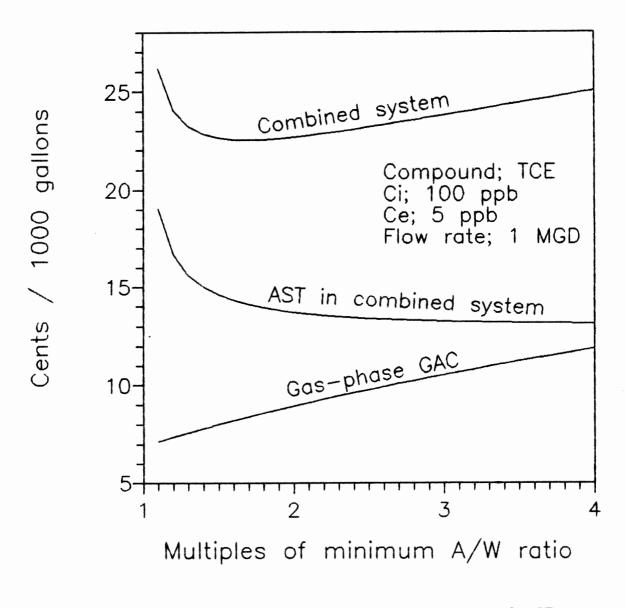


Figure 8. Effect of A/W Ratio on the Cost of AST and Gas-phase GAC

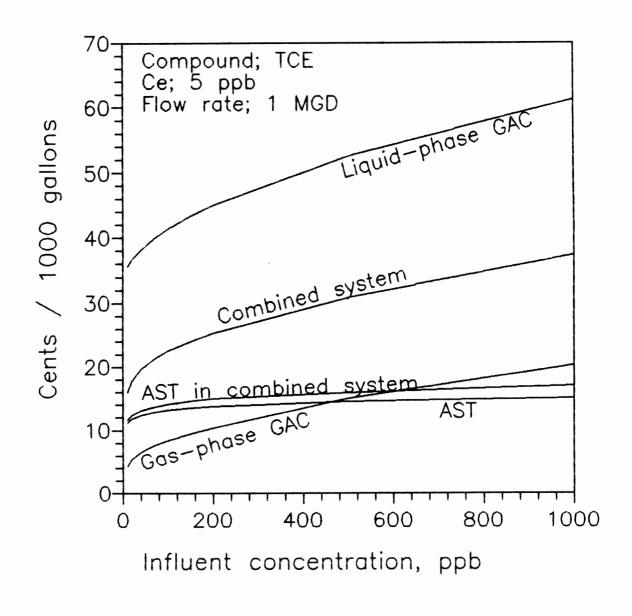


Figure 9. Effect of Influent Concentration (low range) on the Cost of Treatment Processes

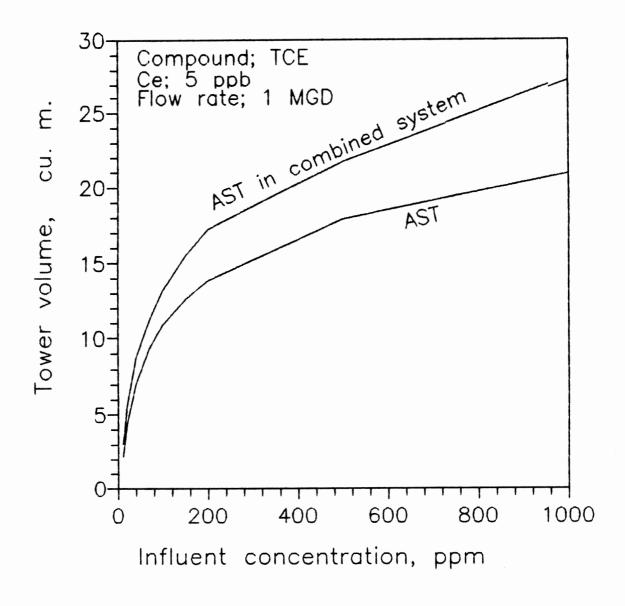


Figure 10. Effect of Influent Concentration (low range) on the Volume of AST

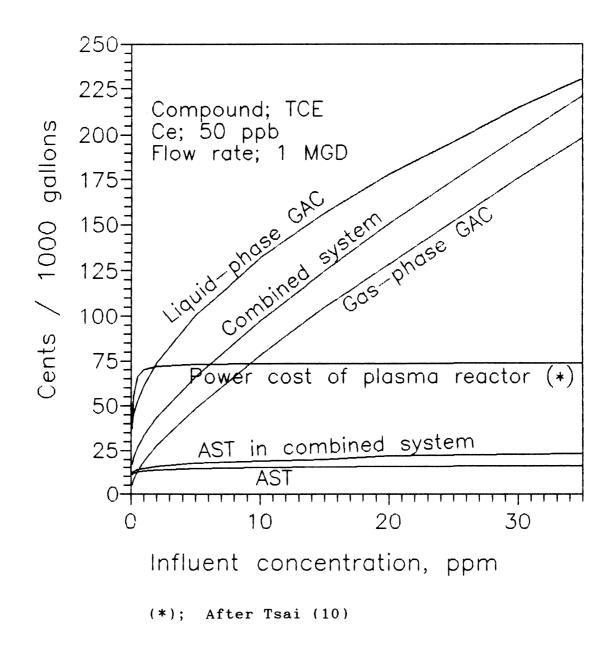


Figure 11. Effect of Influent Concentration (high range) on the Cost of Treatment Processes

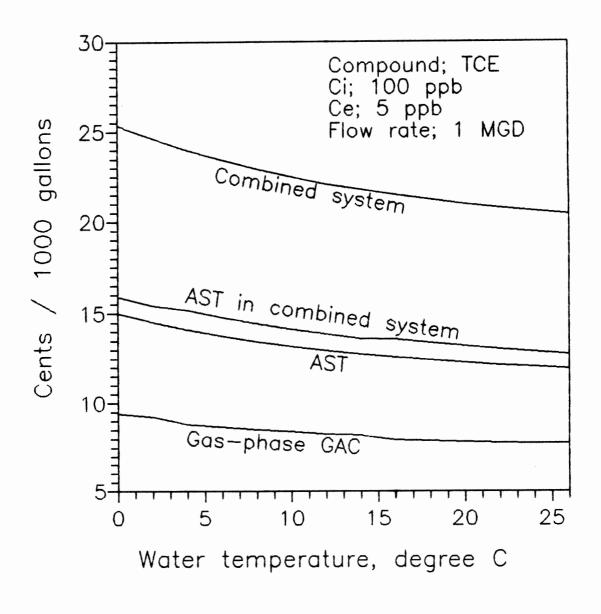


Figure 12. Effect of Water Temperature on the Cost of Treatment Processes

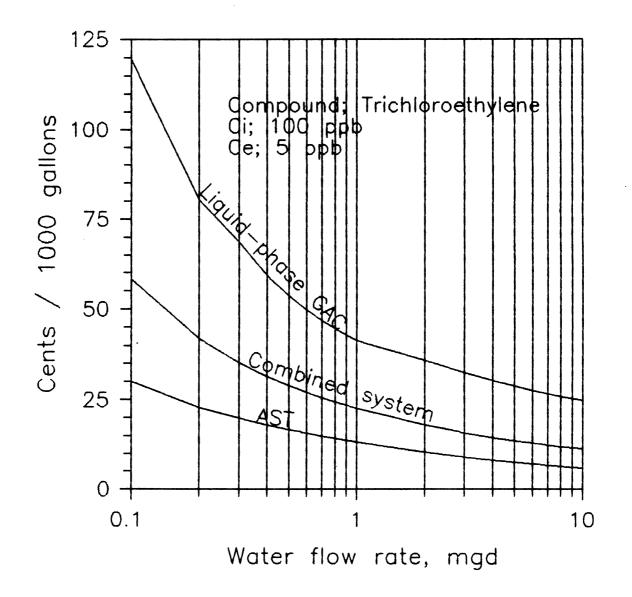


Figure 13. Trichloroethylene

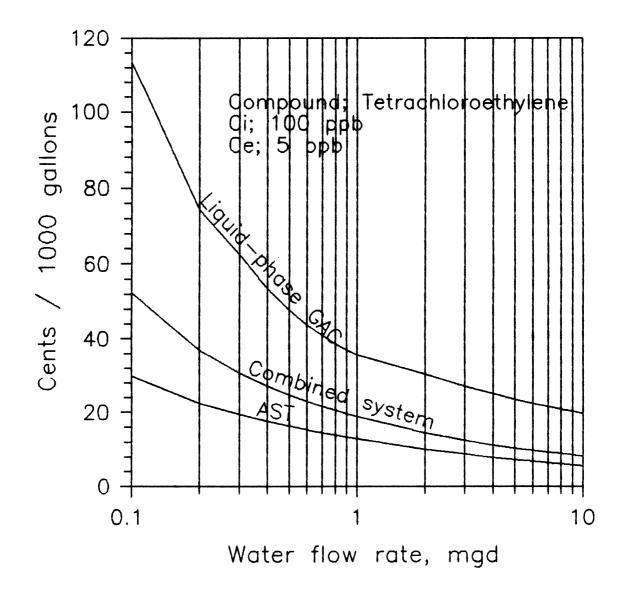


Figure 14. Tetrachloroethylene

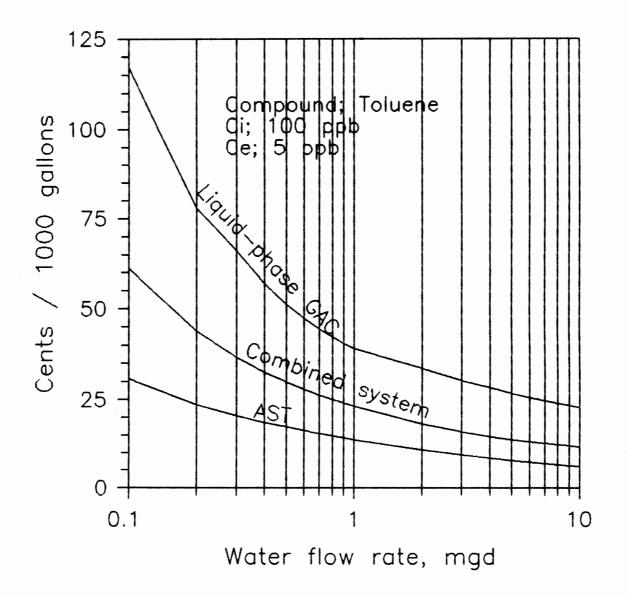


Figure 15. Toluene

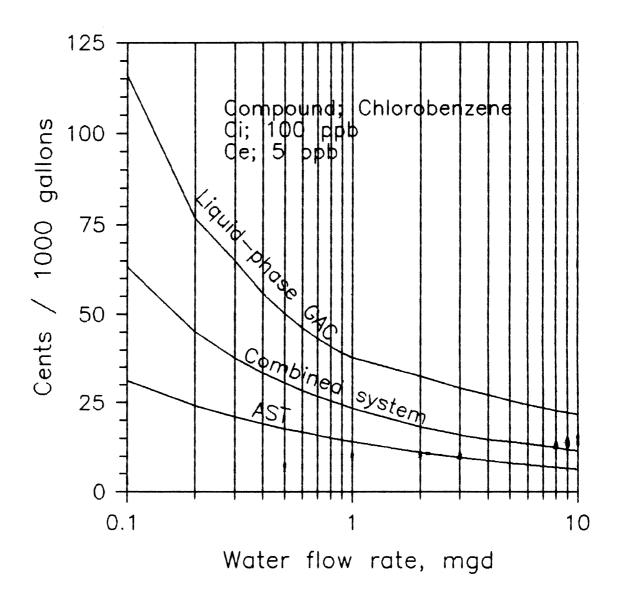


Figure 16. Chlorobenzene

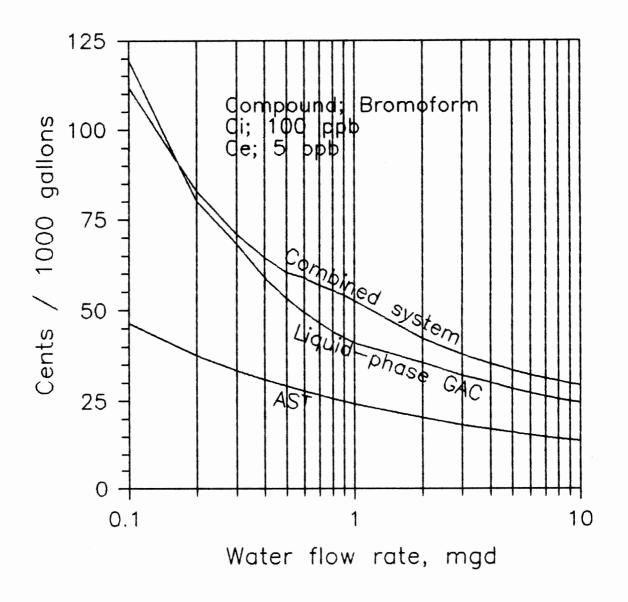


Figure 17. Bromoform

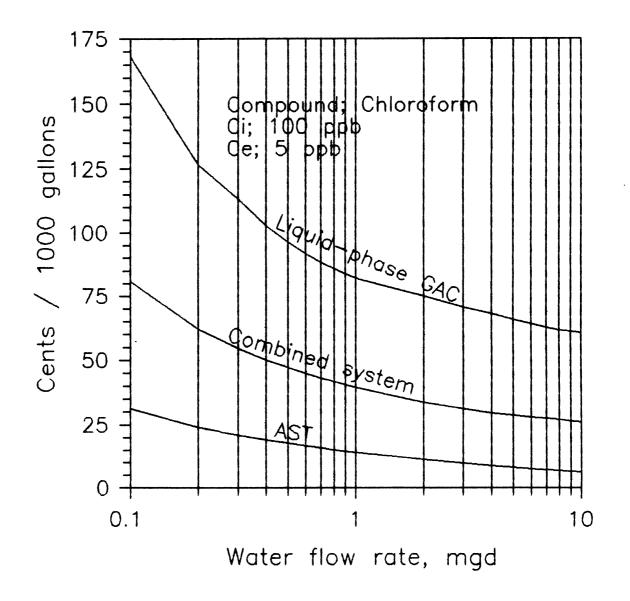


Figure 18. Chloroform

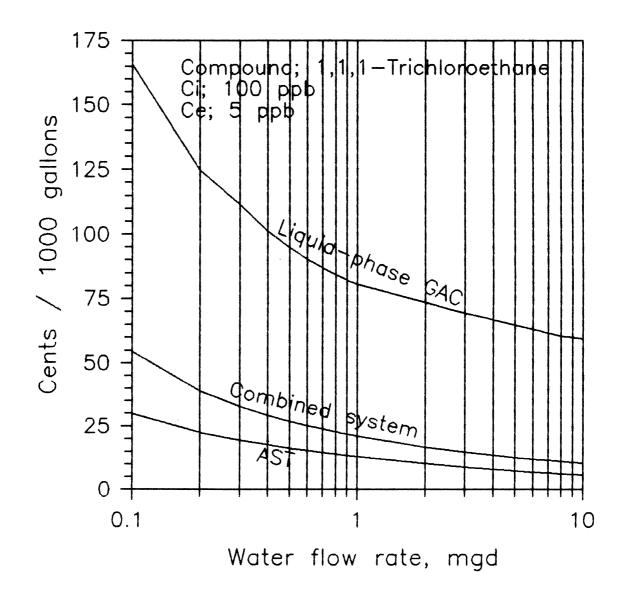


Figure 19. 1,1,1-Trichloroethane

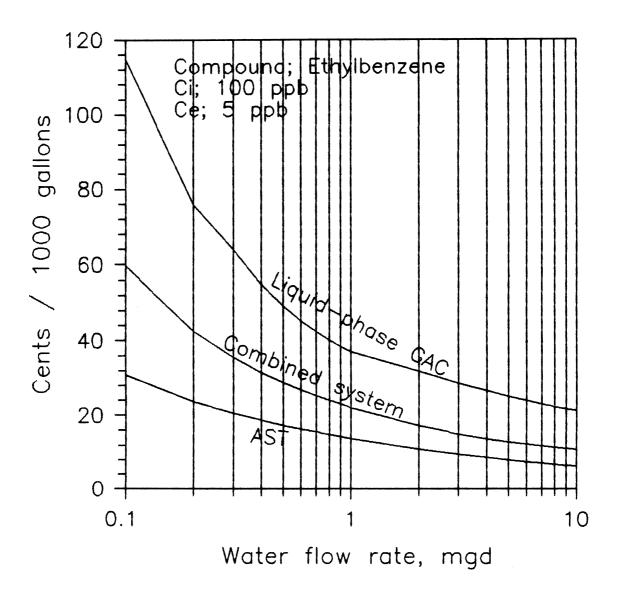


Figure 20. Ethylbenzene

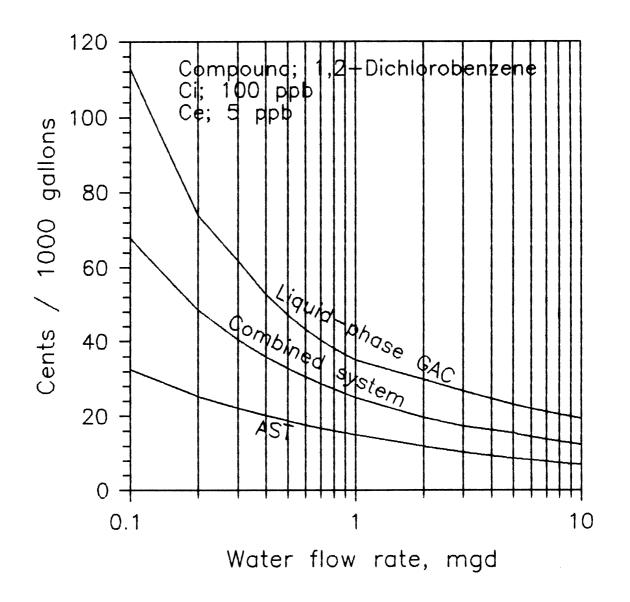


Figure 21. 1,2-Dichlorobenzene

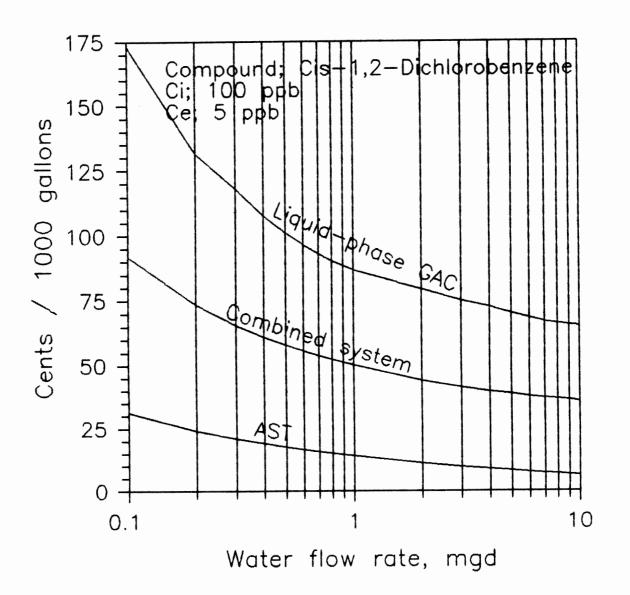


Figure 22. Cis-1,2-Dichlorobenzene

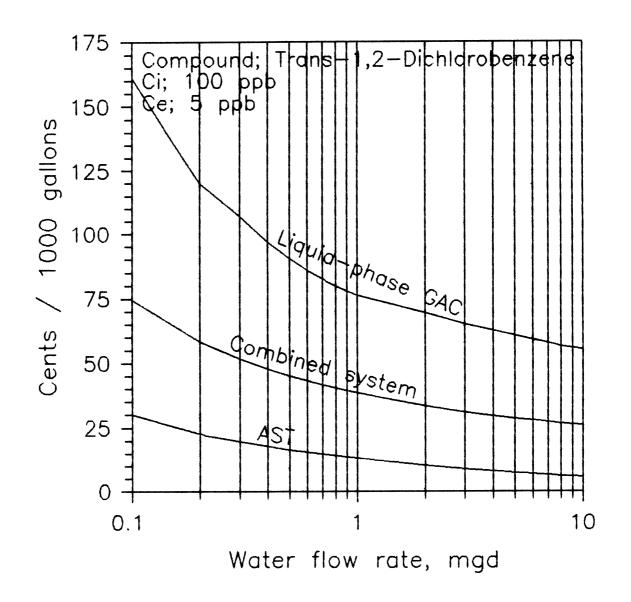


Figure 23. Trans-1,2-Dichlorobenzene

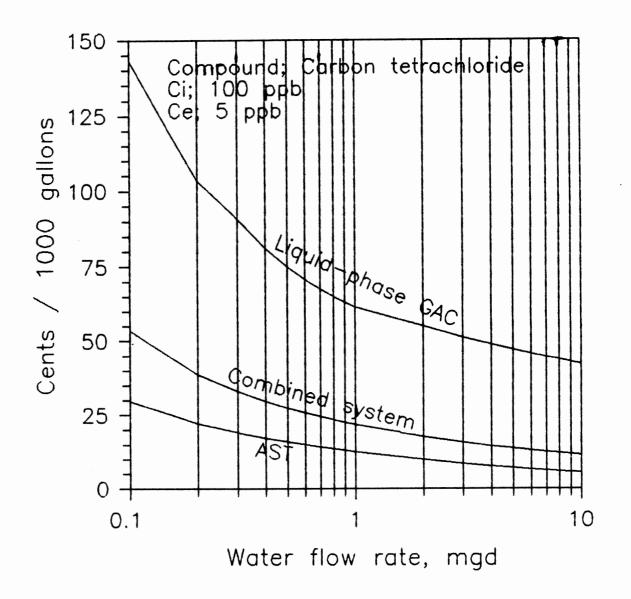


Figure 24. Carbon tetrachloride

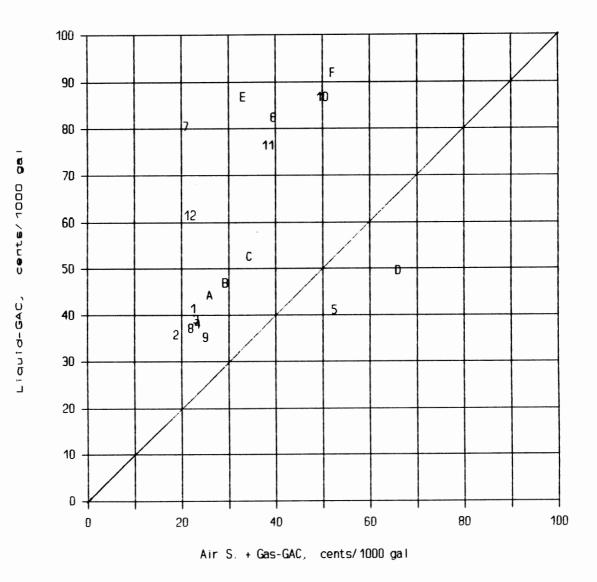


Figure 25. Cost Mapping of the Compounds Studied

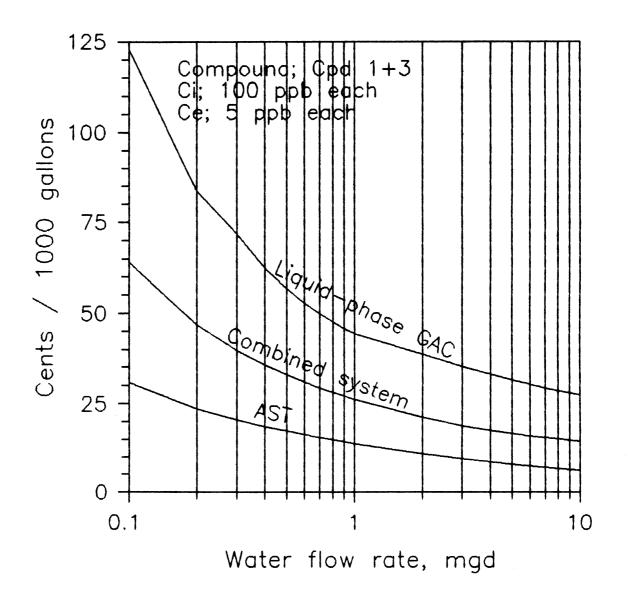


Figure 26. Compounds #1+#3 (System A)

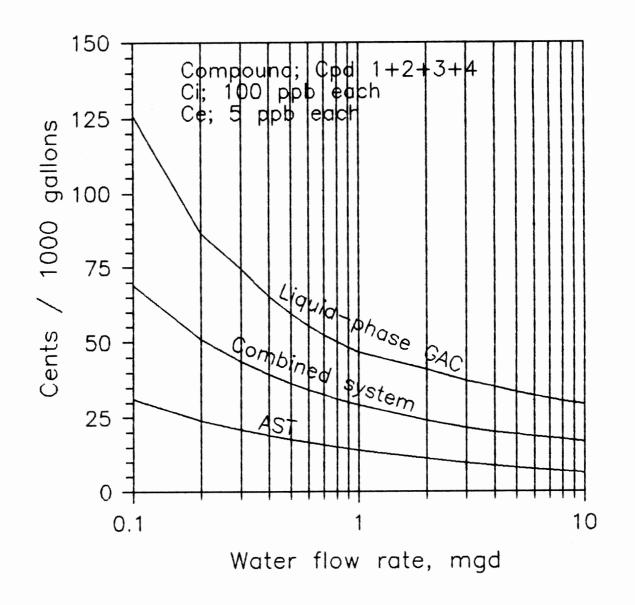


Figure 27. Compounds #1+#2+#3+#4 (System B)

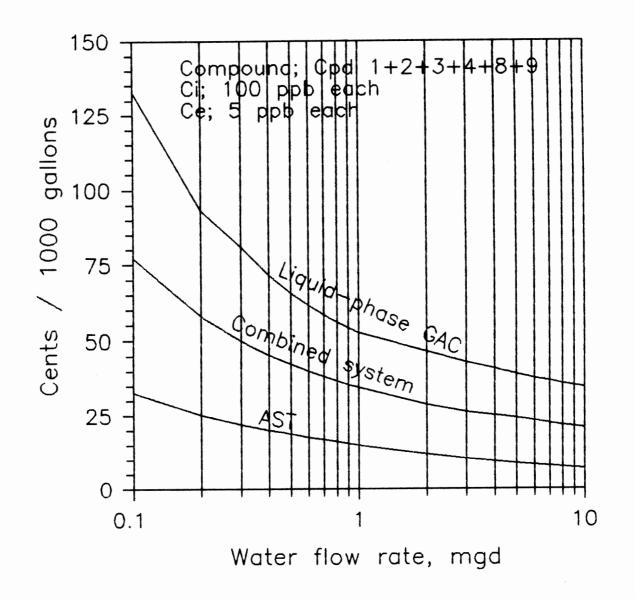


Figure 28. Compounds #1+#2+#3+#4+#8+#9 (System C)

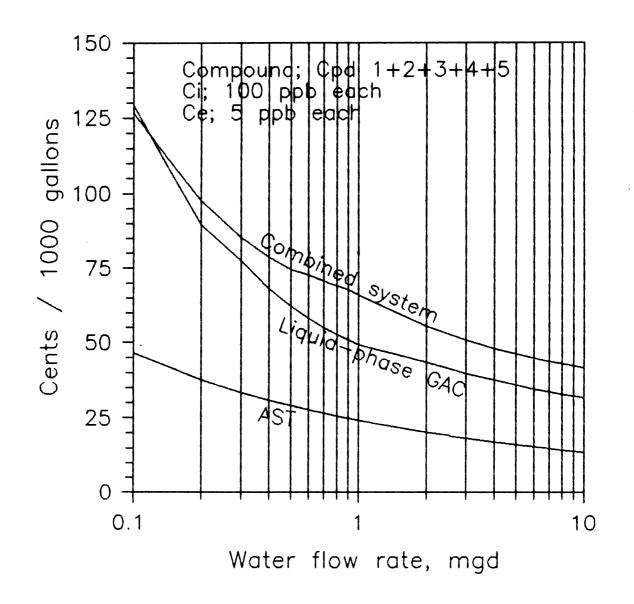


Figure 29. Compounds #1+#2+#3+#4+#5 (System D)

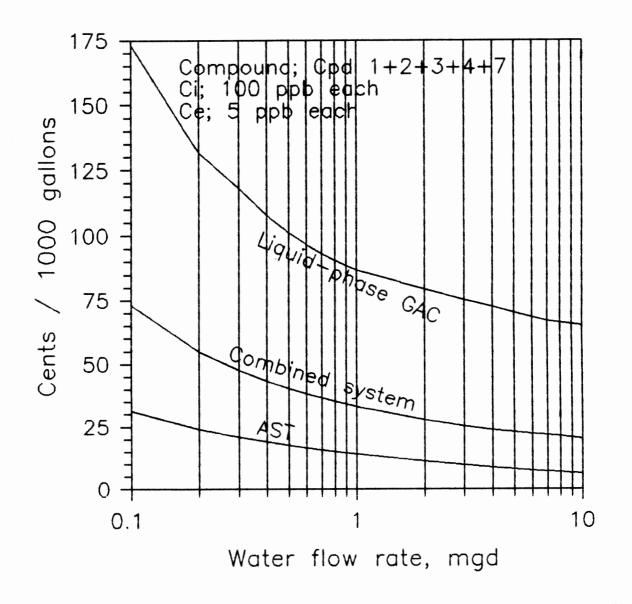


Figure 30. Compounds #1+#2+#3+#4+#7 (System E)

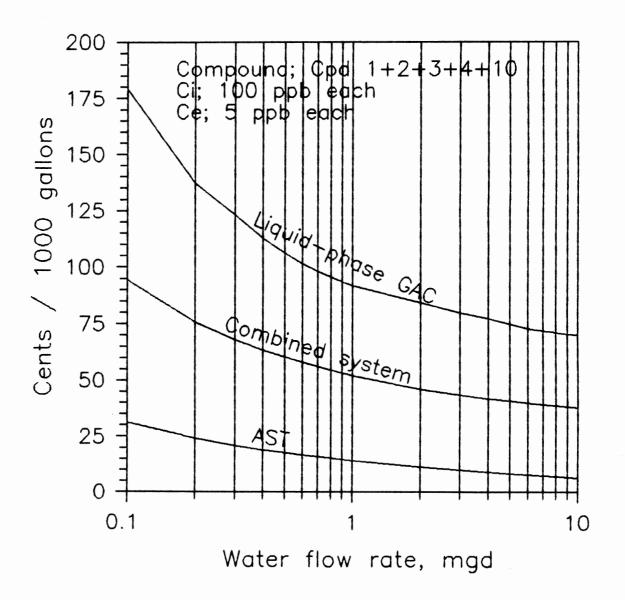


Figure 31. Compounds #1+#2+#3+#4+#10 (System F)

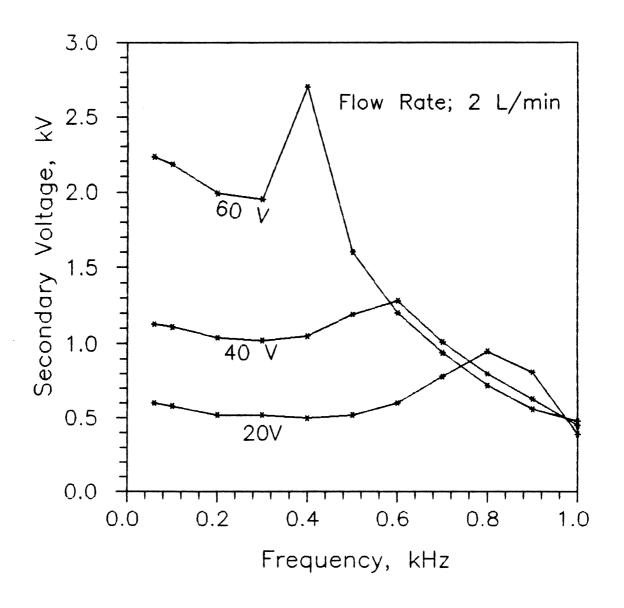


Figure 32. Effect of Frequency and Primary Voltage on Secondary Voltage for Reactor #1

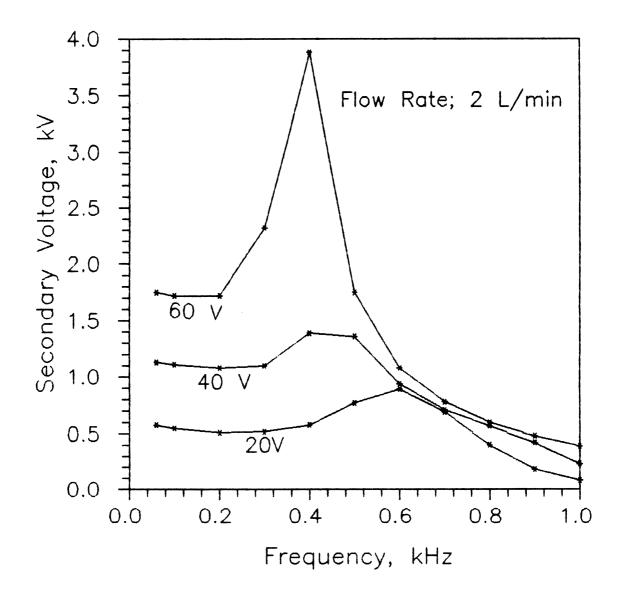


Figure 33. Effect of Frequency and Primary Voltage on Secondary Voltage for Reactor #2

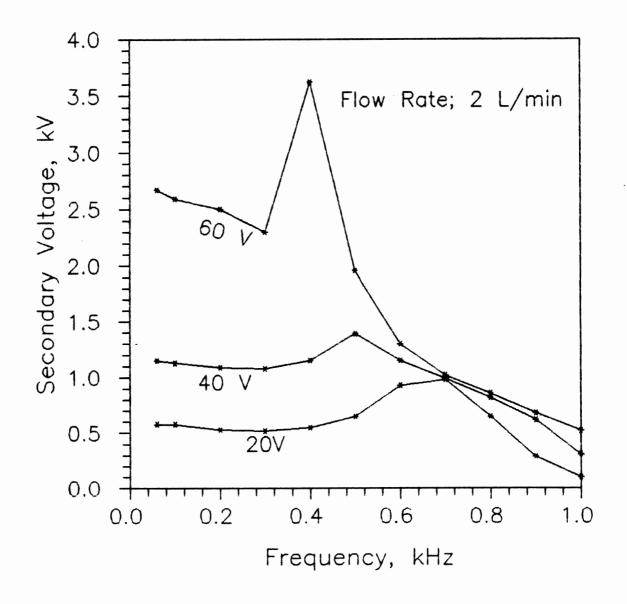


Figure 34. Effect of Frequency and Primary Voltage on Secondary Voltage for Reactor #3

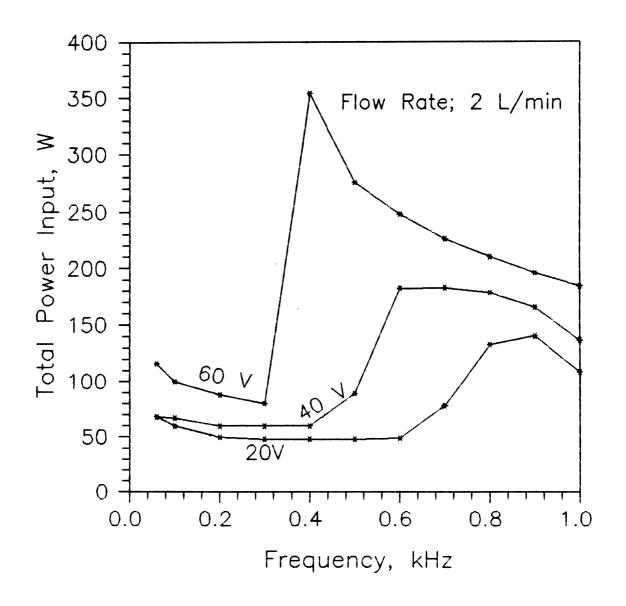


Figure 35. Effect of Frequency and Primary Voltage on Total Power Input for Reactor #1

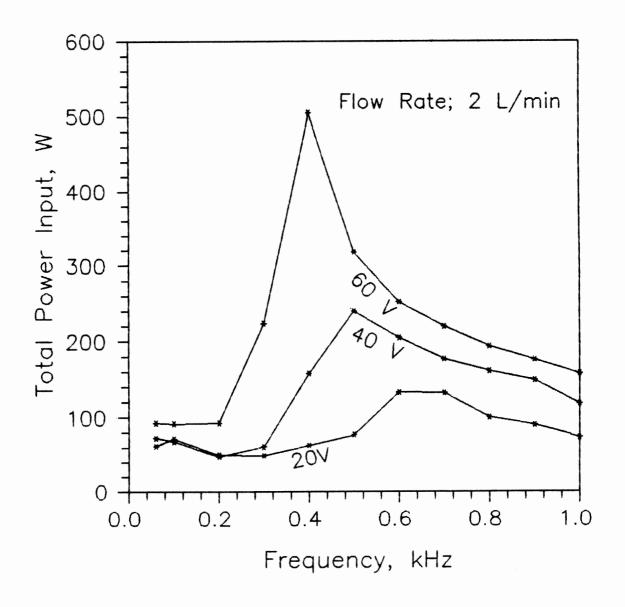


Figure 36. Effect of Frequency and Primary Voltage on Total Power Input for Reactor #2

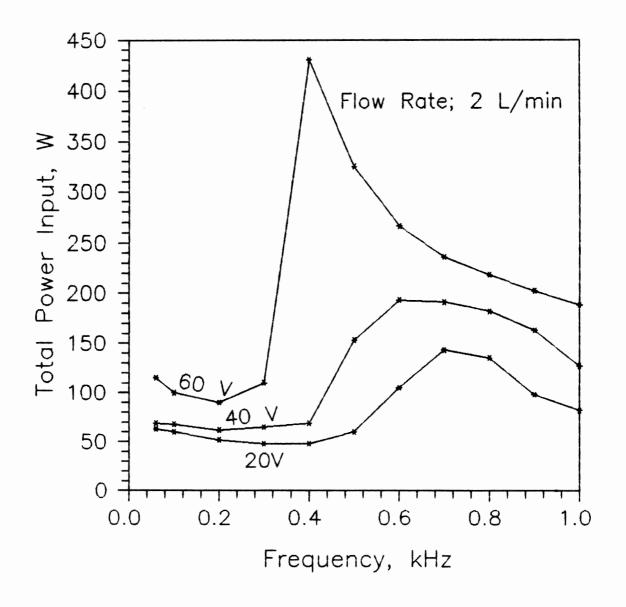


Figure 37. Effect of Frequency and Primary Voltage on Total Power Input for Reactor #3

CHAPTER V

CONCLUSIONS

A coupled computer algorithm was developed for optimum design and preliminary cost estimation of air stripping towers (ASTs) with a granular activated carbon (GAC) adsorption system as an off-gas treatment. The computer program also includes subroutines for the design of liquidphase GAC systems. The newly developed algorithm consisted of seven preexisting subroutines (MPTAD, ONDA, DIFL, DIFG, ET, SPEQ, and USER), five new subroutines (GACBED, GACBEDG, DENVIS, GACCOST, GACCOSTG, and TWCOST), and a new main program.

The optimization was done by determining the best combination of the operating and design variables, and process selections resulting in the least total cost of the systems (AST + gas-phase GAC, or AST alone). The method works for either single or multicomponent systems for ASTs and GAC processes (gas-phase and liquid-phase). This model allows a comparison between an optimized AST + gas-phase GAC and an optimized liquid-phase GAC system.

This is a total integrated model for the optimum design and cost estimation of an AST with off-gas carbon treatment. The least cost design takes into account the operating

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conditions in both unit processes and optimizes the overall design. This model can be used for designing either new systems as it is, or for retrofitting existing systems by running only a portion of the program.

The first phase of this study consisted of development and evaluation of a model of an AST + gas-phase GAC system. The specific findings are summarized below:

The integrated model predicted the least total cost 1. for the AST + gas-phase GAC system to occur in the range of 1.2 to 2.1 times the minimum A/W ratio. This range was established for the 12 compounds used in this study. However, since the model contains a large number of general system or cost parameters that the user must input, the established range may not be absolute but held for the input variables selected in this study. Previous investigations have suggested 3.5 times the minimum A/W ratio to be the best design for an AST (56). A comparison between the AST designed alone and that coupled to a gas-phase GAC system which was designed by the integrated model showed the AST system to be physically as well as operationally different. For instance, with TCE, the total cost difference between the AST + gas-phase GAC system designed by the integrated model versus the two processes designed independently and coupled together was 8.4 %. The integrated model produced the lower cost.

2. The integrated model was designed to be more realistic in what the unit processes could handle as input

streams. It was constructed to handle multicomponent systems in both the AST and carbon units. An analysis of the data showed the cost to treat a multicomponent system was highly dependent on the least strippable component in the air stripper or the least adsorbable component in the liquid-phase GAC adsorption.

3. The integrated model evaluation of the effect of water temperature on system cost showed that as the water temperature increased the total system cost of the coupled system decreased. The model showed the cost of each unit process involved in the coupled system to follow this same trend. This drop in cost for the gas-phase GAC system with increasing temperature is contradictory to existing theory. However, the effect of increased temperature on the AST reduces the off-gas volume to be treated by gas-phase GAC, thereby reducing the cost of the gas-phase GAC and total system.

4. The cost of AST was shown to be only a minor function of air pressure drop. For the twelve compounds evaluated in this study, the pressure drop yielding the least cost for the AST system appeared in the range of 50-62 $N/m^2/m$.

5. Even when off-gas treatment is required, the integrated model showed the AST to generally be a less expensive treatment process for VOCs than a liquid-phase GAC system. This confirms the results of previous studies of Adams and Clark (13). Of the 12 compounds evaluated in this study, only bromoform showed liquid-phase GAC to be less expensive, at flow rates greater than 0.2 MGD, than the combined system.

The integrated model represents a step forward in the design and cost evaluation of an AST with off-gas control using GAC. Instead of designing the units independently, the coupled system is now designed as a package. The current model is by no means perfect. The following are weaknesses that exist in this model.

1. As the A/W ratio decreases as recommended by this study, the tower becomes very tall. Physically, this can be solved by putting towers in series. However, this may not be suitable for the cost data used in this study. To remedy this, more field cost data are needed.

2. Due to the lack of data, gas-phase GAC cost data were obtained from liquid-phase GAC systems. Real gas-phase GAC cost data are needed to verify the cost estimation.

As part of this research a preliminary evaluation of plasma reactors was conducted to investigate their potential as a feasible and economical off-gas control technology for an AST. This portion of the study involved experiments conducted on bench scale plasma reactors. The majority of these experiments dealt with the power drawing characteristics of various plasma reactors. However, a limited number of destruction tests were conducted using TCE. The specific findings of this portion of the study are

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summarized below:

1. The total power demanded by the plasma reactor did not increase as the air flow rate to the unit increased from 1 to 12 l/min. Therefore, the amount of power per unit volume of air decreased as flow rate increased. This phenomenon may explain the drop in TCE destruction efficiency observed by Tsai (10) as the flow rate to the plasma increased.

2. For heavily contaminated air streams, the plasma reactor is a more economical treatment technically than a gas-phase GAC system. However, the breakpoint is at concentrations much higher than those normally seen in the air exhaust stream from an AST. Therefore, this evaluation showed the plasma reactor to be an expensive process for off-gas control for an AST. This result is based on power costs.

3. Destruction tests conducted on an air stream containing 9000 ppm TCE showed the plasma reactor was capable of greater than 90 % destruction efficiency. This work is in agreement with the results obtained by Tsai (10)

4. Studies conducted to investigate the electrical characteristics of the plasma reactors showed that an optimum frequency for the alternating current exists for maximum power input. Also, the optimum frequency is dependent on the reactor (i.e. geometry) and the primary voltage applied. These results are similar to those observed in previous investigations (10, 31).

CHAPTER VI

SUGGESTIONS FOR FUTURE STUDY

The following suggestions are made for future study.

1. This report did not account for naturally occurring organic matter such as humic and fulvic acids due to the lack of a proper model. Depending on the water source, the background organics may reduce the liquid-phase GAC capacity. Future studies should consider this effect.

2. Laboratory work may be conducted to verify the prediction of the multicomponent model.

3. A sensitivity analysis, with model input variables, could be conducted on the model output. The sensitivity analysis may include the effect of individual model uncertainty on the overall cost and design.

4. Further investigations may be done on a more optimized and scaled up design of the plasma reactor to increase its power efficiency.

5. Further studies should include more detailed aspects of plasma reactor such as by-product formation and the effects of temperature and humidity.

6. Evaluation of the total cost of the plasma reactor system including capital cost, 0 & M cost, and power cost should be done.

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APPENDIXES

APPENDIX A

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LIST OF VARIABLES

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From Main Program

A,B,C; constants for Antoine equation COMPOUND; name of the compound CS; the solubility of the compound, ug/l VP; vapor pressure of coumpound at TEMPC, mmHg YNHC; flag for Henry's constant TCOST; total yearly cost of air stripping, \$/year TGAL; unit cost of air stripping, cents/1000-gal DCOST; total yearly cost of discharge reactor, \$/year DGAL; unit cost of discharge reactor, cents/1000-gal CCOST; total yearly cost of liquid-phase GAC, \$/year CGAL; unit cost of liquid-phase GAC, cents/1000-gal CCOSTG; total yearly cost of gas-phase GAC, \$/year CGALG; unit cost of gas-phase GAC, cents/1000-gal TCGALG: TGAL+CGALG TCGALOP; TGAL+CGALG of optimum A/W ratio AWOPT; the index of the optimum A/W ratio

From MPTAD

TAREA; total tower cross sectional area, sq.m. AT; specific surface area of the packing, sq. m. per cu. m. AW; wetted surface area of the packing, m**2/m**3 BP; blower brake power, kw BPW; brake power for the pump, kw CE; effluent conc. desired, ug/l CEA; effluent conc. actual, ug/l CF; packing factor CI; influent conc., ug/l DGKGM3; density of air, kg/m**3, DGGCM3 * TEMPKG/TEMPK * 1000 DGGCM3; density of air at the elevated temperature, g/cm**3 DIFLL; liquid diffusivity, sq.m./sec. DIFCM2L (cm**2/sec) = DIFLL * 10000.0DIFGG; gas-diffusivity of the compound, m**2/sec DIFCM2G (cm**2/sec) = DIFGG * 10000.0 DIFGGG; gas-diffusivity at the elevated temperature, m**2/sec DP; nominal packing size, cm DT; tower diameter, m. DWGCM3; density of water, g/cm**3 DWKGM3 = DWGCM3*1000.0, kg/m**3EAB; energy of molecular attraction EFF; blower (fan*motor) efficiency, % EFFW; pump efficiency, % F(KT/EAB); collision function FR; Froude number G; gravitational constant GM; air loading rate, gas phase mass flux, kg/sq.m-sec HC; Henry's constant, dimensionless form HLL; tower length, m INCREM; increment of XMPL K; boltzmann's constant KLA; overall mass transfer coefficient, sec.**(-1) LM; liquid-phase mass flux

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MA; molecular weight of the air, ma, 28.95
ML; water loading rate, kg/sq.m-sec
MW; molecular weight of the compound
N; constant equal to .283
NFLOWL; number of flow rates for simulation
NVQ; number of air to water ratio for simulation
P1; inlet air pressure to blower, Pa
P2; outlet air pressure from blower, Pa
PACKING; name and type of packing to be used
PRESATM; operating pressure, atm
  PRESHG = PRESATM * 760.0
PRESD; desired air pressure drop across the tower, Pa/m.
PRESE; pressure drop due to tower inlet, outlet, packing support plate,
       Pa
PT; absolute pressure, assumed to be 1 atm or 101,325 N/sq.m.
QMG; mass flow rate of air
FLOWL; water flow rate, mgd or m**3/sec
SFLOWL; starting water flow rate for simulation, mgd
SXMPL; starting XMPL
R; gas constant, 286.7
RAB; mol. separation at collision, nm
    RAB = (RA+RB)/2, where RB = 1.18*VB**.33
                           RA = .3711 \text{ nm} For air
RE; Reynolds number
RECE; removal efficiency
ST; surface tension of water, kg/sec**2
STC; critical surface tension of the packing, N/m
TEMPAIRC; inlet air temp., deg C
TEMPC; water temperature, deg C
   TEMPK = TEMPC + 273.0
TEMPKB; boiling pt. temp of the compound, deg K
TV; tower volume, cu.m.
VB; molal volume of the compound, m**3/kg-mol
    (can be determined from the Lebas method).
VGAS; superficial gas velocity of tower, m/sec
VGKGMS; air viscosity, kg/m-sec
VGGCMS; air viscosity at the elevated temperature, g/cm-sec
VQ; the calculated value of the air to water ratio
VWGCMS; water viscosity at DW, g/cm-sec
   VWKGMS = VWGCMS/10.0, kg/m-sec
VQMIN; minimum air to water ratio
WE; weber number
XMPL; some multiple of VQMIN to acheive the desired operating air
      to water ratio
 From GACBED, GACBEDG
CMASS; total amount of carbon in bed, kg
CARUSE; carbon usage rate, kg/day
BDEPTH; bed depth, m
BAREA; bed area, m**2
BVOL = BDEPTH * BAREA
LIFE; bed life (regeneration cycle), days
VPG; vapor pressure of the coumpound at the elevated temp, mnHg
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TEMPUPG; increase in temp to lower relative humidity, deg C
TEMPKG; elevated temperature, deg K
FLOWG; air flow rate, mgd or m**3/sec
FLOWGG; air flow rate at the elevated temp, mgd or m**3/sec
QB; equilbrium concentration on the carbon in D-R equation,
      PP = (CONC/MW * 22.4 / 1.0E+6)*PRESHG
      QB = 0.46E+6* DENL/MW*EXP(-1.33E-7*(TEMPKG/BETA*ALOG(VPG/PP))**2)
 From SPEQ
DENL; liquid (compound) density, g/cc
TEMPC; system temperature, deg C, assumed to be equal to inlet
       water temperature
BETA; affinity coefficient
 From USER
VSW; liquid superficial velocity, cm/sec
DIA; carbon particle diameter, cm
RHOB; bulk bed density, gm/cm**3
RHOP; apparent particle density, gm/cm**3
EPOR; void fraction of the particle
EBED; void fraction of the bed = 1.0 - RHOB/RHOP
PSDFR; pore surface diffusion flux ratio
EBCT; empty bed contact time of interest, min.
SEBCT; starting empty bed contact time for simulation, min.
NEBCT; number of empty bed contact time for simulation
TAU; packed bed contact time
CI; the initial conc. of the compound, ug/l
CIM; CI/MW, umole/l
CIOS; overshooting concentration of CI
CE; the effluent conc. of the compound, ug/l
CEM; CE/MW, umole/l
KK; Freundlich iso. cap., (umol/gm)(l/umol)**NN
NN; Freundlich isotherm exponent, 1/n, dimensionless
KF; film transfer coefficient, cm/sec
DS; surface diffusion coefficient, cm**2/sec
DG; solute distribution parameter
BI; biot number
SC: Schmidt number
STM; the minimum Stanton number
ETMIN; the minimum EBCT, sec
ETLEN; the length of the minimum EBCT, cm
T95; throughput at 95% of the MTZ
TEI; throughput at (CEM/CIM)*100% of the MTZ
ETMTZ; the EBCT of the MTZ, sec
EMTZL; the length of the MTZ, cm
Q; equilbrium concentration on the carbon,
   Q = KK*CIM**NN, umole/g-carbon
PC; partition coefficient (distribution parameter)
From GAS-PHASE USER;
CIG; the initial conc. of the compound in gas-phase, ug/l
```

122

CIGG; initial concentration at the elevated temperature CIGGOS; overshooting concentration of CIGG VSG; air superficial velocity, cm/sec VGGCMS; viscosity of air, (gm/cm-sec) at the elevated temperature DGGCM3; density of air, (gm/cm**3) at the elevated temperature From Cost calculations (GACCOST, GACCOSTG, TWCOST) CONTAC; least cost contactor selected for liquid phase CONTACG; least cost contactor selected for gas phase REGEN; least cost regeneration selected for liquid phase REGENG; least cost regeneration selected for gas phase CCOST; total system cost for liquid phase carbon adsorption, \$/year CCOSTG; total system cost for gas phase carbon adsorption, \$/year CCOST; unit cost for liquid phase carbon adsorption, cents/1000gal -water CCOSTG; unit cost for gas phase carbon adsorption, cents/1000gal-water GACOP; percentage operation of GAC contactor, % INTEREST; interest, % PAYBACK; pay back period, years UPTIME; reactivator uptime, % CAPITAL; capital cost of the system GACPR; GAC price, \$/lb LOSS; GAC regeneration and handling losses; % LABOR; labor rate, \$/hr ELECT; electric rate, \$/kwh FUEL; fuel oil price, \$/gal NGAS; natural gas price, \$/standard cu.ft. WATER; process water price, \$/1000gal PROFIT; contractor profit factor, % SITE; special site work factor, % FEE; engineering fees factor, % CONTIN; construction contingencies factor, % PACKAGE; package pressure GAC contactors STEEL; conventional steel pressure GAC contactors CONCRETE; conventional gravity GAC contactors BWASH; back wash pumping CC STORAGE; GAC storage CC CP; heat capacity of air, cal/g-deg C HEAT; air heating cost, \$/year VIRGIN; virgin GAC replacement with disposal of spent GAC, \$/year INFRA; infrared reactivation FLUID; fluidized reactivation HEARTH; multihearth reactivtion HAREA; total effective hearth area, caruse/(451b/sqft/day) PRESDG; gas-phase pressure drop through carbon bed, Pa PTOP; percentage operation of packed tower, % CRF; capital recovery factor ECI; Marshall and Swift equipment cost index CCI; engineering news record construction cost index

From ET

BVF; bed void fraction

```
C; liquid phase concentration, ug/l
CH; working character
CHAR; name of the components
CO; initial concentrations, ug/l
DEN; bulk density of adsorbent, g/cm**3
DGX; dimensionless group X: used to find strongest component
DGY; dimensionless group Y: used to find strongest component
FCN; subroutine that sets up the non-linear equations
FNORM; output: sum of the residuals
I: counter
IAST; subroutine to account for competitive effects
IER; output: error parameter
ITMAX; maximum number of iterations
IX; used to keep track of strongest component
J: counter
K; counter
L; counter for error fixing
M; counter
MW; molecular weight
N; number of components total
NN; number of components in a zone
NS; NSIG input
NSIG; number of digits of accuracy desired in the computed root
OATS; bed volumes fed
PAR; parameter set
PAR(1 to N); Freundlich K values
PAR(10 to 10+N); Fruendlich N values
PAR(20 to 20+N); initial concentrations
PAR(30); velocity of the wave, VW, cm/s
PAR(35); velocity of flow, VF, cm/s
PAR(40 \text{ to } 40+I); calculated liquid concentrations
PAR(60 to 60+I); Q's of the previous wave
PAR(80 to 80+1); C's of the previous wave
Q; solid phase concentration, ug/g
QAVE; average Q in zone
SSTC; single solute treatment capacity, mg C/L water
SUM; used to calculate VW and OATS
VF; velocity of flow, cm/s
VW; velocity of wave, cm/s
WK; work vector: LENGTH=N*(3*N+15)/2
X; one dimensional solid-phase concentration, um/g
XK; Freundlich K's (um/g)*((L/um)**1/N
XN; Fruendlich 1/n 's
ZSQ; common block
ZZ; variable used to calculate initial Q's
ZZZ; dimensionless bed length
```

APPENDIX B

.

EXAMPLE OF INPUT FILE

<<< INPUT FILE >>>

- * Do not change any format of this data file.
- * Always include decimal point for the number except integer format is specified. In case of integer input, never use decimal point.

Data entry for Air Stripping Tower

PACKING; name and type of packing to be used DP; nominal packing size, cm CF; packing factor	;INTALOX SADDLES ;7.62 ;16.0
STC; critical surface tension of packing, N/m AT; specific surface area of the packing,	;0.033
sq. m. per cu. m.	;89.0
PRESATM; operating pressure, atm	;1.0
TEMPC; water temperature, deg C	;10.0
SFLOWL; starting water flow rate, mgd	;0.1
TEMPAIRC; inlet air temp., deg C	;20.0
EFF; blower efficiency, % (effic. of fan*motor)	;35.0
EFFW; pump efficiency, %	;70.0
NFLOWL; (integer)	;10

Data entry for Gas-phase Carbon Adsorption

VSG; air superficial velocity, cm/sec	;30.48
TEMPUPG; required temp increase, C, RF;100%->40%	;14.4
DIAG; carbon particle diameter, cm	;0.3715
RHOBG; bulk bed density, gm/cm**3	;0.555
RHOPG; apparent particle density, gm/cm**3	;0.85
EPORG; void fraction of the particle	;0.595
EBCTG; empty bed contact time, sec.	;1.5

Data entry for Liquid-phase Carbon Adsorption

RHOB; bulk bed density, gm/cm**3	;0.470
DIA; carbon particle diameter, cm	;0.0513
RHOP; apparent particle density, gm/cm**3	;0.8034
EPOR; void fraction of the particle	;0.641
VSW; water superficial velocity, cm/sec	;0.3396
EBCT; empty bed contact time, min.	;15.

Data entry for cost calculation

GACOP; percentage operation of GAC contactor, %	;70.
UPTIME; reactivator uptime, %	;75.
LOSS; GAC regeneration and handling losses; %	;12.
INTEREST; interest, %	;10.
PAYBACK; pay back period, years	;20.
GACPR; GAC price, \$/1b	;.9
LABOR; labor rate, \$/hr	;15.
ELECT; electric rate, \$/kwh	;.08
NGAS; natural gas price, \$/std.cu.ft.	;.003

WATER; process water price, \$/1000gal PROFIT; contractor profit factor, % SITE; special site work factor, % FEE; engineering fees factor, % CONTIN; construction contingencies factor, % GACPRG; GAC price for gas phase, \$/lb ECI; Marshall and Swift Equipment Cost Index CCI; ENR Construction Cost Index PTOP; percentage operation of aeretion tower, %	;.35 ;5. ;5. ;10. ;10. ;2. ;904. ;435. ;70.
NCOMPOUND; No. of compounds (integer, Maximum;9)	•
***************************************	*****
(1) COMPOUND; name of the compound	; TRI CHLOROETHYLENE
MW; molecular weight of the compound	;131.39
Constants for Anotine equation, A	;5.3976
В	;631.94
С	;154.59
YNHC; Do you have a value of the Henry's	
constant in dimensionless form ? (Y/N)	;Y
(If no, answer #1. If yes, answer #2.)	
#1. CS; the solubility of the compound, ug/l	;
#2. HC; Henry's constant in dimensionless form	;0.1907
CI; influent conc., ug/l	;100.0
CE; effluent conc. desired, ug/l	;5.0
VB; molal volume of the compound, m ³ /kg-mol	,0.0
(can be determined from the Lebas method).	;0.1071
TEMPBK; boiling pt. temp of the compound, deg K	-
TEMPOR, boiling pt. temp of the compound, deg h	,000.7
Compound data regarding Gas-phase Carbon Adsorpt	ion
RECEG; desired removal, %	;95.0
PSDFRG; pore surface diffusion flux ratio	;16.0
TODANG, pore surface utilitision flux facto	,1010
Data entry for subroutine SPEQ	
BETA; affinity coefficient	;0.816
DENL; liquid (compound) density, g/cc	;1.4642
bland, fiquid (compound) density, gree	,111012
Compound data regarding Liquid-phase Carbon Adso	rption
K; Freundlich isotherm parameter	;196.6
1/N;	;0.4163
PSDFR; pore surface diffusion flux ratio	;3.72

(2) COMPOUND; name of the compound	;TET. CH. ETHYLENE
· · · · · · · · · · · · · · · · · · ·	;165.83
	;7.5406
• · · ·	•
B C	;1694.6
-	;245.29
YNHC; Do you have a value of the Henry's	

constant in dimensionless form ? (Y/N) ;Y (If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/l ; #2. HC; Henry's constant in dimensionless form ;0.3569 CI; influent conc., ug/l :100.0 CE; effluent conc. desired, ug/l ;5.0 VB; molal volume of the compound, m^3/kg-mol (can be determined from the Lebas method). ;0.128 TEMPBK; boiling pt. temp of the compound, deg K ;394.1 Compound data regarding Gas-phase Carbon Adsorption RECEG; desired removal, % ;95.0 PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ BETA; affinity coefficient ;0.976 DENL; liquid (compound) density, g/cc ;1.6227 Compound data regarding Liquid-phase Carbon Adsorption K; Freundlich isotherm parameter ;650.6 1/N;;0.4579 PSDFR; pore surface diffusion flux ratio ;3.72 (3) COMPOUND; name of the compound ; TOLUENE MW; molecular weight of the compound :92.14 Constants for Anotine equation, A ;6.7624 B ;1254.5 С ;211.31 YNHC; Do you have a value of the Henry's constant in dimensionless form ? (Y/N) ;Y (If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/1 ; #2. HC; Henry's constant in dimensionless form ;0.1190 CI; influent conc., ug/l ;100.0 CE; effluent conc. desired, ug/l ;5.0 VB; molal volume of the compound, m³/kg-mol (can be determined from the Lebas method). ;0.1182 TEMPBK; boiling pt. temp of the compound, deg K ;383.6 Compound data regarding Gas-phase Carbon Adsorption RECEG; desired removal, % ;95.0 PSDFRG; pore surface diffusion flux ratio ;16.0

Data entry for subroutine SPEQ BETA; affinity coefficient ;1.0 DENL; liquid (compound) density, g/cc ;0.8669 Compound data regarding Liquid-phase Carbon Adsorption ;348.0 K; Freundlich isotherm parameter 1/N;;0.365 PSDFR; pore surface diffusion flux ratio :3.72 (4) COMPOUND; name of the compound ; CHLOROBENZENE MW; molecular weight of the compound ;112.56 Constants for Anotine equation, A ;5.957 ;1004.3 B С ;180.41 YNHC; Do you have a value of the Henry's constant in dimensionless form ? (Y/N);Y (If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/1; #2. HC; Henry's constant in dimensionless form ;0.08977 CI; influent conc., ug/l ;100.0 CE; effluent conc. desired, ug/l ;5.0 VB; molal volume of the compound, m³/kg-mol (can be determined from the Lebas method). ;0.1169 TEMPBK; boiling pt. temp of the compound, deg K ;405.0 Compound data regarding Gas-phase Carbon Adsorption ;95.0 RECEG; desired removal, % PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ ;1.059 BETA; affinity coefficient DENL; liquid (compound) density, g/cc :1.047 Compound data regarding Liquid-phase Carbon Adsorption K; Freundlich isotherm parameter ;381.0 :0.31 1/N;;3.72 PSDFR; pore surface diffusion flux ratio (5) COMPOUND; name of the compound ; BROMOFORM MW; molecular weight of the compound ;252.73 Constants for Anotine equation, A ;4.9134 B :657.45 С ;134.0 YNHC; Do you have a value of the Henry's constant in dimensionless form ? (Y/N) ;Y

(If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/l ; #2. HC; Henry's constant in dimensionless form ;0.009944 CI; influent conc., ug/l ;100.0 ;5.0 CE; effluent conc. desired, ug/l VB; molal volume of the compound, m^3/kg-mol (can be determined from the Lebas method). ;0.0995 TEMPBK; boiling pt. temp of the compound, deg K ;422.5 Compound data regarding Gas-phase Carbon Adsorption RECEG; desired removal, % ;95.0 PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ ;0.963 BETA; affinity coefficient DENL; liquid (compound) density, g/cc ;2.8899 Compound data regarding Liquid-phase Carbon Adsorption ;161.0 K; Freundlich isotherm parameter 1/N;;0.5629 PSDFR; pore surface diffusion flux ratio ;3.72 (6) COMPOUND; name of the compound ; CHLOROFORM ;119.38 MW; molecular weight of the compound Constants for Anotine equation, A ;5.7 B ;647.54 С ;164.61 YNHC; Do you have a value of the Henry's constant in dimensionless form ? (Y/N);Y (If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/l: #2. HC; Henry's constant in dimensionless form ;0.07594 CI; influent conc., ug/l ;100.0 CE; effluent conc. desired, ug/l ;5.0 VB; molal volume of the compound, m³/kg-mol (can be determined from the Lebas method). ;0.0923 TEMPBK; boiling pt. temp of the compound, deg K ;334.7 Compound data regarding Gas-phase Carbon Adsorption RECEG; desired removal, % ;95.0 PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ

BETA; affinity coefficient	;0.694
DENL; liquid (compound) density, g/cc	;1.4832
	,
Compound data regarding Liquid-phase Carbon Adso	rption
K; Freundlich isotherm parameter	;30.4
1/N;	;0.5325
PSDFR; pore surface diffusion flux ratio	;3.72
*********	*****
(7) COMPOUND; name of the compound	;1,1,1-T.CH.ETHANE
MW; molecular weight of the compound	;133.4
Constants for Anotine equation, A	;13.08
В	;5926.8
C	;514.91
YNHC; Do you have a value of the Henry's	
constant in dimensionless form ? (Y/N)	;Y
(If no, answer #1. If yes, answer #2.)	
#1. CS; the solubility of the compound, ug/l	
#1. CS, the solubility of the compound, ug/1	;
#2. HC; Henry's constant in dimensionless form	;0.3516
CI; influent conc., ug/l	;100.0
CE; effluent conc. desired, ug/l	;5.0
VB; molal volume of the compound, m^3/kg-mol	,
(can be determined from the Lebas method).	;0.1145
TEMPBK; boiling pt. temp of the compound, deg K	;347.1
Compound data regarding Gas-phase Carbon Adsorpt	ion
RECEG; desired removal, %	;95.0
PSDFRG; pore surface diffusion flux ratio	;16.0
Data entry for subroutine SPEQ	
BETA; affinity coefficient	;0.841
DENL; liquid (compound) density, g/cc	;1.339
Compound data regarding Liquid-phase Carbon Adso	rption
K; Freundlich isotherm parameter	;29.7
1/N;	;0.495
PSDFR; pore surface diffusion flux ratio	;3.72
****************	*****
(8) COMPOUND; name of the compound	;ETHYLBENZENE
MW; molecular weight of the compound	;106.17
Constants for Anotine equation, A	;11.612
В	;4616.7
C	;409.12
YNHC; Do you have a value of the Henry's	
constant in dimensionless form ? (Y/N)	;Y
(If no, answer #1. If yes, answer #2.)	

#1. CS; the solubility of the compound, ug/l ; #2. HC; Henry's constant in dimensionless form ;0.1332 CI; influent conc., ug/l ;100.0 ;5.0 CE; effluent conc. desired, ug/l VB; molal volume of the compound, m³/kg-mol (can be determined from the Lebas method). ;0.1404 TEMPBK; boiling pt. temp of the compound, deg K ;409.2 Compound data regarding Gas-phase Carbon Adsorption ;95.0 RECEG; desired removal, % PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ BETA; affinity coefficient ;1.15 DENL; liquid (compound) density, g/cc ;0.867 Compound data regarding Liquid-phase Carbon Adsorption K; Freundlich isotherm parameter ;507.0 1/N;;0.53 PSDFR; pore surface diffusion flux ratio ;3.72 (9) COMPOUND; name of the compound ;1,2-DICH.BENZENE MW; molecular weight of the compound ;147.0 Constants for Anotine equation, A ;6.886 B ;1584.8 С ;210.14 YNHC; Do you have a value of the Henry's constant in dimensionless form ? (Y/N):Y (If no, answer #1. If yes, answer #2.) #1. CS; the solubility of the compound, ug/l; #2. HC; Henry's constant in dimensionless form ;0.06015 CI; influent conc., ug/l ;100.0 CE; effluent conc. desired, ug/l ;5.0 VB; molal volume of the compound, m³/kg-mol (can be determined from the Lebas method). ;0.1378 TEMPBK; boiling pt. temp of the compound, deg K ;453.5 Compound data regarding Gas-phase Carbon Adsorption RECEG; desired removal, % ;95.0 PSDFRG; pore surface diffusion flux ratio ;16.0 Data entry for subroutine SPEQ BETA; affinity coefficient ;1.157

DENL; liquid (compound) density, g/cc	;1.3048
Compound data regarding Liquid-phase Carbon Adso	rption
K; Freundlich isotherm parameter 1/N; PSDFR; pore surface diffusion flux ratio	;865.0 ;0.38 ;3.72

End of input file

APPENDIX C

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SOURCE PROGRAM (FORTRAN 77)

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```
С
IMPLICIT REAL (A-Z)
     CHARACTER*40 PACKING, COMPOUND (20), CPD, CONTAC1, CONTACG1, REGEN1,
    & REGENG1, CONTAC(10), CONTACG(10, 100), REGEN(10), REGENG(10, 100)
     CHARACTER*1 YNHC
     DIMENSION HC(20), MW(20), VB(20), TEMPKB(20), CI(20), CE(20), CIGG(20),
    & CEA(20,100),CEA1(20),RECEG(20),VPG(20),PSDFR(20),PSDFRG(20),
    & BETA(20), DENL(20), KK(20), NN(20), DIFLL(20), DIFGG(20), DIFGGG(20),
```

- & VQ(100), TAREA(10,100), HLL(10,100), TV(10,100), TGAL(10,100),
- & TCGALG(10,100), TCGALOP(10), DGAL(100), ETMING(100), ETMTZG(100),
- & EMTZLG(100), CARUSEG(100), BAREAG(100), PRESD(10,100), LIFEG(100),
- & CGALG(10,100),CGAL(10),KKG(20),NNG(20)
- INTEGER NFLOWL, NVQ, I, J, K, L, LL(100), LLL, II(100), JJ, AWOPT(10),

```
& NCOMPOUND
```

MAIN PROGRAM

С С

C FROM SUBROUTINE ET

INTEGER M DOUBLE PRECISION BVF, DEN EXTERNAL FCN COMMON /ZSQ/ BVF, DEN, M

OPEN (UNIT = 7, FILE = 'MVOC.DAT', FORM = 'FORMATTED', ACCESS = 'SEQUENTIAL', STATUS = 'OLD')& OPEN (UNIT = 8, FILE = 'MVOC.OUT', STATUS = 'UNKNOWN')

С DATA ENTRY OR ESTIMATION FOR EACH PROCESS

C AIR STRIPPING TOWER

READ (UNIT=7, FMT=100, END=10) PACKING, DP, CF, STC, AT, PRESATM, TEMPC, SFLOWL, TEMPAIRC, EFF, EFFW, NFLOWL &

PRESHG = PRESATM * 760.0TEMPK = TEMPC + 273.0

C GAS-PHASE CARBON ADSORPTION

READ (UNIT=7, FMT=200, END=10) VSG, TEMPUPG, DIAG, RHOBG, & RHOPG, EPORG, EBCTG TEMPKG = TEMPK + TEMPUPGCP = (.79*(6.50+0.001*(TEMPK+TEMPUPG/2.))+.21*(8.27+0.000258*)& (TEMPK+TEMPUPG/2.)-187700./(TEMPK+TEMPUPG/2.)**2.))/29.

С LIQUID-PHASE CARBON ADSORPTION

READ (UNIT=7, FMT=110, END=10) RHOB, DIA, RHOP, EPOR, VSW, EBCT

```
С
    COST CALCULATION
      READ (UNIT=7, FMT=320, END=10) GACOP, UPTIME, LOSS, INTEREST, PAYBACK,
           GACPR, LABOR, ELECT, NGAS, WATER, PROFIT, SITE, FEE, CONTIN, GACPRG,
     8
           ECI, CCI, PTOP
     &
      INT = INTEREST/100.
      CRF = INT*(1.+INT)**PAYBACK/((1.+INT)**PAYBACK-1.)
С
    COMPOUNDS
      READ (UNIT=7, FMT=115, END=10) NCOMPOUND
      DO 15 I = 1, NCOMPOUND
      READ (UNIT=7, FMT=120, END=10) COMPOUND(I), MW(I), A, B, C
C Calculation of the compound vapor pressure using Antoine equation:
C Vapor pressure should be in mmHg to use the subroutine SPEQ and
C the equation for Henry's constant, which are all that need vapor
C pressure in this program. Following formula gives vapor pressure in
C mmHg while LN formula gives it in bar. Accordingly, A,B,C values are
C different in the two formulae.
C Following formula needs TEMPC while LN formula does TEMPK.
      VP = 10.0 * * (A - B/(TEMPC+C))
      READ (UNIT=7, FMT=130, END=10) YNHC
      IF ((YNHC .EQ. 'N') .OR. (YNHC .EQ. 'n')) THEN
         READ (UNIT=7, FMT=140, END=10) CS
         HC(I) = (16034.*MW(I)*VP)/(CS*TEMPK)
         READ (UNIT=7, FMT=140, END=10) CI(I)
         GOTO 20
      ELSE
         READ (UNIT=7, FMT=150, END=10) HC(I)
      ENDIF
      READ (UNIT=7, FMT=160, END=10) CI(I)
20
      READ (UNIT=7, FMT=170, END=10) CE(I), VB(I), TEMPKB(I)
      READ (UNIT=7, FMT=180, END=10) RECEG(I), PSDFRG(I)
         VPG(I) = 10.0 * * (A - B/(TEMPC+TEMPUPG+C))
      READ (UNIT=7, FMT=180, END=10) BETA(I), DENL(I)
      READ (UNIT=7, FMT=190, END=10) KK(I), NN(I), PSDFR(I)
15
      CONTINUE
10
      CLOSE (UNIT=7)
С
      CALCULATION OF DENSITY AND VISCOSITY OF AIR
С
    Before the elevation of temperature.
      DGKGM3 = (28.964 * PRESATM) / (.08216 * TEMPK)
      VGKGMS = 1.7E-7 * TEMPK**.818
```

```
At the elevated temperature (Units are different also.)
С
     DGGCM3 = (28.964*PRESATM)/(.08216*TEMPKG * 1000.0)
     VGGCMS = 1.7E-6 * TEMPKG**.818
     CALL DENVIS (DWGCM3, VWGCMS, TEMPC)
          DWKGM3 = DWGCM3 \times 1000.0
          VWKGMS = VWGCMS/10.0
     DO 17 I = 1, NCOMPOUND
     CALL DIFL(DIFLL(I), MW(I), VB(I), VWKGMS)
     CALL DIFG(DIFGG(I), MW(I), VB(I), TEMPKB(I), TEMPK)
     CALL DIFG(DIFGGG(I), MW(I), VB(I), TEMPKB(I), TEMPKG)
17
     CONTINUE
SIMULATION
C
C DESIGN AND COST ESTIMATION OF AIR STRIPPING TOWER
С
   Vary the plant capacity, mgd.
     DO 40 I = 1, NFLOWL
        FLOWL = SFLOWL * I
   Vary the air to water ratio to find the optimum value.
С
     NVQ = 30
     SXMPL = 1.1
     INCREM = .1
     DO 40 J = 1,NVQ
        XMPL = SXMPL + (J-1.) * INCREM
С
   Initialization.
     TGAL(I,J) = 10000.
     SPRESD = 50.
     DO 45 K = 1,151
        PRESD1 = SPRESD + K-1.
     CALL MPTAD(VQ(J), TAREA(I,J), HLL(I,J), TV(I,J), CEA1, II(J), JJ,
    & DWKGM3, VWKGMS, TEMPC, CI, CE, HC, XMPL, PRESD1, DGKGM3,
    & CF, FLOWL, TEMPAIRC, EFF, PRESATM, EFFW, AT, STC, DP, VGKGMS,
    & DIFLL, DIFGG, BP, BPW, NCOMPOUND)
     DO 46 L=1, NCOMPOUND
         CEA(L,J)=CEA1(L)
46
     CONTINUE
     CALL TWCOST(TCOST, TV(I, J), BP, BPW, PTOP, FLOWL, LABOR, ELECT,
```

```
æ
              PROFIT, FEE, ECI, CCI, CRF)
         TGAL1 = (TCOST*1000.)/(FLOWL*1.0E+6*365.) * 100.
     IF (TGAL1 .LT. TGAL(I,J)) THEN
         TGAL(I,J) = TGAL1
         PRESD(I,J) = PRESD1
     ELSE
        GOTO 40
    ENDIF
45
    CONTINUE
40
    CONTINUE
C If off gas treatment is not required,
     IF (RECEG(1) .EQ. 0.0) THEN
C Find the least cost of tower for varying air to water ratio.
    DO 47 I = 1, NFLOWL
       TCGALOP(I) = 10000.0
    DO 47 J = 1, NVQ
       IF (TGAL(I,J) .LE. TCGALOP(I)) THEN
          TCGALOP(I) = TGAL(I,J)
          AWOPT(I) = J
       ENDIF
47
    CONTINUE
    GOTO 48
    ENDIF
C COST CALCULATION FOR DISCHARGE REACTOR
    DO 50 J = 1, NVQ
C Starting flow rate, mgd
    FLOWG = SFLOWL * VQ(J)
C Best result of Mr. Tsai's experiment will be used (7L/min;130w;95%)
C Unit price is independent of flow rate.
    KW = FLOWG/22.82688 \times 1114.2857
    KWH = KW * 365 . * 24.
    DCOST = KWH*ELECT
    DGAL(J) = (DCOST*1000.)/(SFLOWL*1.0E+6*365.) * 100.
50
    CONTINUE
DO 51 J = 1, NVQ
```

```
С
    Flow rate at the elevated temperature.
           FLOWG = SFLOWL * VQ(J)
           FLOWGG = FLOWG*TEMPKG/TEMPK
      DO 55 K = 1, NCOMPOUND
C Determination of the effluent gas concentration in ug/l
C CEA is used in multiple component instead of CE.
          CIG = (CI(K)-CEA(K,J))/VQ(J)
С
    Concentration at the elevated temperature.
           CIGG(K) = CIG * FLOWG/FLOWGG
      CALL SPEQ(KKG(K), NNG(K), CIGG(K), DENL(K), MW(K), PRESHG,
     ۶
                TEMPKG, BETA(K), VPG(K))
55
     CONTINUE
      CALL ET (FCN, CPD, CIGGOS, CUSEG, NCOMPOUND, RHOBG, RHOPG, VSG,
     &
             COMPOUND, KKG, NNG, CIGG, MW)
C Identification of the limiting compound
      DO 56 L=1,NCOMPOUND
         IF (CPD .EQ. COMPOUND(L)) THEN
            LL(J)=L
             GOTO 60
         ENDIF
56
      CONTINUE
60
      CONTINUE
C Desired effluent concentration of the limiting compound
          CEGGOS = CIGGOS * (100.- RECEG(LL(J)))/100.
C Mass transfer zone length of gas-phase GAC.
      FLAG = 0.0
     CALL USER(ETMING(J), ETMTZG(J), EMTZLG(J), RHOBG, RHOPG,
        CIGGOS, CEGGOS, MW(LL(J)), KKG(LL(J)), NNG(LL(J)), VGGCMS, VSG, DIAG,
     &
     &
        DGGCM3, EPORG, PSDFRG(LL(J)), DIFGGG(LL(J)), FLAG)
C Actual design
     CALL GACBEDG(CARUSEG(J), BAREAG(J), BDEPTHG, LIFEG(J), CUSEG,
         FLOWGG, VSG, EBCTG, RHOBG)
     &
51
     CONTINUE
C GAS-PHASE GAC COST
      DO 52 I = 1, NFLOWL
        FLOWL = SFLOWL * I
      DO 52 J = 1,NVQ
```

```
FLOWGG = FLOWL*VQ(J)*TEMPKG/TEMPK
```

```
CARUSEG1 = CARUSEG(J) * I
        BAREAG1 = BAREAG(J) * I
        BVOLG = BDEPTHG*BAREAG1
        CMASSG = BVOLG * RHOBG * 1000.0
     CALL GACCOSTG(CCOSTG, CONTACG1, REGENG1, BAREAG1,
    å
          BVOLG, FLOWGG, CARUSEG1, CMASSG, LIFEG(J), DGGCM3, TEMPUPG, CP,
    &
          GACOP, UPTIME, LOSS, GACPR, GACPRG, LABOR, ELECT, NGAS,
          WATER, PROFIT, SITE, FEE, CONTIN, ECI, CCI, CRF,
    &
          RHOBG, RHOPG, DIAG, VGGCMS, VSG, BDEPTHG, PRESATM, TEMPKG, EFF)
    &
          CONTACG(I,J) = CONTACG1
          REGENG(I,J) = REGENG1
          CGALG(I,J) = (CCOSTG*1000.)/(FLOWL*1.0E+6*365.) * 100.
          TCGALG(I,J) = TGAL(I,J)+CGALG(I,J)
52
     CONTINUE
C Find the least cost for varying air to water ratio.
     DO 53 I = 1, NFLOWL
        TCGALOP(I) = 10000.0
     DO 54 J = 1, NVQ
        IF (TCGALG(I,J) .LE. TCGALOP(I)) THEN
            TCGALOP(I) = TCGALG(I,J)
            AWOPT(I) = J
        ENDIF
54
     CONTINUE
     IF (BDEPTHG*100. .LT. 2.*EMTZLG(AWOPT(I))) THEN
          PRINT *, 'Bed depth is not enough for gas-phase GAC where;'
          PRINT *, ' '
          PRINT *, ' Raw water flow = ', SFLOWL*I
PRINT *, ' EBCT = ', EBCTG
          PRINT *, ',
          PRINT *, 'Increase EBCT!'
          STOP
     ENDIF
53
     CONTINUE
48
     CONTINUE
CALL ET(FCN, CPD, CIOS, CUSE, NCOMPOUND, RHOB, RHOP, VSW,
            COMPOUND, KK, NN, CI, MW)
    &
C Identification of the limiting compound
     DO 66 L=1, NCOMPOUND
        IF (CPD .EQ. COMPOUND(L)) THEN
            LLL=L
            GOTO 68
        ENDIF
```

```
66 CONTINUE
68 CONTINUE
```

C Mass transfer zone length of liquid-phase GAC.

```
FLAG = 1.0
CALL USER(ETMIN, ETMTZ, EMTZL, RHOB, RHOP, CIOS, CE(LLL),
      MW(LLL), KK(LLL), NN(LLL), VWGCMS, VSW, DIA, DWGCM3, EPOR,
&
      PSDFR(LLL), DIFLL(LLL), FLAG)
æ
CALL GACBED (CARUSEL, BAREAL, BDEPTH, LIFE, CUSE,
    SFLOWL, VSW, EBCT, RHOB)
&
IF (BDEPTH*100. .LT. 2.*EMTZL) THEN
      PRINT *, 'Bed depth is not enough for liquid-phase GAC where;'
      PRINT *, ''
      PRINT *, '
PRINT *, '
                    EBCT = ', EBCT
      PRINT *, 'Increase EBCT!'
      STOP
ENDIF
```

```
C LIQUID-PHASE GAC COST
```

```
DO 57 I = 1,NFLOWL
FLOWL = SFLOWL * I
CARUSE = CARUSEL * I
BAREA = BAREAL * I
BVOL = BDEPTH*BAREA
CMASS = BVOL * RHOB * 1000.0
CALL GACCOST(CCOST,CONTAC1,REGEN1,BVOL,FLOWL,CARUSE,
& CMASS,LIFE,GACOP,UPTIME,LOSS,GACPR,LABOR,ELECT,NGAS,
& WATER,PROFIT,SITE,FEE,CONTIN,ECI,CCI,CRF)
CONTAC(I) = CONTAC1
REGEN(I) = REGEN1
CGAL(I) = (CCOST*1000.)/(FLOWL*1.0E+6*365.) * 100.
```

```
57 CONTINUE
```

C RESULTS OF AIR STRIPPING TOWER.

```
WRITE (8,*) 'RESULTS OF CALCULATIONS FOR PACKED TOWER'
       WRITE (8,*) ' '
       WRITE (8,*) 'The calculated value of the air to water ratio = ',
                     VQ(AWOPT(I))
     &
      WRITE (8,*) 'The multiple of minimum air to water ratio
                                                                          = '、
                     1.1+(AWOPT(I)-1.)*INCREM
     &
                                                                          = '.
      WRITE (8,*) 'Pressure drop across the tower, sq.m./m.
                     PRESD(I,AWOPT(I))
     &
      WRITE (8,*) 'Total tower cross sectional area, sq.m.
                                                                          = ',
                     TAREA(I,AWOPT(I))
     &
      WRITE (8,*) 'Tower length in meters
                                                                          = ',
                     HLL(I,AWOPT(I))
     &
                                                                          = ',
      WRITE (8,*) 'Total tower volume in cu.m.
                     TV(I,AWOPT(I))
     &
      WRITE (8,*) ''
      WRITE (8,*)'Air flow rate and tower diameter has been determined
     &by ', COMPOUND(JJ)
      WRITE (8,*)'Tower length has been determined by ',
     æ
                    COMPOUND(II(AWOPT(I)))
      WRITE (8,*) ''
      WRITE (8,*)'CALCULATION OF REMOVAL EFFICIENCIES OF ALL COMPONENTS'
      WRITE (8, *) 'FOR A GIVEN TOWER DESIGN.'
      DO 80 J = 1, NCOMPOUND
      IF ((VB(J) .LT. .015) .OR. (VB(J) .GT. .5)) THEN WRITE (8,*) '
          WRITE (8,*) 'Your system does not match the accuracy ranges of'
          WRITE (8,*) 'the equations to get DIFL of', COMPOUND(J)
          WRITE (8,*) 'Anyway VB has been used to get the DIFL.'
      ENDIF
      WRITE (8,*) ''
      WRITE (8,*)
WRITE (8,*) 'Name of the compound = ', COMPOUND(J)
WRITE (8,*) 'Influent conc. in ug/l = ', CI(J)
WRITE (8,*) 'Effluent conc. desired in ug/l = ', CE(J)
WRITE (8,*) 'Actual effluent conc. in ug/l = ', CEA(J,AWOPT(I))
      WRITE (8,*) 'Removal efficiency in %
                                                        = ',
                     (1.-CEA(J,AWOPT(I))/CI(J))*100
     &
      CONTINUE
C RESULTS OF GAS-PHASE CARBON ADSORPTION
      WRITE (8,*) ''
      WRITE (8,*) 'RESULTS OF CALCULATIONS FOR GAS-PHASE CARBON ADSORPTI
     &ON'
      WRITE (8,*) ''
      WRITE (8,*) 'Minimum EBCT, (sec.) = ',ETMING(AWOPT(I))
      WRITE (8,*) 'EBCT of the MTZ, ETMTZ, (sec) = ', ETMTZG(AWOPT(I))
      WRITE (8,*) 'The length of the MTZ, EMTZL, (cm.) = ',
     &
                      EMTZLG(AWOPT(I))
      WRITE (8,*) 'The first component to elute = ',
```

COMPOUND(LL(AWOPT(I))) & WRITE (8,*) 'Carbon usage rate, kg/day = ',CARUSEG(AWOPT(I))*I WRITE (8,*) 'Bed depth, m = ', BDEPTHG WRITE (8,*) 'Total bed area, m**2 = ', BAREAG(AWOPT(I))*I WRITE (8,*) 'Bed life (regeneration cycle), days = ', LIFEG(AWOPT(I)) &

C RESULTS OF LIQUID-PHASE CARBON ADSORPTION

```
WRITE (8,*) ''
WRITE (8,*) 'RESULTS OF CALCULATIONS FOR LIQUID-PHASE CARBON ADSOR
&PTION'
WRITE (8,*) ''
WRITE (8,*) 'Minimum EBCT, (sec) = ', ETMIN
WRITE (8,*) 'EBCT of the MTZ, ETMTZ, (sec) = ', ETMTZ
WRITE (8,*) 'The length of the MTZ, EMTZL, (cm.) = ', EMTZL
WRITE (8,*) 'The first component to elute = ',COMPOUND(LLL)
WRITE (8,*) 'Carbon usage rate, kg/day = ', CARUSE*I
 WRITE (8, *) 'Bed depth, \mathbf{m} = \mathbf{i}, BDEPTH
 WRITE (8,*) 'Total bed area, m**2 = ', BAREA*I
 WRITE (8,*) 'Bed life (regeneration cycle), days = ', LIFE
```

C RESULTS OF COST CALCULATION

С

С

```
WRITE (8,*) ''
      WRITE (8,*) 'RESULTS OF COST CALCULATION'
      WRITE (8,*) ''
      WRITE (8,*) 'Least cost contactor selected for liquid-phase;'
      WRITE (8,*) CONTAC(I)
      WRITE (8,*) ''
      WRITE (8,*) 'Least cost regeneration selected for liquid-phase;'
      WRITE (8,*) REGEN(I)
      WRITE (8,*) ''
      WRITE (8,*) 'Least cost contactor selected for gas-phase;'
      WRITE (8, *) CONTACG(I, AWOPT(I))
      WRITE (8,*) ''
      WRITE (8,*) 'Least cost regeneration selected for gas-phase;'
      WRITE (8,*) REGENG(I,AWOPT(I))
      WRITE (8,*) ''
      WRITE (8,*) 'Liquid-phase carbon adsorption, cents/1000gal = ',
                   CGAL(I)
     &
      WRITE (8,*) ''
      WRITE (8,*) 'Gas-phase carbon adsorption, cents/1000gal-water = ',
                   CGALG(I,AWOPT(I))
     &
      WRITE (8,*) ''
      WRITE (8,*) 'Packed tower air stripping, cents/1000gal = ',
     &
                   TGAL(I,AWOPT(I))
C RESULTS OF DISCHARGE REACTOR
       WRITE (8,*) ''
       WRITE (8,*) 'Plasma reactor, cents/1000gal-water = ',
```

```
С
                 DGAL(AWOPT(I))
     &
70
     CONTINUE
This part is for a temporary use.
С
С
С
   VARIABLE = FLOWL
С
С
      WRITE (8,*) 'UNIT COSTS'
С
      DO 1010 I=1, NFLOWL
С
      J = AWOPT(I)
С
     WRITE (8,900) SFLOWL*I, TGAL(I,25), TGAL(I,J), CGALG(I,J),
С
                       TCGALG(I,J),CGAL(I)
     å
C1010 CONTINUE
     WRITE (8,*) ''
С
С
С
      WRITE (8,*) 'TOTAL REACTOR VOLUMES'
С
      DO 1020 I=1,NFLOWL
С
      J = AWOPT(I)
С
     WRITE (8,900) SFLOWL*I, TV(I,25), TV(I,J), BDEPTHG*BAREAG(J)*I,
С
                               BDEPTH*BAREAL*I
     &
C1020 CONTINUE
CLOSE (UNIT=8)
100
     FORMAT (9(/), 54x, A25, 3(/, 54x, F20.10), /, 7(/, 54x, F20.10),
       /,54X,120)
    å
     FORMAT (2(/), 6(/,54X,F20.10))
110
     FORMAT (/, 54X, 120)
115
120
     FORMAT (/, 54X, A25,4(/,54X,F20.10))
     FORMAT (/, 54X, A1)
130
     FORMAT (3(/), 54X, F20.10)
140
150
     FORMAT (5(/), 54X, F20.10)
     FORMAT (/, 54X, F20.10)
160
170
     FORMAT (54X, F20.10, /, 2(/,54X,F20.10))
     FORMAT (2(/), 2(/,54X, F20.10))
180
190
     FORMAT (2(/), 3(/,54X, F20.10))
200
     FORMAT (2(/), 7(/, 54X, F20.10))
     FORMAT (2(/), 18(/,54X,F20.10))
320
900
     FORMAT (6(1X, E11.5))
     STOP
     END
SUBROUTINE MPTAD (VQ, TAREA, HLL, TV, CEA, II, JJ, DWKGM3,
```

- + VWKGMS, TEMPC, CI, CE, HC, XMPL, PRESD, DGKGM3, CF, FLOWL, TEMPAIRC, EFF,
- + PRESATM, EFFW, AT, STC, DP, VGKGMS, DIFLL, DIFGG, BP, BPW, NCOMPOUND)

C This subroutine was originally developed by Dr. David W. Hand and

```
C Dr. John C. Crittenden at Michigan Technological University.
С
  The following modifications were made for this study.
С
С
       Original program
С
          * Written in BASIC
С
          * Handles single component system
С
       Modification
          * Written in FORTRAN 77
С
С
          * Handles multicomponent system
С
  For the development of equations, see 'Design and Evaluation of
С
   an Air-Stripping Tower for Removing VOCs From Groundwater',
С
С
   J. AWWA, p87-97, September, 1986.
С
IMPLICIT REAL (A-Z)
      DIMENSION CI(20), CE(20), CEA(20), HC(20), DIFLL(20), DIFGG(20), KLA(20)
      INTEGER I, II, JJ, NCOMPOUND
С
   Conversion of the unit of the variable (mgd \rightarrow cu.m/sec)
      FLOWL = FLOWL / 22.82688
C VQM, HL; Dummy variables to find maximum values of VQMIN & HLL
С
           among all compounds.
C Initialization.
     VQM = 0.0
     HL = 0.0
С
   CALCULATION OF DESIGN PARAMETERS FOR ALL COMPOUNDS
С
   Calculation of the minimum air to water ratio, VQMIN, of each
   compound.
С
С
   VQMIN is calculated from the following equation.
    VQMIN = (CI - CE)/(HC*CI)
C
     DO 10 I = 1, NCOMPOUND
     VQMIN = (CI(I) - CE(I)) / (HC(I) * CI(I))
      IF (VQMIN .GT. VQM) THEN
         JJ=I
         VQM=VQMIN
      ENDIF
10
     CONTINUE
      VQMIN=VQM
С
   CALCULATION OF A REASONABLE VALUE OF THE AIR TO WATER RATIO
     VQ = XMPL * VQMIN
С
    DETERMINATION OF THE TOWER DIAMETER
```

```
FF = ALOG(PRESD)/2.3025851
      A0 = -6.6599 + 4.3077 * FF - 1.3503 * (FF * 2.) + .15931 * (FF * 3.)
      A1 = 3.0945 - 4.3512*FF + 1.624*(FF**2.) - .20855*(FF**3.)
      A2 = 1.7611 - 2.3394*FF + .89914*(FF**2.) - .11597*(FF**3.)
      EE = -1.*ALOG(VQ*(((DGKGM3/DWKGM3) - ((DGKGM3/DWKGM3)**2.))**.5))
           /2.3025851
     &
      MM = 10.**(A0 + A1*EE + A2*(EE**2.))
      GM = ((MM*DGKGM3*(DWKGM3-DGKGM3))/(CF*(VWKGMS**.1)))**.5
      VQM = VQ*(DGKGM3/DWKGM3)
      ML = GM/VQM
      FLOWLM = FLOWL*DWKGM3
      TAREA = FLOWLM/ML
С
       DT = (4.*TAREA/3.1415926)**.5
      FLOWG = FLOWL * VQ
    DETERMINATION OF THE MASS TRANSFER COEFFICIENT, KLa
С
    AND CALCULATION OF THE TOWER LENGTH
С
      DO 20 I = 1, NCOMPOUND
      CALL ONDA(KLA(I), TEMPC, ML, AT, VWKGMS, DWKGM3, STC, DP, GM,
         VGKGMS, DGKGM3, HC(I), DIFLL(I), DIFGG(I))
     +
      CSS = (1./(VQ*HC(I)))*(CI(I)-CE(I))
      HTU = FLOWL/(TAREA*KLA(I))
      NTU = ((CI(I)-CE(I))/(CI(I)-CSS-CE(I)))*ALOG((CI(I)-CSS)/CE(I))
      HLL = HTU * NTU
      IF (HLL .GT. HL) THEN
          II=I
          HL=HLL
      ENDIF
20
      CONTINUE
      HLL=HL
      TV = TAREA * HLL
C CALCULATION OF REMOVAL EFFICIENCIES OF OTHER COMPONENTS
C FOR A GIVEN TOWER DESIGN.
      DO 30 I=1, NCOMPOUND
      RR = VQ*HC(I)
      QWA = FLOWL/TAREA
      BB = (HLL*KLA(I)*(RR-1.))/(QWA*RR)
      CEA(I) = (CI(I)*(RR-1.))/(RR*(EXP(BB))-1.)
30
      CONTINUE
C BRAKE POWER CALCULATION FOR BLOWER (BP) AND PUMP (BPW)
      VGAS = FLOWG/TAREA
```

```
PRESE = 275.*VGAS**2.
     RG = 286.7
     NN = .283
     P1 = PRESATM * 101330.
     P2 = PRESD + HLL + P1 + PRESE
     QMG = FLOWG * DGKGM3
     BP = ((QMG*RG*(TEMPAIRC+273.))/(1000.*NN*EFF/100.))
           *((P2/P1)**NN -1.)
    ۶.
     BPW = (DWKGM3*FLOWL*HLL*9.8)/(1000.*EFFW/100.)
С
   CONVERSION BACK TO THE ORIGINAL UNIT
     FLOWL = FLOWL * 22.82688
     RETURN
     END
SUBROUTINE ONDA (KLA, TEMPC, ML, AT, VWKGMS, DWKGM3, STC,
    +
           DP, GM, VGKGMS, DGKGM3, HC, DIFLL, DIFGG)
С
C This subroutine was a part of the program, PTAD,
C developed by Dr. David Hand.
С
C This program will use the ONDA et.al. correlation to calculate
C the overall mass transfer coefficient. The ONDA correlation
C includes both the liquid and gas phase mass transfer resistances.
C This correlation has been shown to be valid for liquid loading rates
C between .8 And 43 kg/m**2-sec, gas loading rates between .014 And 1.7
C kg/m**2-sec, and packing sizes between 10 and 50 mm.
C The liquid-phase mass transfer coefficient; KL
C The gas-phase mass transfer coefficient; KG
C The wetted surface area; AW
     IMPLICIT REAL (A-Z)
     ST = 7.558301E-2 - (1.3143*10.**(-4.))*TEMPC
    1
           -(4.7616*10.**(-7.))*(TEMPC**2.)
     RE = ML/(AT*VWKGMS)
     FR =(AT*(ML**2.))/(DWKGM3*DWKGM3*9.810001)
     WE = (ML * *2.) / (DWKGM3 * AT * ST)
     AW = AT * (1. - EXP(-1.45 * ((STC/ST) * *.75) * (RE * *.1) * (FR * * (-.05)))
    1
                  *(WE**.2)))
     KL=(.0051*((ML/(AW*VWKGMS))**(2./3.))*((VWKGMS/(DWKGM3*DIFLL))**
    & (-.5))*((AT*DP/100.)**.4))/((DWKGM3/(VWKGMS*9.810001))**(1./3.))
     KG = 5.23*((GM/(AT*VGKGMS))**.7)*((VGKGMS/(DGKGM3*DIFGG)))
    &
            **(1./3.))*((AT*DP/100.)**(-2.))*AT*DIFGG
     RL = 1./(KL*AW)
     RG = 1./(KG*AW*HC)
```

RT = RL + RG KLA =(1./(RL + RG)) RETURN END

```
SUBROUTINE DIFL (DIFLL, MW, VB, VWKGMS)
```

```
С
C This subroutine was a part of the program, PTAD,
C developed by Dr. David Hand.
С
C The liquid-diffusivity (DIFLL) of compounds will be calculated
C by this subroutine.
C If the molecular weight (MW) of the compound is greater than 1000,
C DIFLL is calculated from the following equation:
    DIFLL = 2.74*10**(-5)*(MW)**(-1/3)
С
C If MW is less than 1000 the following equation can be used:
С
    DIFLL = 13.26*10**(-5) / (VWKGMS**1.14*VB**.589)
С
    This equation is only valid for VB values between
С
    .015 And 0.5 M**3/kg-mol
     IMPLICIT REAL (A-Z)
     IF (MW .GT. 1000.) THEN
         DIFLL = 2.74 \times 10. \times (-5.) \times MW \times (-1./3.)
     ELSE
         DIFLL =1.326E-4/((VWKGMS*1000.)**1.14*(VB*1000.)**.589)/10000.
     ENDIF
     RETURN
     END
SUBROUTINE DIFG (DIFGG, MW, VB, TEMPKB, TEMPK)
C
C This subroutine was a part of the program, PTAD,
C developed by Dr. David Hand.
C
C The gas-diffusivity (DIFGG) of compounds will be calculated
C by this subroutine.
C The correlation to be used is the WILKE-LEE modification of
C HIRSCHFELDER-BIRD-SPOTZ method. This correlation is taken from
C TREYBAL (1980) and is given by the following equation:
С
    DIFGG = (10**-4*(1.084-.249*((1/MA+1/MB)**.5)*TEMPK**(3/2))
           *((1/MA+1/MB)**.5))/(PT*((RAB)**2)*F(KT/EAB))
С
C PT is assumed to be 1 atm, or PT = 101,325 N/sq.m
C RAB = (RA+RB)/2, where RB = 1.18 \times VB \times 33 And RA = .3711 nm for air.
```

```
IMPLICIT REAL (A-Z)
```

```
MA = 28.95
 RB = 1.18 * (VB * * .33333)
 RA = .3711
 RAB = (RA+RB)/2.
 EKB= 1.21*TEMPKB
 EKA = 78.6
 EKEAB = (EKB \times EKA) \times .5
TKEAB = TEMPK/EKEAB
EE = ALOG(TKEAB)/2.303
YVAL = 10.**(-.14329 - .48343*(EE) + .1939*(EE**2) + .13612*(EE**3)
        -.20578*(EE**4) +.083899*(EE**5) -.011491*(EE**6))
1
SQM = (1./MA + 1./MW) **.5
PT = 101325.
DIFGG = (.0001*(1.084 - (.249*SQM))*(TEMPK**1.5)*SQM)
       /(PT*RAB*YVAL*RAB)
1
```

RETURN END

SUBROUTINE GACBEDG(CARUSEG, BAREAG, BDEPTHG, LIFEG, CUSEG, + FLOWGG, VSG, EBCTG, RHOBG)

IMPLICIT REAL (A-Z)

C Calculation of the carbon usage rate in kg/day for the starting
Water flow rate: 100% saturation can be achieved through
C serial operation, but a safety factor of 5% will be used
C (95% saturation) because it is a regenerated carbon and
C 100% saturation is not achieved generally.

CARUSEG = CUSEG*FLOWGG*3.785 * 100./95.

C CONVERSION OF THE UNIT OF THE VARIABLE (MGD --> CU.M/SEC) FLOWGG = FLOWGG / 22.82688

C CALCULATE THE BED DIMENSIONS AND LIFE

BDEPTHG = (VSG * EBCTG)/100. BAREAG = FLOWGG*1.0E+2/VSG BVOLG = BDEPTHG*BAREAG CMASSG = BVOLG * RHOBG * 1000.0 LIFEG = CMASSG/CARUSEG

C CONVERSION BACK TO THE ORIGINAL UNIT FLOWGG = FLOWGG * 22.82688

RETURN

SUBROUTINE SPEQ(KKG, NNG, CIG, DENL, MW, PRESHG, TEMPK, BETA, VP)

```
С
С
  This subroutine is a part of the original program, SPEQ, that was
С
  developed by Mr. Randy D. Cortright at Michigan Technological
С
  University.
С
IMPLICIT REAL (A-Z)
     INTEGER I, MAX
C Initialize the values for the numerical intergration.
C the values of CONC and H were multiplied by 10 to reduce
C computation time with negligible differences in the resulting
C KKG and NNG (less than 1% error and 10 times faster).
     NA = 0.0
     QA = 0.0
     SUM = 0.0
     CONC = 1.0E-8
     H = 1.0E - 8
     EXC = 1.0E-6
     I = 1
     MAX = 10
30
     IF (CONC .LE. CIG) THEN
С
C CALCULATE THE SURFACE LOADING AT THE GAS CONC
С
        PP = (CONC/MW * 22.4 / 1.0E+6)*PRESHG
        QB = 0.46E+6* DENL/MW*EXP(-1.33E-7*(TEMPK/BETA*ALOG(VP/PP))**2)
С
C CALCULATE THE VALUE OF
С
        NB = 1.0/(2.66E-7 * ALOG(VP/PP) * (TEMPK/BETA)**2)
С
C TRAPEZOID RULE
С
        SUM = SUM + ((QB - QA)/2.0) * (NB+NA)
        NA = NB
        QA = QB
С
C INCREMENT THE GAS CONC
C
        IF (I .LE. MAX) THEN
          I = I + 1
          CONC = CONC + H
          GOTO 30
```

```
ELSE
С
          MAX = MAX + MAX
          IF (CONC .GT. EXC) THEN
            H = H * 10.0
            EXC = EXC + 10.0
          ENDIF
          CONC = CONC + H
          I = I + 1
          GOTO 30
       END IF
     ELSE
C HERE, NNG IS ACTUALLY 1/NNG.
       NNG = QA/SUM
       KKG = QA/((CONC/MW) * * NNG)
     ENDIF
     RETURN
     END
SUBROUTINE GACBED (CARUSE, BAREA, BDEPTH, LIFE, CUSE,
```

```
& FLOWL, VSW, EBCT, RHOB)
```

IMPLICIT REAL (A-Z)

- C Calculation of the carbon usage rate in kg/day for the starting C flow rate. A safety factor of 5% will be used (95% saturation). CARUSE = CUSE*FLOWL*3.785 * 100./95.
- C CONVERSION OF THE UNIT OF THE VARIABLE (MGD --> CU.M/SEC) FLOWL = FLOWL / 22.82688
- C CALCULATE THE BED DIMENSIONS AND LIFE

BDEPTH = (VSW * EBCT * 60.0)/100.0 BAREA = FLOWL*1.0E+2/VSW BVOL = BDEPTH*BAREA CMASS = BVOL * RHOB * 1000.0 LIFE = CMASS/CARUSE

C CONVERSION BACK TO THE ORIGINAL UNIT FLOWL = FLOWL * 22.82688

> RETURN END

SUBROUTINE USER(ETMIN, ETMTZ, EMTZL, RHOB, RHOP, CI, CE, MW, KK, NN,

& VWGCMS, VSW, DIA, DWGCM3, EPOR, PSDFR, DIFLL, FLAG)

```
С
  This subroutine was developed by Dr. David W. Hand, Dr. John C.
С
  Crittenden, and Mr. Randy D. Cortright at Michigan Technological
С
С
  University.
С
IMPLICIT REAL (A-Z)
     EBED = 1.0 - RHOB/RHOP
С
  CALC. THE EQUILBRIUM CONCENTRATION ON THE CARBON AND IN THE LIQUID
С
С
  HERE, NN IS ACTUALLY 1/NN.
С
     CIM = CI/MW
     CEM = CE/MW
     Q = KK * CIM * * NN
С
С
  CALCULATE THE LIQUID DIFFUSIVITY. Here, cm**2/sec will be used.
С
     DIFCM2L = DIFLL * 10000.0
С
C CALCULATE THE REYNOLDS AND SCHMIDT NUMBERS.
  (EBED in the gas-phase Reynolds equation was missing.)
С
     RE = (DIA*VSW*DWGCM3)/(VWGCMS*EBED)
     SC = (VWGCMS/(DWGCM3*DIFCM2L))
C CALCULATE THE MASS (FILM) TRANSFER COEFFICIENT. This part is the
C only difference between gas and liquid phase calculation.
C FLAG = 1.0 for liquid-phase, FLAG = 0.0 for gas-phase.
     IF (FLAG .EQ. 1.) THEN
         KF = (2.4 * VSW) / ((RE * *.66) * (SC * *.58))
     ELSE
         KF = (DIFCM2L/DIA) * (2.0 + 1.1 * RE**0.6 * SC**0.333333)
     ENDIF
C CALCULATE THE PORE AND SURFACE DIFFUSION COEFFICIENT
     DS = (EPOR*DIFCM2L*CIM*PSDFR)/(1000.0*RHOP*KK*CIM**NN)
C CALCULATE THE PARTITION COEFFICIENT (DISTRIBUTION PARAMETER)
     PC = (RHOP * Q * (1.0 - EBED) * 1000.0) / (EBED * CIM)
С
  CALCULATE THE BIOT NUMBER
С
С
     BI = (KF * DIA/2.0 * (1.0 - EBED))/(PC * DS * EBED)
```

```
C CALCULATE THE MINIMUN STANTON NUMBER AND THE EBCT MINIMUM
С
             STM = STMIN(BI, NN)
             ETMIN = (STM * DIA/2.0) / (KF * (1.0 - EBED))
C CALCULATE THE THROUGHPUT FOR (CEM/CIM)*100% AND 95 PERCENT
C BREAKTHRU AND FIND THE EBCT FOR THE MASS TRANSFER ZONE
             CALL TPUT(NN, BI, AO, A1, A2, A3, A4)
             T95 = A0 + A1 * (0.95 * A2) + A3/(1.01 - 0.95 * A4)
             TEI = A0 + A1 * (CEM/CIM)**A2 + A3/(1.01 - (CEM/CIM)**A4)
             ETMTZ = ETMIN * (T95 - TEI)
             EMTZL = ETMTZ * VSW
             RETURN
             END
С
С
      Function STMIN, subroutines TPUT and T1-T10 are parts of
      the subroutine USER.
С
С
С
С
      FUNCTION STMIN FOR FINDING THE MINIMUN STANTON NUMBER REQUIRED
      FOR CONSTANT PATTERN
С
С
             REAL FUNCTION STMIN(BI,N)
             IMPLICIT REAL (A-Z)
             INTEGER 1, J, M
             DIMENSION FN(10), A01(10), A11(10), A02(10)
             DATA (FN(I), I = 1,10)/0.05,0.10,0.20,0.30,0.40,0.50,0.60,0.70,
                                                                 0.80,0.90/
           $
             DATA (A01(I), I = 1, 10)/2.10526E-2, 2.10526E-2, 4.21053E-2,
                                                                 1.05263E-1,2.31579E-1,5.26316E-1,
           $
                                                                 1.15789, 1.78947, 3.68421, 6.31579/
           $
             DATA (A11(I), I = 1, 10)/1.98947, 2.18947, 2.37895, 2.54737, 2.68421,
                                                                 2.73684, 3.42105, 7.10526, 13.1579, 56.8421/
           $
             DATA (A02(I), I = 1, 10)/0.22, 0.24, 0.28, 0.36, 0.50, 0.80, 1.50, 2.50, 0.80, 0.50, 0.80, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.50, 0.5
            $
                                                                 5.00,12.00/
С
С
С
             M = 10
             IF((BI .GE. 0.5) .AND. (BI .LE. 10.0)) THEN
                    J = 1
10
                    IF(J .LE. M) THEN
                           IF ((N . GE. FN(J)) . AND. (N . LT. FN(J+1))) THEN
                                 A0 = A01(J) + (A01(J+1)-A01(J)) * ((N - FN(J))/
                                                                                                          (FN(J+1) - FN(J)))
           $
                                 A1 = A11(J) + (A11(J+1)-A11(J)) * ((N - FN(J))/
           $
                                                                                                          (FN(J+1) - FN(J)))
                                 STMIN = AO * BI + A1
```

```
GO TO 30
            ELSE
               \mathbf{J} = \mathbf{J} + \mathbf{1}
               GO TO 10
            END IF
         ELSE
            WRITE (8,*)' THE VALUE OF 1/N IS OUT OF RANGE FOR STMIN'
         ENDIF
      ELSEIF (BI .GT. 10.0) THEN
         J = 1
20
         IF(J .LE. M) THEN
            IF ((N . GE. FN(J)) . AND. (N . LT. FN(J+1))) THEN
               AO = AO2(J) + (AO2(J+1)-AO2(J)) * ((N - FN(J))/
                                                (FN(J+1) - FN(J)))
     $
               STMIN = A0 * BI
               GO TO 30
            ELSE
               \mathbf{J} = \mathbf{J} + \mathbf{1}
               GO TO 20
            END IF
         ELSE
            WRITE (8,*)' THE VALUE OF 1/N IS OUT OF RANGE FOR STMIN'
         ENDI F
      ELSE
         WRITE (8,*)' THE VALUE OF THE BIOT NUMBER IS OUT OF RANGE'
         WRITE (8,*)' BIOT NUMBER = ',BI
      ENDIF
30
      RETURN
      END
SUBROUTINE TPUT(N, BI, AO, A1, A2, A3, A4)
С
C SUBROUTINE TPUT TO FIND THE CONSTANTS TO FIND EBCTMIN.
С
      REAL N
      IF (N .LT. 0.075) THEN
         CALL T1(BI, A0, A1, A2, A3, A4)
      ELSEIF((N .GE. 0.075) .AND. (N .LT. 0.15)) THEN
         CALL T2(BI, A0, A1, A2, A3, A4)
      ELSEIF((N .GE. 0.15) .AND. (N .LT. 0.25)) THEN
         CALL T3(BI, A0, A1, A2, A3, A4)
      ELSEIF((N .GE. 0.25) .AND. (N .LT. 0.35)) THEN
         CALL T4(BI,A0,A1,A2,A3,A4)
      ELSEIF((N .GE. 0.35) .AND. (N .LT. 0.45)) THEN
         CALL T5(BI, A0, A1, A2, A3, A4)
```

```
ELSEIF((N.GE. 0.45) .AND. (N.LT. 0.55)) THEN
```

```
CALL T6(BI, A0, A1, A2, A3, A4)
     ELSEIF((N .GE. 0.55) .AND. (N .LT. 0.65)) THEN
        CALL T7(BI, A0, A1, A2, A3, A4)
     ELSEIF((N .GE. 0.65) .AND. (N .LT. 0.75)) THEN
        CALL T8(BI, A0, A1, A2, A3, A4)
     ELSEIF((N .GE. 0.75) .AND. (N .LT. 0.85)) THEN
        CALL T9(BI, A0, A1, A2, A3, A4)
     ELSEIF((N .GE. 0.85) .AND. (N .LT. 1.00)) THEN
        CALL T10(BI, A0, A1, A2, A3, A4)
     ELSE
        WRITE (8,*)' THE VALUE OF 1/N IS OUT OF RANGE'
     ENDIF
     RETURN
     END
SUBROUTINE T1(BI,A0,A1,A2,A3,A4)
```

```
IF(BI .LT. 1.25) THEN
   A0 = -5.447214
   A1 = 6.598598
   A2 = 0.026569
   A3 = 0.019384
   A4 = 20.45047
ELSEIF((BI .GE. 1.25) .AND. (BI .LT. 3.0)) THEN
   A0 = -5.465811
   A1 = 6.592484
   A2 = 0.025290
   A3 = 0.004988
   A4 = 0.503250
ELSEIF((BI .GE. 3.0) .AND. (BI .LT. 5.0)) THEN
   A0 = -5.531155
   A1 = 6.584935
   A2 = 0.023580
   A3 = 0.009019
   A4 = 0.273076
ELSEIF((BI .GE. 5.0) .AND. (BI .LT. 7.0)) THEN
   A0 = -5.606508
   A1 = 6.582188
   A2 = 0.022088
   A3 = 0.013126
   A4 = 0.214246
ELSEIF((BI .GE. 7.0) .AND. (BI .LT. 9.0)) THEN
   A0 = -5.606500
   A1 = 6.504701
   A2 = 0.020872
   A3 = 0.017083
   A4 = 0.189537
ELSEIF((BI .GE. 9.0) .AND. (BI .LT. 12.0)) THEN
   A0 = -5.664173
   A1 = 6.456597
   A2 = 0.018157
```

```
A3 = 0.019935
        A4 = 0.149314
     ELSEIF((BI .GE. 12.0) .AND. (BI .LT. 19.5)) THEN
        A0 = -0.662780
        A1 = 1.411252
        A2 = 0.060709
        A3 = 0.020229
        A4 = 0.143293
     ELSEIF((BI .GE. 19.5) .AND. (BI .LT. 62.5)) THEN
        A0 = -0.662783
        A1 = 1.350940
        A2 = 0.031070
        A3 = 0.020350
        A4 = 0.129998
     ELSEIF(BI .LT. 62.5) THEN
        A0 = 0.665879
        A1 = 0.711310
        A2 = 2.987309
        A3 = 0.016783
        A4 = 0.361023
     ENDIF
     RETURN
     END
SUBROUTINE T2(BI, A0, A1, A2, A3, A4)
     IF(BI .LT. 1.25) THEN
        A0 = -1.919873
        A1 = 3.055368
        A2 = 0.055488
        A3 = 0.024284
        A4 = 15.311766
     ELSEIF((BI .GE. 1.25) .AND. (BI .LT. 3.0)) THEN
        A0 = -2.278950
        A1 = 3.393925
        A2 = 0.046838
        A3 = 0.004751
        A4 = 0.384675
     ELSEIF((BI .GE. 3.0) .AND. (BI .LT. 5.0)) THEN
        A0 = -2.337178
        A1 = 3.379926
        A2 = 0.043994
        A3 = 0.008650
        A4 = 0.243412
     ELSEIF((BI .GE. 5.0) .AND. (BI .LT. 7.0)) THEN
        A0 = -2.407407
        A1 = 3.374131
        A2 = 0.041322
        A3 = 0.012552
        A4 = 0.196565
     ELSEIF((BI .GE. 7.0) .AND. (BI .LT. 9.0)) THEN
        A0 = -2.477819
        A1 = 3.370954
```

A2 = 0.038993A3 = 0.016275A4 = 0.176437ELSEIF((BI .GE. 9.0) .AND. (BI .LT. 13.0)) THEN A0 = -2.566414A1 = 3.370950A2 = 0.035003A3 = 0.019386A4 = 0.150788ELSEIF((BI .GE. 13.0) .AND. (BI .LT. 23.0)) THEN A0 = -2.567201A1 = 3.306341A2 = 0.020940A3 = 0.019483A4 = 0.136813ELSEIF((BI .GE. 23.0) .AND. (BI .LT. 65.0)) THEN A0 = -2.568618A1 = 3.241783A2 = 0.009595A3 = 0.019610A4 = 0.121746ELSEIF(BI .GE. 65.0) THEN A0 = -2.568360A1 = 3.191482A2 = 0.001555A3 = 0.019682A4 = 0.110113ENDIF RETURN END SUBROUTINE T3(BI,A0,A1,A2,A3,A4) IF (BI .LT. 1.25) THEN A0 = -1.441000A1 = 2.569000A2 = 0.060920A3 = 0.002333A4 = 0.371100ELSEIF((BI .GE. 1.25) .AND. (BI .LT. 3.0)) THEN A0 = -1.474313A1 = 2.558300A2 = 0.058480A3 = 0.005026A4 = 0.241265ELSEIF((BI .GE. 3.0) .AND. (BI .LT. 5.0)) THEN A0 = -1.506696A1 = 2.519259A2 = 0.055525A3 = 0.008797A4 = 0.187510ELSEIF((BI .GE. 5.0) .AND. (BI .LT. 7.0)) THEN A0 = -1.035395

A1 = 1.983018A2 = 0.069283A3 = 0.012302A4 = 0.167924ELSEIF((BI .GE. 7.0) .AND. (BI .LT. 9.0)) THEN A0 = -0.169192A1 = 1.077521A2 = 0.144879A3 = 0.015500A4 = 0.168083ELSEIF((BI .GE. 9.0) .AND. (BI .LT. 11.5)) THEN A0 = -1.402932A1 = 2.188339A2 = 0.052191A3 = 0.018422A4 = 0.133574ELSEIF((BI .GE. 11.5) .AND. (BI .LT. 19.0)) THEN A0 = -1.369220A1 = 2.118545A2 = 0.039492A3 = 0.018453A4 = 0.127565ELSEIF((BI .GE. 19.0) .AND. (BI .LT. 62.5)) THEN A0 = -1.514159A1 = 2.209450A2 = 0.017937A3 = 0.018510A4 = 0.118517ELSEIF(BI .GE. 62.5) THEN A0 = 0.680346A1 = 0.649006A2 = 2.570086A3 = 0.014947A4 = 0.369818ENDIF RETURN END SUBROUTINE T4(BI, A0, A1, A2, A3, A4)IF (BI .LT. 1.25) THEN A0 = -1.758696A1 = 2.846576A2 = 0.049530A3 = 0.003022A4 = 0.156816ELSEIF ((BI .GE. 1.25) .AND. (BI .LT. 3.0)) THEN A0 = -1.657862A1 = 2.688895A2 = 0.048409A3 = 0.005612

ELSEIF ((BI .GE. 3.0) .AND. (BI .LT. 5.0)) THEN

A4 = 0.140937

```
A0 = -0.565664
   A1 = 1.537833
   A2 = 0.084451
   A3 = 0.008808
   A4 = 0.139086
ELSEIF ((BI .GE. 5.0) .AND. (BI .LT. 7.0)) THEN
   A0 = -0.197077
   A1 = 1.118564
   A2 = 0.117894
   A3 = 0.011527
   A4 = 0.135874
ELSEIF ((BI .GE. 7.0) .AND. (BI .LT. 9.0)) THEN
   A0 = -0.197070
   A1 = 1.069216
   A2 = 0.119760
   A3 = 0.013925
   A4 = 0.132691
ELSEIF ((BI .GE. 9.0) .AND. (BI .LT. 12.5)) THEN
   A0 = -0.173358
   A1 = 1.00000
   A2 = 0.120311
   A3 = 0.015940
   A4 = 0.133973
ELSEIF ((BI .GE. 12.5) .AND. (BI .LT. 25.0)) THEN
   A0 = -0.173350
   A1 = 0.919411
   A2 = 0.071768
   A3 = 0.014156
   A4 = 0.086270
ELSEIF ((BI .GE. 25.0) .AND. (BI .LT. 67.5)) THEN
   A0 = 0.666471
   A1 = 0.484570
   A2 = 1.719440
   A3 = 0.013444
   A4 = 0.259545
ELSEIF (BI .GE. 67.5) THEN
  A0 = 0.696161
   A1 = 0.516951
  A2 = 2.054587
  A3 = 0.012961
   A4 = 0.303218
ENDIF
RETURN
END
```

SUBROUTINE T5(BI,A0,A1,A2,A3,A4)

```
IF (BI .LT. 1.25) THEN

A0 = -0.534251

A1 = 1.603834

A2 = 0.094055

A3 = 0.004141

A4 = 0.137797
```

```
ELSEIF((BI .GE. 1.25) .AND. (BI .LT. 3.0)) THEN
        A0 = -0.166270
        A1 = 1.190897
        A2 = 0.122280
        A3 = 0.006261
        A4 = 0.134278
     ELSEIF((BI .GE. 3.0) .AND. (BI .LT. 5.0)) THEN
        A0 = -0.166270
        A1 = 1.131946
        A2 = 0.115513
        A3 = 0.008634
        A4 = 0.126813
     ELSEIF((BI .GE. 5.0) .AND. (BI .LT. 7.5)) THEN
        A0 = -0.166270
        A1 = 1.089789
        A2 = 0.112284
        A3 = 0.010463
        A4 = 0.124307
     ELSEIF((BI .GE. 7.5) .AND. (BI .LT. 10.5)) THEN
        A0 = 0.491912
        A1 = 0.491833
        A2 = 0.487414
        A3 = 0.011371
        A4 = 0.147747
     ELSEIF((BI .GE. 10.5) .AND. (BI .LT. 13.5)) THEN
        A0 = 0.564119
        A1 = 0.419196
        A2 = 0.639819
        A3 = 0.011543
        A4 = 0.149005
     ELSEIF((BI .GE. 13.5) .AND. (BI .LT. 20.0)) THEN
        A0 = 0.640669
        A1 = 0.432466
        A2 = 1.048056
        A3 = 0.011616
        A4 = 0.212726
     ELSEIF((BI .GE. 20.0) .AND. (BI .LT. 62.5)) THEN
        A0 = 0.672353
        A1 = 0.397007
        A2 = 1.153169
        A3 = 0.011280
        A4 = 0.216883
     ELSEIF(BI .GE. 62.5) THEN
        A0 = 0.741435
        A1 = 0.448054
        A2 = 1.929879
        A3 = 0.010152
        A4 = 0.306448
     ENDIF
     RETURN
     END
```

SUBROUTINE T6(BI,A0,A1,A2,A3,A4)

```
IF(BI .LT. 2.25) THEN
   A0 = -0.040800
   A1 = 1.099652
   A2 = 0.158995
   A3 = 0.005467
   A4 = 0.139116
ELSEIF((BI .GE. 2.25) .AND. (BI .LT. 7.00)) THEN
   A0 = -0.040800
   A1 = 0.982757
   A2 = 0.111618
   A3 = 0.008072
   A4 = 0.111404
ELSEIF((BI .GE. 7.0) .AND. (BI .LT. 12.0)) THEN
   A0 = 0.094602
   A1 = 0.754878
   A2 = 0.092069
   A3 = 0.009877
   A4 = 0.090763
ELSEIF((BI .GE. 12.0) .AND. (BI .LT. 19.5)) THEN
   A0 = 0.023000
   A1 = 0.802068
   A2 = 0.057545
   A3 = 0.009662
   A4 = 0.084532
ELSEIF((BI .GE. 19.5) .AND. (BI .LT. 62.5)) THEN
   A0 = 0.02300
   A1 = 0.793673
   A2 = 0.039324
   A3 = 0.009326
   A4 = 0.082751
ELSEIF(BI .GE. 62.5) THEN
   A0 = 0.529213
   A1 = 0.291801
   A2 = 0.082428
   A3 = 0.008317
   A4 = 0.075461
ENDIF
RETURN
END
```

SUBROUTINE T7(BI,A0,A1,A2,A3,A4)

```
IF (BI .LT. 1.25) THEN

A0 = 0.352536

A1 = 0.692114

A2 = 0.263134

A3 = 0.005482

A4 = 0.121775

ELSEIF((BI .GE. 1.25) .AND. (BI .LT. 4.0)) THEN

A0 = 0.521979

A1 = 0.504220

A2 = 0.327290

A3 = 0.005612
```

```
A4 = 0.128679
     ELSEIF((BI .GE. 4.0) .AND. (BI .LT. 10.0)) THEN
        A0 = 0.676253
        A1 = 0.334583
        A2 = 0.482297
        A3 = 0.005898
        A4 = 0.138946
     ELSEIF((BI .GE.10.0) .AND. (BI .LT. 32.0)) THEN
        A0 = 0.769531
        A1 = 0.259497
        A2 = 0.774068
        A3 = 0.005600
        A4 = 0.165513
     ELSEIF((BI .GE. 32.0) .AND. (BI .LT. 75.0)) THEN
        A0 = 0.849057
        A1 = 0.215799
        A2 = 1.343183
        A3 = 0.004725
        A4 = 0.223759
     ELSEIF(BI .GE. 75.0) THEN
        A0 = 0.831231
        A1 = 0.227304
        A2 = 1.174756
        A3 = 0.004961
        A4 = 0.212109
     ENDIF
     RETURN
     END
SUBROUTINE T8(BI, A0, A1, A2, A3, A4)
     IF(BI .LT. 2.25) THEN
        A0 = 0.575024
        A1 = 0.449062
        A2 = 0.278452
        A3 = 0.004122
```

```
A4 = 0.121682
ELSEIF((BI .GE. 2.25) .AND. (BI .LT. 8.0)) THEN
   A0 = 0.715269
   A1 = 0.307172
   A2 = 0.442104
   A3 = 0.004371
   A4 = 0.138351
ELSEIF((BI .GE. 8.0) .AND. (BI .LT. 18.5)) THEN
   A0 = 0.787940
   A1 = 0.243548
   A2 = 0.661599
  A3 = 0.004403
   A4 = 0.162595
ELSEIF((BI .GE. 18.5) .AND. (BI .LT. 62.5)) THEN
  A0 = 0.829492
  A1 = 0.204078
```

A2 = 0.784529

```
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```

```
A3 = 0.004050
        A4 = 0.179003
     ELSEIF(BI .GE. 62.5) THEN
        A0 = 0.847012
        A1 = 0.190678
        A2 = 0.931686
        A3 = 0.003849
        A4 = 0.183239
     ENDIF
     RETURN
     END
SUBROUTINE T9(BI, A0, A1, A2, A3, A4)
     IF(BI .LT. 2.25) THEN
        A0 = 0.708905
        A1 = 0.314101
        A2 = 0.357499
        A3 = 0.003276
        A4 = 0.119300
     ELSEIF((BI .GE. 2.25) .AND. (BI .LT. 9.0)) THEN
        A0 = 0.784576
        A1 = 0.239663
        A2 = 0.484422
        A3 = 0.003206
        A4 = 0.134987
     ELSEIF((BI .GE. 9.0) .AND. (BI .LT. 57.0)) THEN
       A0 = 0.839439
       A1 = 0.188966
       A2 = 0.648124
       A3 = 0.003006
        A4 = 0.157697
     ELSEIF( BI .GE. 57.0) THEN
       A0 = 0.882747
       A1 = 0.146229
       A2 = 0.807987
       A3 = 0.002537
       A4 = 0.174543
     ENDIF
     RETURN
     END
SUBROUTINE T10(BI, A0, A1, A2, A3, A4)
     IF(BI .LT. 2.25) THEN
       A0 = 0.865453
       A1 = 0.157618
       A2 = 0.444973
       A3 = 0.001650
       A4 = 0.148084
     ELSEIF((BI .GE. 2.25) .AND. (BI .LT. 10.0)) THEN
       A0 = 0.854768
```

```
A1 = 0.171434
   A2 = 0.495042
   A3 = 0.001910
   A4 = 0.142251
ELSEIF((BI .GE. 10.0) .AND. (BI .LT. 58.0)) THEN
  A0 = 0.866180
   A1 = 0.163992
  A2 = 0.573946
  A3 = 0.001987
  A4 = 0.157594
ELSEIF(BI .GE. 58.0) THEN
  A0 = 0.893192
  A1 = 0.133039
  A2 = 0.624100
  A3 = 0.001740
  A4 = 0.164248
ENDIF
RETURN
END
```

SUBROUTINE DENVIS(DWGCM3,VWGCMS,TEMPC)

æ

```
С
C Subroutine DENVIS is used to obtain the density and viscosity
C of water.
С
D1 = 999.83952+16.945176*TEMPC-7.9870401E-3*TEMPC**2-46.170461E-6
   & *TEMPC**3+105.56302E-9*TEMPC**4-280.54253E-12*TEMPC**5
    D2 = 1.+16.87985E-3*TEMPC
    DWGCM3 = (D1/D2)/1000.
    IF (TEMPC .LE. 20.) THEN
      VWGCMS = (10.**(1301./(998.333+8.1855*(TEMPC-20.)+
           .00585*(TEMPC-20.)**2.)-1.30233))/100.
   å
    ELSE
      VWGCMS = (10.**((1.3272*(20.-TEMPC)-.001053*(TEMPC-20.)**2.)/
           (TEMPC+105.))*1.002)/100.
   &
    ENDIF
    RETURN
    END
SUBROUTINE TWCOST (TCOST, TV, BP, BPW, PTOP, FLOWL, LABOR, ELECT,
```

PROFIT, FEE, ECI, CCI, CRF)

IMPLICIT REAL (A-Z)

```
DIMENSION Y(5), ADMIN(4)
      INTEGER I
    CONVERSION OF THE UNIT OF THE VARIABLE (M**3 --> FT**3)
С
      TV = TV * 35.318
C VARIABLE = PACKED TOWER VOLUME
С
    Y(1) = CC, Y(2) = MM, Y(3) = LABOR
С
    Y(4) = BLOWER ENERGY, Y(5) = PUMP ENERGY
С
С
    Y(1), Y(2), and Y(3) were developed for the curves given in
С
    Gumerman's report; p460, p466, and p467.
С
    Gumerman, R.C., R.L. Culp, and S.P. Hansen, 'Estimating Water
С
    Treatment Costs, Vol. 2, Cost Curves Applicable to 1 to 200 mgd
С
    Treatment Plants, EPA-600/2-79-162b, Aug. 1979.
      Y(1) = 10.**(2.480708+0.699403*ALOG10(TV*100./PTOP))
      Y(2) = 10.**(3.71184-.951171*ALOG10(TV)+.20046*(ALOG10(TV))**2.)
      Y(3) = 10.**(1.84073 - .399972*ALOG10(TV) + .121128*(ALOG10(TV))**2.)
      Y(4) = BP*365.*24.
      Y(5) = BPW * 365 . * 24.
C ADMINISTRATION, LABORATORY AND MAINTENANCE BUILDING
  VARIABLE = FLOW RATE, MGD
С
С
С
    ADMIN(1) = CC, ADMIN(2) = MM, ADMIN(3) = LABOR
С
    ADMIN(4) = BUILDING ENERGY
С
    Following equations were developed for the curves given in
С
    Gumerman's report p469, p472, and p473.
      ADMIN(1) = 10.**(4.3617+.633898*ALOG10(FLOWL*100./PTOP))
                 -.0380989*(ALOG10(FLOWL*100./PTOP))**2.)
     &
      ADMIN(2) = 10.**(3.29564+.293344*ALOG10(FLOWL))
                 +.0639727*(ALOG10(FLOWL))**2.)
     &
      ADMIN(3) = 10.**(3.17059+.68173*ALOG10(FLOWL))
     &
                 -.105693*(ALOG10(FLOWL))**2.)
      ADMIN(4) = 10.**(4.7412+.638106*ALOG10(FLOWL))
     &
                 -.0357398*(ALOG10(FLOWL))**2.)
      DO 5 I = 1,4
         Y(I) = Y(I) + ADMIN(I)
5
      CONTINUE
C PROFIT AND FEES FOR CONSTRUCTION COST
C Contingencies and site work (miscellaneous) were included in the
C original report.
      AUXIL = PROFIT + FEE
```

```
AUXIL = 1. + AUXIL/100.
     Y(1) = Y(1) * AUXIL * CCI/259.
    Following equations were developed for the curve given in
С
С
    'Plant Design and Economics for Chemical Engineers', 4th ed.,
С
    McGraw-Hill, p527, figure 14-41, 1990.
     PUMP = 10.**(5.42915-1.46769*ALOG10(2298.25*BPW*100./PTOP))
                 +.237617*(ALOG10(2298.25*BPW*100./PTOP))**2.)
    &
     Y(1) = Y(1) + PUMP * ECI / 904.
C Conversion to $
     Y(1) = Y(1) * CRF
     Y(2) = Y(2) * ECI / 545.
     Y(3) = Y(3) * LABOR
     DO 10 I = 4.5
        Y(I) = Y(I) * ELECT
10
     CONTINUE
С
   CALCULATION OF TOTAL YEARLY COST
     TCOST = Y(1) + Y(2) + Y(3) + Y(4) + Y(5)
С
   CONVERSION BACK TO THE ORIGINAL UNIT
     TV = TV / 35.318
     RETURN
     END
SUBROUTINE GACCOST (CCOST, CONTAC, REGEN, BVOL, FLOWL, CARUSE,
          CMASS, LIFE, GACOP, UPTIME, LOSS, GACPR, LABOR, ELECT, NGAS,
    &
    &
          WATER, PROFIT, SITE, FEE, CONTIN, ECI, CCI, CRF)
С
С
  Data used in this subroutine was obtained from 'Cost Estimates for
  GAC Treatment Systems', J.Q. Adams and R.M. Clark, J. AWWA, p35-42,
С
С
  Jan., 1989.
С
IMPLICIT REAL (A-Z)
     DIMENSION A(37), B(37), C(37), D(37), Y(37)
     INTEGER I
     CHARACTER*40 CONTAC, REGEN
     DATA A/16125, 3*0, 100, 256, 766.6, 100100, 3*0, 1115, 1460, 93700, 0, 15150,
           0,540,1160,47200,20400,700000,49245,500,0,2920,1038000,0,
    +
           15600,2920,111110,144000,354600,12250,0,2920,648400/
    +
     DATA B/7632,2983,203.2,47817.6,34.2,248.6,.00224,155.6,12,47817.6,
    +
           1000,7.33,12.6,1999.1,12,350,19127,23.6,.3,21.8,9.7,148.4,
```

```
346.5,25,956,69,8131.7,43.8,830.2,210.2,1084,198330.4,6387,
     +
     +
             312.1,4456.6,282,287714.9/
      DATA C/.523,.4289,1.12,1,.601,.2104,2.491,.997,1,1,.813,1,.698,
             .712,1,.916,1,.753,1.068,.933,1.1,.933,.988,.753,.397,.5,
     +
             .494,1,.353,.4,1,.434,.755,.649,.401,.7,.899/
      DATA D/37*1/
    CONVERSION OF THE UNITS OF THE VARIABLES
С
      BVOL = BVOL * 35.318
      CARUSE = CARUSE * 2.2046
      CMASS = CMASS * 2.2046
С
    Filter surface area for this cost calculation was based on a
С
    hydraulic loading rate of 12.22 m/hour. So the area of liquid-
    phase GAC will be recalculated for this purpose.
C
      FAREA = FLOWL/22.82688*3600./12.22*10.764
      IF (BVOL .GT. 400) D(1)=1.102
      IF (BVOL .LT. 3000) D(8)=.958
      IF (BVOL .GT. 5000) D(14)=1.027
      IF (FAREA .LT. 7000) D(19)=1.152
C VARIABLE = GAC CONTACTOR VOLUME
      I = 1
         Y(I) = A(I) + B(I) * (BVOL*100./GACOP)**C(I) * D(I)
      I = 8
         Y(I) = A(I) + B(I) * (BVOL*100./GACOP)**C(I) * D(I)
      I = 14
        Y(I) = A(I) + B(I) * (BVOL*100./GACOP)**C(I) * D(I)
      I = 21
         Y(I) = A(I) + B(I) * (BVOL*100./GACOP)**C(I) * D(I)
      I = 5
         Y(I) = A(I) + B(I) * BVOL **C(I) * D(I)
C VARIABLE = GAC CONTACTOR TOTAL CROSS SECTIONAL AREA
      I = 2
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 3
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 6
        Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 7
        Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 9
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
     DO 10 I = 11,13
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
10
     CONTINUE
     I = 15
        Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
```

```
I = 16
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 18
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
      I = 19
         Y(I) = A(I) + B(I) * FAREA**C(I) * D(I)
C VARIABLE = TOTAL EFFECTIVE HEARTH AREA, CARUSE/(45LB/SQFT/DAY)
      HAREA = CARUSE/45.0
      I = 32
         Y(I) = A(I) + B(I) * (HAREA*100./UPTIME)**C(I) * D(I)
      DO 20 I = 33,37
         Y(I) = A(I) + B(I) * HAREA**C(I) * D(I)
20
      CONTINUE
C VARIABLE = FLOW RATE
C PUMPING ENERGY REQUIREMENT
      I = 4
         Y(I) = A(I) + B(I) * FLOWL**C(I) * D(I)
      I = 10
         Y(I) = A(I) + B(I) * FLOWL**C(I) * D(I)
      I = 17
         Y(I) = A(I) + B(I) * FLOWL**C(I) * D(I)
C VARIABLE = CARBON USAGE RATE
      I = 22
         Y(I) = A(I) + B(I) * (CARUSE*100./UPTIME)**C(I) * D(I)
      DO 30 I = 23, 31
         Y(I) = A(I) + B(I) * CARUSE **C(I) * D(I)
30
      CONTINUE
      I = 27
         Y(I) = A(I) + B(I) * (CARUSE*100./UPTIME)**C(I) * D(I)
C VARIABLE = BACKWASH PUMP CAPACITY (SET MAX = 18 GPM/SQ FT)
      I = 20
         Y(I) = A(I) + B(I) * 18.**C(I) * D(I)
C PROFIT, SITE WORK, FEES, AND CONTINGENCIES FOR CONSTRUCTION COST
      AUXIL = PROFIT + SITE + FEE + CONTIN
      AUXIL = 1. + AUXIL/100.
      Y(1) = Y(1) * AUXIL
      Y(8) = Y(8) * AUXIL
      Y(14) = Y(14) * AUXIL
      Y(20) = Y(20) * AUXIL
      Y(21) = Y(21) * AUXIL
      Y(22) = Y(22) * AUXIL
      Y(27) = Y(27) * AUXIL
      Y(32) = Y(32) * AUXIL
```

```
Y(1) = Y(1) * CRF * CCI / 380.
      DO 40 I = 2,4
          Y(I) = Y(I) * ELECT
40
      CONTINUE
      Y(5) = Y(5) * ECI / 761.
      Y(6) = Y(6) * LABOR
      Y(7) = Y(7) * LABOR
      Y(8) = Y(8) * CRF * CCI / 380.
      DO 50 I = 9,11
          Y(I) = Y(I) * ELECT
50
      CONTINUE
      Y(12) = Y(12) * ECI / 761.
      Y(13) = Y(13) * LABOR
      Y(14) = Y(14) * CRF * CCI/380.
      DO 60 I = 15, 17
          Y(I) = Y(I) * ELECT
60
      CONTINUE
      Y(18) = Y(18) * ECI / 761.
      Y(19) = Y(19) * LABOR
      Y(20) = Y(20) * CRF * CCI / 380.
      Y(21) = Y(21) * CRF * CCI / 380.
      Y(22) = Y(22) * CRF * CCI / 380.
      Y(23) = Y(23) * ELECT
      Y(24) = Y(24) * ELECT
      Y(25) = Y(25) * ECI/761.
      Y(26) = Y(26) * LABOR
      Y(27) = Y(27) * CRF * CCI / 380.
      Y(28) = Y(28) * ELECT
      Y(29) = Y(29) * ECI / 761.
      Y(30) = Y(30) * LABOR
      Y(31) = Y(31) * NGAS
      Y(32) = Y(32) * CRF * CCI / 380.
      Y(33) = Y(33) * ELECT
      Y(34) = Y(34) * ELECT
      Y(35) = Y(35) * ECI / 761.
      Y(36) = Y(36) * LABOR
      Y(37) = Y(37) * NGAS
С
    CALCULATION OF PRICE FOR EACH UNIT
      IF (FAREA .LE. 50.0) THEN
          PACKAGE = Y(1)+Y(2)+Y(4)+Y(5)+Y(6)
      ELSE
С
      FAREA should be less than 200. Otherwise this may not be valid.
          PACKAGE = Y(1)+Y(3)+Y(4)+Y(5)+Y(7)
      ENDIF
С
      CC OF BACKWASH, Y(20), will be added for conventional contactor.
С
      initial GAC cost also will be added for conventional contactor.
      STEEL = Y(8)+Y(9)+Y(10)+Y(11)+Y(12)+Y(13)+Y(20)+CMASS*GACPR*CRF
      CONCRETE = Y(14)+Y(15)+Y(16)+Y(17)+Y(18)+Y(19)+Y(20)
                   +CMASS*GACPR*CRF
     &
```

STORAGE = Y(21)

```
CLOSS = CMASS*LOSS*365./LIFE*GACPR
      CWATER = CARUSE * 28.5 * 365. / 1000.0 * WATER
      CLABOR = CARUSE*0.4*365./1000.0*LABOR
      INFRA = Y(22)+Y(23)+Y(24)+Y(25)+Y(26)+CLOSS+CWATER+CLABOR
      FLUID = Y(27)+Y(28)+Y(29)+Y(30)+Y(31)+CLOSS+CLOSS+CWATER+CLABOR
      HEARTH = Y(32)+Y(33)+Y(34)+Y(35)+Y(36)+Y(37)+CLOSS+CLOSS+CWATER
               +CLABOR
     æ
    Virgin GAC replacement with disposal of spent GAC by incineration.
С
    Formula for this option was developed for the curve given by J.
С
С
    Adams and R. Clark (figure 6).
С
    Here, ALOG is the Natural logarithm, Ln, not the ALOG10.
      IF (CARUSE .LT. 273.97) THEN
          VIRGIN = CARUSE*365.*(1.9-.27639202*ALOG(1+5.9207397
                *(3.65E-3*CARUSE))+.17468663*(3.65E-3*CARUSE)) + CLABOR
     &
         ELSE IF (CARUSE .LT. 1095.89) THEN
            VIRGIN = CARUSE*365.*(1.5299251-.10618521*ALOG(.99916691
                *(3.65E-3*CARUSE))+.010547582*(3.65E-3*CARUSE)) + CLABOR
     &
         ELSE IF (CARUSE .LT. 2000.0) THEN
            VIRGIN = CARUSE * 365. * (1.50366667 - 7.1783333E - 5 * CARUSE) + CLABOR
С
      From now on, flat line is assumed.
         ELSE
            VIRGIN = CARUSE*365.*1.3601+CLABOR
      ENDIF
      VIRGIN = VIRGIN * ECI/761.
С
    SELECTION OF THE MOST ECONOMICAL PROCESS FOR ADSORPTION AND
С
      REGENERATION
      IF (PACKAGE .EQ. AMIN1(PACKAGE, CONCRETE, STEEL)) THEN
               CON = PACKAGE
               CONTAC = 'PACKAGE PRESSURE GAC CONTACTORS'
          ELSE IF (STEEL .EQ. AMIN1(PACKAGE, CONCRETE, STEEL)) THEN
               CON = STEEL
               CONTAC = 'CONVENTIONAL STEEL PRESSURE GAC CONTACTORS'
          ELSE
               CON = CONCRETE
               CONTAC = 'CONVENTIONAL CONCRETE GRAVITY GAC CONTACTORS'
      ENDIF
      IF (INFRA .EQ. AMIN1(INFRA, FLUID, HEARTH, VIRGIN)) THEN
               REG = INFRA
               REGEN = 'INFRARED REGENERATION'
          ELSE IF(FLUID .EQ. AMIN1(INFRA, FLUID, HEARTH, VIRGIN)) THEN
               REG = FLUID
               REGEN = 'FLUID-BED REGENERATION'
          ELSE IF (HEARTH . EQ. AMIN1 (INFRA, FLUID, HEARTH, VIRGIN)) THEN
               REG = HEARTH
               REGEN = 'MULTIHEARTH REGENERATION'
          ELSE
               REG = VIRGIN
               REGEN = 'VIRGIN GAC REPLACEMENT WITH DISPOSAL'
      ENDIF
```

C CALCULATION OF TOTAL YEARLY COST

CCOST = CON + STORAGE + REG

C CONVERSION BACK TO THE ORIGINAL UNITS BVOL = BVOL / 35.318 CARUSE = CARUSE / 2.2046 CMASS = CMASS / 2.2046

> RETURN END

÷

SUBROUTINE GACCOSTG(CCOST, CONTAC, REGEN, BAREAG, BVOLG, FLOWGG,

- CARUSE, CMASS, LIFE, DGGCM3, TEMPUPG, CP,
- & GACOP, UPTIME, LOSS, GACPR, GACPRG, LABOR, ELECT, NGAS,
- & WATER, PROFIT, SITE, FEE, CONTIN, ECI, CCI, CRF,
- & RHOBG, RHOPG, DIAG, VGGCMS, VSG, BDEPTHG, PRESATM, TEMPKG, EFF)

C Data used in this subroutine was obtained from 'Cost Estimates for C GAC Treatment Systems', J.Q. Adams and R.M. Clark, J. AWWA, p35-42, C Jan., 1989.

```
С
```

```
IMPLICIT REAL (A-Z)
DIMENSION A(37),B(37),C(37),D(37),Y(38)
INTEGER I
CHARACTER*40 CONTAC,REGEN
```

DATA A/16125,3*0,100,256,766.6,100100,3*0,1115,1460,93700,0,15150, 0,540,1160,47200,20400,700000,49245,500,0,2920,1038000,0,+ 15600,2920,111110,144000,354600,12250,0,2920,648400/ DATA B/7632,2983,203.2,47817.6,34.2,248.6,.00224,155.6,12,47817.6, 1000,7.33,12.6,1999.1,12,350,19127,23.6,.3,21.8,9.7,148.4, + + 346.5,25,956,69,8131.7,43.8,830.2,210.2,1084,198330.4,6387, ÷ 312.1,4456.6,282,287714.9/ DATA C/.523,.4289,1.12,1,.601,.2104,2.491,.997,1,1,.813,1,.698, .712,1,.916,1,.753,1.068,.933,1.1,.933,.988,.753,.397,.5, + + .494,1,.353,.4,1,.434,.755,.649,.401,.7,.899/ DATA D/37*1/

C High surface loading rate will be allowed for the gas-phase GAC. C So, design bed area (BAREA) will be used

C (Just need unit conversion).

C CONVERSION OF THE UNITS OF THE VARIABLES

BAREAG = BAREAG * 10.764 BVOLG = BVOLG * 35.318 CARUSE = CARUSE * 2.2046

```
CMASS = CMASS * 2.2046
      IF (BVOLG .GT. 400) D(1)=1.102
      IF (BVOLG .LT. 3000) D(8)=.958
      IF (BVOLG .GT. 5000) D(14)=1.027
      IF (BAREAG .LT. 7000) D(19)=1.152
C VARIABLE = GAC CONTACTOR VOLUME
      I = 1
        Y(I) = A(I) + B(I) * (BVOLG*100./GACOP)**C(I) * D(I)
      I = 8
        Y(I) = A(I) + B(I) * (BVOLG*100./GACOP)**C(I) * D(I)
      I = 21
        Y(I) = A(I) + B(I) * (BVOLG*100./GACOP)**C(I) * D(I)
      I = 5
         Y(I) = A(I) + B(I) * BVOLG**C(I) * D(I)
C VARIABLE = GAC CONTACTOR TOTAL CROSS SECTIONAL AREA
      I = 2
        Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
      I = 3
        Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
      I = 6
         Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
      I = 7
        Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
      I = 9
         Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
      DO 10 I = 11,13
         Y(I) = A(I) + B(I) * BAREAG**C(I) * D(I)
10
      CONTINUE
C VARIABLE = TOTAL EFFECTIVE HEARTH AREA, CARUSE/(45LB/SQFT/DAY)
      HAREA = CARUSE/45.0
      I = 32
         Y(I) = A(I) + B(I) * (HAREA*100./UPTIME)**C(I) * D(I)
      DO 20 I = 33.37
         Y(I) = A(I) + B(I) * HAREA**C(I) * D(I)
20
      CONTINUE
C VARIABLE = Flow rate
   BP = air blower break power requirement, (instead of pumping
С
С
         energy requirement in liquid-phase GAC).
   Ergun equation to get the pressure drop through the bed
С
C
    10.764 = unit ajustment of BAREAG
      EBEDG = 1.0 - RHOBG/RHOPG
      D1 = (150.*(1.-EBEDG))/(DIAG*((FLOWGG/22.82688*100.*DGGCM3)))
```

```
(BAREAG/10.764*VGGCMS)))
     &
      D2 = (DGGCM3*VSG**2.*BDEPTHG*(1.-EBEDG)*10.)/(DIAG*EBEDG**3.)
      PRESDG = (D1 + 1.75) * D2
C BRAKE POWER CALCULATION FOR BLOWER (BP) IN KW.
      VGAS = VSG/100.
      PRESE = 275.*VGAS**2.
      RG = 286.7
      NN = .283
      P1 = PRESATM * 101330.
      P2 = PRESDG + P1 + PRESE
      QMG = FLOWGG/22.82688*DGGCM3*1000.
      BP = ((QMG*RG*TEMPKG)/(1000.*NN*EFF/100.))
             *((P2/P1)**NN -1.)
     &
С
    BLOWER ENERGY REQUIREMENT, IN KWH/YEAR
      Y(4) = BP*365.*24.
      Y(10) = Y(4)
C VARIABLE = CARBON USAGE RATE
      I = 22
         Y(I) = A(I) + B(I) * (CARUSE*100./UPTIME)**C(I) * D(I)
      DO 30 I = 23,31
         Y(I) = A(I) + B(I) * CARUSE**C(I) * D(I)
30
      CONTINUE
      I = 27
         Y(I) = A(I) + B(I) * (CARUSE*100./UPTIME)**C(I) * D(I)
C VARIABLE = BACKWASH PUMP CAPACITY (SET MAX = 18 \text{ GPM/SQ FT})
      I = 20
         Y(I) = A(I) + B(I) * 18.**C(I) * D(I)
C PROFIT, SITE WORK, FEES, AND CONTINGENCIES FOR CONSTRUCTION COST
      AUXIL = PROFIT + SITE + FEE + CONTIN
      AUXIL = 1. + AUXIL/100.
      Y(1) = Y(1) * AUXIL
      Y(8) = Y(8) * AUXIL
      Y(20) = Y(20) * AUXIL
      Y(21) = Y(21) * AUXIL
      Y(22) = Y(22) * AUXIL
      Y(27) = Y(27) * AUXIL
      Y(32) = Y(32) * AUXIL
C CONVERSION TO $
      Y(1) = Y(1) * CRF * CCI / 380.
      DO 40 I = 2,4
         Y(I) = Y(I) * ELECT
40
      CONTINUE
      Y(5) = Y(5) * ECI / 761.
```

```
Y(6) = Y(6) * LABOR
      Y(7) = Y(7) * LABOR
      Y(8) = Y(8) * CRF * CCI / 380.
      DO 50 I = 9,11
         Y(I) = Y(I) * ELECT
50
      CONTINUE
      Y(12) = Y(12) * ECI / 761.
      Y(13) = Y(13) * LABOR
      Y(20) = Y(20) * CRF * CCI / 380.
      Y(21) = Y(21) * CRF * CCI / 380.
      Y(22) = Y(22) * CRF * CCI / 380.
      Y(23) = Y(23) * ELECT
      Y(24) = Y(24) * ELECT
      Y(25) = Y(25) * ECI/761.
      Y(26) = Y(26) * LABOR
      Y(27) = Y(27) * CRF * CCI / 380.
      Y(28) = Y(28) * ELECT
      Y(29) = Y(29) * ECI / 761.
      Y(30) = Y(30) * LABOR
      Y(31) = Y(31) * NGAS
      Y(32) = Y(32) * CRF * CCI / 380.
      Y(33) = Y(33) * ELECT
      Y(34) = Y(34) * ELECT
      Y(35) = Y(35) * ECI / 761.
      Y(36) = Y(36) * LABOR
      Y(37) = Y(37) * NGAS
    CALCULATION OF PRICE FOR EACH UNIT
С
      IF (BAREAG .LE. 50.0) THEN
         PACKAGE = Y(1)+Y(2)+Y(4)+Y(5)+Y(6)
      ELSE
С
      Barea should be less than 200. Otherwise this may not be valid.
         PACKAGE = Y(1)+Y(3)+Y(4)+Y(5)+Y(7)
      ENDIF
С
      Initial GAC cost is included in package contactor. However,
С
      the GAC price was based on liquid-phase GAC. So, the difference
С
      will be added for gas-phase contactor.
      PACKAGE = PACKAGE + CMASS*(GACPRG-GACPR)*CRF
С
      Gas-phase does not include backwash pumping CC
С
      Therefore Y(20) will not be added to conventional contactor.
С
      The amount of Y(20) will be subtracted from package contactor
С
      which contains backwash pump.
С
      Process energy requirements are also for backwash pumping.
С
      So, Y(9) will not be added to conventional contactor and will be
С
      subtracted from package contactor.
      PACKAGE = PACKAGE - Y(9) - Y(20)
С
      Initial GAC cost also will be added for conventional contactor.
```

```
STEEL = Y(8)+Y(10)+Y(11)+Y(12)+Y(13)+CMASS*GACPRG*CRF
```

STORAGE = Y(21)

```
CLOSS = CMASS*LOSS*365./LIFE*GACPRG
      CWATER = CARUSE*28.5*365./1000.0*WATER
      CLABOR = CARUSE * 0.4 * 365./1000.0 * LABOR
      INFRA = Y(22)+Y(23)+Y(24)+Y(25)+Y(26)+CLOSS+CWATER+CLABOR
      FLUID = Y(27)+Y(28)+Y(29)+Y(30)+Y(31)+CLOSS+CLOSS+CWATER+CLABOR
      HEARTH = Y(32)+Y(33)+Y(34)+Y(35)+Y(36)+Y(37)+CLOSS+CLOSS+CWATER
               +CLABOR
     &
    Virgin GAC replacement with disposal of spent GAC by incineration.
С
С
    Formula for this option was developed for the curve given by J.
С
    Adams and R. Clark (figure 6).
С
    Here, ALOG is the Natural logarithm, Ln, not the ALOG10.
      IF (CARUSE .LT. 273.97) THEN
          VIRGIN = CARUSE*365.*(1.9-.27639202*ALOG(1+5.9207397
                *(3.65E-3*CARUSE))+.17468663*(3.65E-3*CARUSE)) + CLABOR
     &
         ELSE IF (CARUSE .LT. 1095.89) THEN
            VIRGIN = CARUSE*365.*(1.5299251-.10618521*ALOG(.99916691
                *(3.65E-3*CARUSE))+.010547582*(3.65E-3*CARUSE)) + CLABOR
     æ
         ELSE IF (CARUSE .LT. 2000.0) THEN
            VIRGIN = CARUSE * 365 * (1.50366667 - 7.1783333E - 5 * CARUSE) + CLABOR
С
      From now on, flat line is assumed.
         ELSE
            VIRGIN = CARUSE*365.*1.3601+CLABOR
      ENDIF
      VIRGIN = VIRGIN * ECI/761.
С
      The GAC price is based on liquid-phase GAC in virgin carbon
С
      replacement. So, the difference will be added for gas-phase
С
      contactor.
      VIRGIN = VIRGIN + CARUSE*365.*(GACPRG-GACPR)
С
    SELECTION OF THE MOST ECONOMICAL PROCESS FOR ADSORPTION AND
С
        REGENERATION
      IF (PACKAGE .EQ. AMIN1(PACKAGE, STEEL)) THEN
               CON = PACKAGE
               CONTAC = 'PACKAGE PRESSURE GAC CONTACTORS'
          ELSE
               CON = STEEL
               CONTAC = 'CONVENTIONAL STEEL PRESSURE GAC CONTACTORS'
      ENDIF
      IF (INFRA .EQ. AMIN1(INFRA, FLUID, HEARTH, VIRGIN)) THEN
               REG = INFRA
               REGEN = 'INFRARED REGENERATION'
          ELSE IF(FLUID .EQ. AMIN1(INFRA, FLUID, HEARTH, VIRGIN)) THEN
               REG = FLUID
               REGEN = 'FLUID-BED REGENERATION'
```

```
ELSE IF (HEARTH .EQ. AMIN1 (INFRA, FLUID, HEARTH, VIRGIN)) THEN
             REG = HEARTH
             REGEN = 'MULTIHEARTH REGENERATION'
         ELSE
             REG = VIRGIN
             REGEN = 'VIRGIN GAC REPLACEMENT WITH DISPOSAL'
     ENDIF
С
   CALCULATION OF TOTAL YEARLY COST
С
   Gas-phase adsorption shows that optimum relative humidity is 40%.
   So, air will be heated.
С
С
   heat capacity of air = CP, cal/g-deg C
   1 \text{ cal} = 0.00397 \text{ Btu}
С
С
   typical heating value of natural gas = 1050 Btu/cuft
     HEAT = FLOWGG/22.82688*1.0E+6*DGGCM3*CP*TEMPUPG*0.00397
           *86400.*365./1050.*NGAS
    &
     Y(38) = HEAT
        CCOST = CON + STORAGE + REG + HEAT
С
   CONVERSION BACK TO THE ORIGINAL UNITS
     BAREAG = BAREAG / 10.764
     BVOLG = BVOLG / 35.318
     CARUSE = CARUSE / 2.2046
     CMASS = CMASS / 2.2046
     RETURN
     END
SUBROUTINE ET(FCN, CPD, SCIOS, SCUSE, N, SRHOB, SRHOP, SVSW, COMPOUND,
    +
                  SXK, SXN, SCI, SMW)
С
С
  This subroutine was developed by Mr. Thomas F. Speth, Dr. John C.
С
  Crittenden, and Dr. David W. Hand at Michigan Technological
С
  University.
С
IMPLICIT DOUBLE PRECISION (A-H, O-Z)
     CHARACTER*40 COMPOUND(20), CHAR(20), CH, CPD
     DOUBLE PRECISION MW(20)
     DIMENSION XN(20), XK(20), CO(20, 20), C(20, 20), Q(20, 20), VW(20)
    $,OATS(20),WK(200),X(20),PAR(100),CI(20)
C Variables in single precision in main program
     REAL SCIOS, SCUSE, SRHOB, SRHOP, SVSW, SXK(20), SXN(20), SCI(20), SMW(20)
С
      EXTERNAL FCN
     COMMON /ZSQ/ BVF, DEN, M
```

C Conversion to double precision

```
RHOB=SRHOB
      RHOP=SRHOP
      VSW=SVSW
      DO 5 I=1,N
        XK(I) = SXK(I)
        XN(I)=SXN(I)
        CI(I) = SCI(I)
        MW(I) = SMW(I)
        CHAR(I)=COMPOUND(I)
5
      CONTINUE
      DO 10 I=1,N
       CO(I,1)=CI(I)/MW(I)
       XN(I)=1.0DO/XN(I)
10
      CONTINUE
                           CHANGE UNITS
С
С
      BVF=1.0D0-RHOB/RHOP
      VF=VSW/BVF
      DEN=RHOP*1000.0D0
С
                 SET ZONE ONE CONCENTRATIONS TO ZERO
С
С
      DO 20 I=1,N
       VW(I)=0.0D0
       PAR(60+1)=0.0D0
       PAR(80+I)=0.0D0
20
      CONTINUE
С
                   SOLVE FOR EACH ZONE SEPARATELY
С
С
      DO 100 J=1,N
      L=0
      M=J
      NS=9
      NN=N+1-J
      ZZ = 1.0D0
      NSIG=NS
      SUM=0.0D0
С
                 CALCULATE INITIAL GUESSES OF Q's
С
С
        DO 22 I=1,N
21
         Q(I,J)=ZZ*XK(I)*CO(I,J)**(1.0D0/XN(I))
        CONTINUE
22
С
                 PUT Q INTO ONE-DIMENSIONAL FORM
С
С
        DO 24 I=1,N
        X(I)=Q(I,J)
24
        CONTINUE
```

```
С
С
                      SET IAST PARAMETERS
С
       DO 26 I=1,NN
        X(I) = X(M-1+I)
        PAR(I) = XK(M-1+I)
        PAR(10+I) = XN(M-1+I)
        PAR(20+I)=CO(M-1+I,J)
        PAR(60+I) = PAR(60+M-1+I)
        PAR(80+I) = PAR(80+M-1+I)
26
       CONTINUE
       PAR(30) = VW(J-1)
       PAR(35) = VF
       ITMAX=100
С
       CALL ZSPOW(FCN, NSIG, NN, ITMAX, PAR, X, FNORM, WK, IER)
С
С
                          FIX ANY ERRORS
С
       IF (IER .EQ. 129 .OR. IER .EQ. 131) THEN
        IF (L.EQ. 0) THEN
         ZZ=2.0D0*ZZ
         L=L+1
         GOTO 21
        ENDIF
        IF (L .EQ. 1) THEN
         ZZ=3.0D0*ZZ
         L=L+1
         GOTO 21
        ENDIF
        IF (L .EQ. 2) THEN
         ZZ=ZZ/20.0D0
         L=L+1
         GOTO 21
        ENDIF
        IF (L.EQ. 3) THEN
         PRINT *, 'THERE IS A PROBLEM WITH THE INITIAL CONCENTRATIONS
     $THAT THE PROGRAMS FIXING ROUTINE DID NOT HELP. ZONE=', J
        ENDIF
       ENDIF
С
       IF (IER .EQ. 130) THEN
        NSIG=NSIG-1
        IF (NSIG .LT. 0) THEN
         PRINT *, 'THE NUMBER OF SIGNIFICANT FIGURES HAS DROPPED BELOW
     $ZERO. THERE ARE NO RESULTS FOR ZONE ',J
        ENDIF
        GOTO 21
       ENDI F
С
С
            SET X TO TWO-DIMENSIONAL OUTPUT FOR PRINT OUT
С
       IF (M .GT. 1) THEN
        DO 30 I=1,M-1
```

```
Q(I,J)=0.0D0
30
         CONTINUE
        ENDIF
        DO 31 I=1,NN
         Q(I+M-1,J)=X(I)
31
        CONTINUE
С
С
                CALCULATE THE LIQUID CONCENTRATIONS
С
        IF (M .GT. 1) THEN
         DO 33 I=1,M-1
          C(I, J) = 0.0D0
33
         CONTINUE
        ENDIF
        DO 34 I=1,NN
         C(I+M-1,J)=PAR(40+I)
34
        CONTINUE
С
С
             DETERMINE THE STRONGEST COMPONENT IN ZONE J
С
        DGX=0.0D0
        DO 35 I=M,N
        DG=DEN*Q(I,J)/(C(I,J)*BVF)
         IF (DG .GT. DGX) THEN
         DGX=DG
         IX = I
        ENDIF
35
       CONTINUE
С
С
                     SET STRONGEST COMPONENT TO ZONE J
С
       CH=CHAR(IX)
       CHAR(IX) = CHAR(J)
       CHAR(J)=CH
С
       WM=MW(IX)
       MW(IX) = MW(J)
       MW(J) = WM
С
       XXK = XK(IX)
       XK(IX) = XK(J)
       XK(J) = XXK
С
       XXN=XN(IX)
       XN(IX)=XN(J)
       XN(J) = XXN
С
      DO 37 K=1,J
       XCO=CO(IX,K)
       CO(IX,K)=CO(J,K)
       CO(J,K)=XCO
С
        XC=C(IX,K)
        C(IX,K)=C(J,K)
```

```
C(J,K)=XC
С
       XQ=Q(IX,K)
       Q(IX,K)=Q(J,K)
       Q(J,K)=XQ
37
      CONTINUE
С
С
                 SET C'S AND Q'S FOR NEXT ZONE
С
      DO 38 I=1,N
       PAR(60+I)=Q(I,J)
       PAR(80+I)=C(I,J)
38
      CONTINUE
С
С
           CALCULATE VELOCITY OF THE WAVE FOR ZONE J
С
      IF (J.EQ. 1) THEN
       VW(J)=VF*BVF*CO(1,J)/(Q(1,J)*DEN+C(1,J)*BVF)
      ENDIF
      IF (J .GE. 2) THEN
       SUM=(Q(J,1)*DEN+BVF*C(J,1))*VW(1)
      ENDIF
      IF (J.GT. 2) THEN
       DO 40 K=2, J-1
        SUM=SUM+((Q(J,K)*DEN+BVF*C(J,K))*(VW(K)-VW(K-1)))
40
       CONTINUE
      ENDIF
      IF (J.GE. 2) THEN
       VW(J) = (BVF*VF*CO(J,J) - SUM+(Q(J,J)*DEN+BVF*C(J,J))*VW(J-1)
    (Q(J,J)*DEN+BVF*C(J,J))
      ENDIF
С
С
                     SET CO FOR NEXT ZONE
С
      DO 50 I=J+1,N
       CO(I,J+1)=C(I,J)
50
      CONTINUE
      DO 60 I=1,J
       CO(I, J+1)=0.0D0
60
      CONTINUE
С
100
     CONTINUE
С
С
                    CALCULATE BED VOLUMES FED
С
     DO 110 I=1,N
SUM=(Q(I,1)*DEN+C(I,J)*BVF)*VW(1)
      IF (I .GE. 2) THEN
       DO 105 K=2,I
        SUM=SUM+(Q(I,K)*DEN+C(I,K)*BVF)*(VW(K)-VW(K-1))
105
       CONTINUE
      ENDIF
      OATS(I)=SUM/(CO(I,I)*VW(I))
```

```
110
        CONTINUE
С
                                  PUT INTO ug/L UNITS
С
С
        DO 200 J=1,N
         DO 200 I=1,N
           C(I,J)=C(I,J)*MW(I)
        CONTINUE
200
        CPD=CHAR(N)
        CIOS=C(N,N)
C CARBON USE RATE
        CUSE=DEN*1000.0D0/OATS(N)
C Conversion back to single precision
         SCIOS=CIOS
         SCUSE=CUSE
        RETURN
         END
С
С
                                 SUBROUTINE FCN
С
С
          THIS SUBROUTINE WILL SET UP THE EQUATIONS THAT WILL BE USED IN
С
С
       THE ZSPOW SUBROUTINE.
С
С
         SUBROUTINE FCN(X, F, NN, PAR)
С
         IMPLICIT DOUBLE PRECISION (A-H,O-Z)
         DIMENSION X(NN), F(NN), PAR(100)
         COMMON /ZSQ/ BVF, DEN, M
         QT=0.0D0
         QNQ=0.0D0
         DO 1010 I=1,NN
          QT=QT+X(I)
          QNQ=QNQ+PAR(10+I)*X(I)
 1010 CONTINUE
 С
                                   CALCULATE F(I)
 С
 С
         IF (M.EQ. 1) THEN
          DO 1020 I=1,NN
            F(I)=-PAR(20+I)+X(I)/QT*(QNQ/PAR(10+I)/PAR(I))**PAR(10+I)
 1020
           CONTINUE
         ENDIF
         IF (M.GT. 1) THEN
           DO 1030 I=1,NN
            F(I) = -X(I)/QT*(QNQ/PAR(10+I)/PAR(I))**PAR(10+I)+((X(I)-PAR(60+I)))**PAR(10+I)+((X(I)-PAR(60+I)))**PAR(10+I)+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I)))**PAR(10+I))+((X(I)-PAR(60+I))))**PAR(10+I))+((X(I)-PAR(60+I)))
        $)*DEN*PAR(30))/((PAR(35)-PAR(30))*BVF)+PAR(80+I)
```

```
1030
      CONTINUE
      ENDIF
С
С
                  CALCULATE LIQUID CONCENTRATION
С
      IF (M .EQ. 1) THEN
      DO 1040 I=1,NN
        PAR(40+I)=X(I)*(QNQ/(PAR(10+I)*PAR(I)))**PAR(10+I)/QT
1040
       CONTINUE
      ENDI F
      IF (M .GT. 1) THEN
      DO 1050 I=1,NN
        PAR(40+I)=((X(I)-PAR(60+I))*DEN*PAR(30))/((PAR(35)-PAR(30)))
     $*BVF)+PAR(80+I)
1050
       CONTINUE
      ENDIF
      RETURN
      END
```

VITA

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Doctor of Philosophy

Thesis: PERFORMANCE AND ECONOMICS OF AIR STRIPPING TOWER WITH OFF-GAS CONTROL BY EITHER GAS-PHASE CARBON ADSORPTION OR PLASMA REACTOR IN COMPARISON TO LIQUID-PHASE CARBON ADSORPTION

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