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School of Mechanical Engineering

1974

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OPTIMIZATION OF A NON-IDEAL STAGED COMPRESSION FACILITY

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The classical dynamic programming solution to determine the optimal interstage pressures of a multistage adiabatic gas compressor is based on the assumptions of

1) ideal gas behavior
2) all non-condensibles, i.e., no composition changes
3) no costs for interstage cooling
4) compressor capital costs dependent only on the overall compressor duty.

This paper presents an optimal design study of a wet CO_2 compression facility in which none of the above assumptions are valid. The staged system is modeled using the modular DYSYM/DYFLO flowsheet simulation program which readily allows the non-idealities in the condensation and compression units to be incorporated. Because temperature, pressure, and composition must be specified at each stage, a serial decomposition is not feasible. Instead, the optimal design is obtained by using a direct search optimization technique to drive the simulation program.

INTRODUCTION

The compression of gases is one of the more common and often one of the most expensive component operations found in commercial flow processes. In process applications involving large gas flows compression is typically accomplished by using centrifugal compressors and if large pressure increases, e.g., pressure ratios greater than three are required the compression is performed sequentially in stages with each stage contributing only a fraction of the overall pressure rise. Conventionally, in such staged systems each stage operates essentially adiabatically and hence, both to avoid excessive temperature rises as well as to reduce gas volumes, the outlet of each compressor stage is cooled to some suitable temperature prior to being subjected to the succeeding stages of compression. This paper presents an optimal design study of such a staged compression facility in which a process gas consisting of a mixture of CO_2 and water vapor at specified delivery conditions is to be compressed at least cost to a given final pressure.

The problem of designing an optimal staged compression facility has been considered previously by various authors. Happel (1958) was apparently the first to formally solve the now classical ideal gas case. In this formulation, the process gas is assumed to be ideal and is compressed in a specified number of reversible adiabatic stages from an initial pressure to a specified final pressure. It is assumed that the costs for interstage cooling are negligible (or fixed); that there are no composition or flow changes between stages; and that the capital cost (and hence the fixed annual charges) of the compressor is independent of the choice of interstage pressures. Under these assumptions, optimization of the annual cost of operation reduces merely to the determination of the interstage pressures which will reduce the total power requirements to a minimum. By resorting to the calculus and some algebraic manipulation, it is shown that in the three stage case the optimum interstage pressures correspond to an equal distribution of load among each of the stages, i.e., constant pressure ratios in each stage. By using the strategy of dynamic programming, Aris et al. (1960) have in a later paper proved this to be the case for an arbitrary number of stages. At the present time, this constant pressure ratio rule of thumb has found its way into most engineering design handbooks (Perry, 1963, for example).

Although not considered by Aris et al., the dynamic programming strategy can, in principle, be employed to solve the case in whcih cooling costs for each stage are included in the model. Moreover, it can also accommodate non-ideal gas behavior providing a suitable equation of state is available. These extensions will, of course, require the use of numerical iteration rather than the analytical solution procedures employed in the previous references. However, if in addition to the above complications, the interstage compositions and hence flows are allowed to vary, then both because of the "curse of dimensionality" (Bellman, 1957) as well as due to the fact that the individual stage costs are no longer separable, dynamic programming is inappropriate. Moreover, as is known to compressor technologists, in the presence of unequal interstage flows the constant pressure ratio rule of thumb will lead to a suboptimal design (Shain, 1966). This is the case with the system considered in this paper.

DESCRIPTION OF THE PROBLEM

The wet CO_2 compression facility under study is shown in Figure 1. The process gas consists of 40% CO_2 and 60% water vapor (volume basis) with negligible amounts of inerts. The gas is available at the rate of 4000 moles/hr at a temperature of 92° C and a pressure of 3 psig. This stream, originating in the CO_2 removal section of an ammonia plant, is to be compressed to 35 atm and delivered at 30°C to a drier for further processing. Because of the large required pressure rise, multiple staging is clearly indicated. Moreover, because of the presence of the condensible component, water vapor, each stage of compression must be preceeded by a partial condenser and a vapor/liquid separating drum equipped with demister. The complete multistage compressor system is to be designed to minimize total annual costs. The systems variables are the temperature, pressure, and composition between stages and the capacities of the various units. These variables are related through the design relations for each of the process units and the equilibrium relationships involving the temperature, pressure, and composition at each vapor/liquid separator.

It should be noted that all of the assumptions made in the classical ideal gas case are violated in the above system. Specifically,

1) the gas behavior is not ideal; at the higher pressures the CO_2 rich stream deviates significantly from ideality.
2) the composition of the process gas changes, hence all physical properties of the stream will change.
3) the interstage flows vary because of condensate removal.
4) costs of interstage cooling are significant and are not independent of the interstage pressures.
5) the compressor capital cost and duty is dependent on the interstage process stream conditions.

In spite of these complicating factors, the system can be optimized readily and conveniently by using the modular DYSYM flowsheet simulator to describe the above process combined with a direct search optimization method for adjusting the values of the independent process variables.

DYSYM

DYSYM, a Purdue expansion of the DYFLO system developed by Franks (1971) is a Fortran library of process unit modules together with utility subroutines designed for simulating steady state and dynamic flow processes. The unit modules model individual unit operations and may involve simple arithmetic operations, or may require the iterative solution of algebraic equations, or, as in the case of a nonideal gas compressor, may require the integration of the appropriate differential equation. The utility subroutines include routines which organize iterative calculations such as integration, or calculate the enthalpy of a stream given its temperature, pressure, and composition, or simply perform common conversions. By means of DYSYM, process flowsheets can be modeled by connecting together process unit modules as they occur in the system diagram. The composition, flow, temperature, enthalpy, and pressure of each process stream is stored in a common array (entitled STRM) and is passed from unit to unit according to the connections specified by the user. Physical property constants for each species involved in the process such as those required by vapor pressure relations, enthalpy relations, etc. are stored in a common DATA array which can be accessed as necessary.

MODEL FORMULATION

The entire multistage compressor system can be modeled by using two process modules: a condenser module, VVCON2, and a compressor module, COMP2S.

The heat exchanger module, VVCON2, contains two sections: in one the vapor temperature is greater than the dew point and condensation does not occur; in the other the temperature remains at the dew point and condensation does occur. In the first section the program solves the pair of differential heat balances

$$\frac{d(F_v h_v)}{dz} = -U\left(\frac{dA}{dz}\right)(T_v - T_w)$$

$$\frac{d(F_w h_w)}{dz} = \pm U\left(\frac{dA}{dz}\right)(T_v - T_w)$$

$$T_w = f(h_w),\; T_v = f(h_v)$$

(the (-) applies for counter flow of vapor and cooling water)

where F_v and F_w are the flow rates of vapor and cooling water, h_v and h_w are the unit enthalpies of vapor and cooling water, T_v and T_w are the temperature of vapor and cooling water, U is the overall heat transfer coefficient, and (dA/dz) is the value of the heat exchanger area per unit length.

In the second section of the program the vapor and condensate temperatures are set to the dew point and the program solves the following differential equations

$$\frac{dz}{dF_v} = \left(\frac{1}{UA(T_v - T_w)}\right) \cdot \frac{dq}{dF_v}$$

$$\frac{dh_w}{dF_v} = \pm \frac{1}{F_w} \times \frac{dq}{dF_v}$$

((-) corresponds to counter flow)

The derivative, dq/dF_v, is computed from the backward difference equation

$$\frac{dq}{dF_v} = -\frac{(F_v h_v + F_1 h_1)_j - (F_v h_v + F_1 h_1)_{j-1}}{\Delta F_v}$$

Note that the independent variable is chosen to be the vapor velocity rather than distance. This change leads to improved stability in the solution of the equations. The first differential equation is essentially a differential heat balance for the vapor stream and condensate. The second is a total differential heat balance for the vapor, condensate, and cooling water. An information flow diagram for this module is shown in Figure 2.

The compressor stage module, COMP2S, solves the differential flow energy balance

$$\frac{dW}{dp} = -V$$

and the differential equation which applies for the condition of constant entropy

$$\frac{dT}{dp} = \frac{T}{C_p}\left(\frac{\partial V}{\partial T}\right)_p$$

Values for V and $(\frac{\partial V}{\partial T})_p$ are obtained from the equation of state for the gas. In the present example the equation of state is that due to van der Waals

$$(p + \frac{a}{V^2})(V - b) = RT$$

An information flow diagram for this module is shown in Figure 3. In these equations a, b, R are constants in the equation of state, p is the pressure in atm, V is the molar gas volume, q is the rate of heat removal by the cooling water, and W is the flow work for compression.

Since these two process units occur as a fixed entity replicated at each stage, the simulator can be arranged so that by changing a single parameter a system with any number of stages can be evaluated. The overall simulator organization is shown in Figure 4. Given the number of stages, the set of interstage pressures and temperatures, the simulator performs the integrations necessary to calculate the output from the condenser and generates values for the cooling water flows required, the condensate flow, and the exchanger areas. It then takes the output vapor from the condenser and simulates the compressor operation to calculate the compressed output stream. This requires integration of the flow work so as to generate the value of the brake horse power required for that stage. Upon completion of passage through the required number of stages, the compressed gas stream is sent to the final cooler/condenser in which the temperature is adjusted to the specified value and cooling water flow and exchanger area calculated. With the completion of this pass, necessary auxiliary calculations are performed and the value of the optimization criterion is obtained. Upon completion of the design evaluation, control is passed to the optimization routine which determines suitable changes in the interstage conditions which will lead to an improved value of the design criterion.

In this application, the criterion for optimal design specifications is that which leads to a minimum annual total cost, a combination of annual fixed charges and annual operating costs. The fixed charges are taken to be a constant fraction of the investment in compressor stages, heat exchangers, vapor-liquid separation drums, and demisters. Annual operating costs are taken to be the cost of cooling water plus electrical power. Details of the cost function are given in the Appendix.

By using the interstage pressures and temperature as design variables all of these costs can be calculated directly by means of the simulator. The only explicit constraints which must be imposed on the design or independent variables are that the ratio of the inlet to outlet pressures at each stage be greater than 1 and that the interstage temperatures must be within reasonable bounds.

Hence,

$$1.22 = P_1 \leq P_2$$

$$P_2 \leq P_3$$

$$P_3 \leq P_4 = 35$$

and $26°C \leq T \leq 90°C$.

In addition the temperature difference between the inlet vapor and the outlet cooling water must be equal to or greater than 5°C.

THE SEARCH METHOD

The adjustment of the trial values of the interstage temperature and pressures was performed using the search logic of the Complex Method due to Box (1965). This method is one of the more successful of the direct search methods which can accommodate inequality constraints on the independent variables and which requires only cost function values in order to find the minimum. The technique is an adaptation of the Simplex Method of Spendley, Hext, and Himsworth (1962) and like that method conducts the search by means of a flexible pattern consisting of about 2N points. In the algorithm the initial search pattern is randomly generated and successive new points are obtained by projecting the worst point in each pattern a suitable distance through the centroid of the remaining points.

Specifically, given a problem

$$\begin{array}{lll} \text{Minimize} & f(x) & \\ \text{Subject to} & g_m(x) \leq 0 & m = 1, \ldots, M \\ & a_i \leq x_i \leq b_i & i = 1, \ldots, N \end{array}$$

and a starting point x^1 which satisfies all of the constraints (is feasible) and is interior to all of them, the method proceeds as follows:

1) Generate Starting Pattern

A starting set of K (= about 2N points) is obtained by setting

$$x_i^k = a_i + r_i^k (b_i - a_i) \qquad \begin{array}{l} i = 1, \ldots, N \\ k = 1, \ldots, K \end{array}$$

where the r_i^k are pseudo-random numbers uniformly distributed on the interval 0 to 1. If any trial point violates the constraints, it is retracted half-way towards the centroid of the vertices already feasible until it too becomes feasible.

2) Project the Worst Point

The objective function values at each point are determined and the vertex corresponding to the highest value is identified. A replacement for this point is generated by projecting the rejected vertex a certain distance through the centroid of the remaining points. That is,

$$x^{new} = \bar{x} + \alpha(\bar{x} - x^R)$$

where x^R is the rejected point

α is a suitably chosen step-size parameter (1.3 recommended)

$\bar{x} = \frac{1}{K-1} (\sum_{k=1}^{K} x^k - x^R)$ is the centroid of the remaining points.

3) Test the New Point

If the new point is feasible but again yields the worst function value or is infeasible, retract it half-way towards the previously calculated centroid. If repeated retractions fail, save the best point and proceed with step (1). Otherwise, continue with step (4).

4) Check for Convergence

The search is terminated when the search pattern has shrunk so that the points are sufficiently close together and/or if the differences between the objective function values of the points become small enough. If the convergence test fails, return to (2) and continue the search.

Although the above search algorithm is very conservative in that it always operates on the worst rather than the best point and thus often can be quite slow, it will converge to the minimum providing that the constrained region being searched is convex.

RESULTS

Optimal process designs were obtained for six different cases. Each case could be defined by merely changing a few parameters in the simulator. The results are summarized in Table 1. These case studies provide comparisons between the following situations:

1) Use of ideal gas versus real gas equation of state (Cases I and II).

2) Three or four compressor stages (Cases III and VI).

3) Effects of varying water vapor composition at fixed dry gas rate for the three stage case. (Case III 60%, Case VII 30%, Case VIII 15%)

4) Optimal design versus the design obtained using the fixed pressure ratio rule of thumb (Cases III and II for three stages, Cases VI and V for four stages).

5) Effects of varying water costs (Case III, 10¢/gal; Case IV, 2¢/1000 gal).

Proceeding in the above order, it is first of all apparent that the non-ideality does introduce a significant change in the resulting optimal design. As expected the calculated total required power is higher in the ideal gas case and consequently so is the annual cost. Comparison of Cases III and IV shows that four compression stages are not necessary. Although the cost of the four stage design is only marginally higher, it is apparent that the third stage provides only one atmosphere of pressure rise and hence ought to be deleted.

As might be expected, the reduction of water content from 60% did have a dramatic effect on the cooling water requirement and hence the annual costs. The difference in the cost of Cases VII (30%) and VIII (15%) is small. Virtually all of the condensation takes place in the first condenser and hence after this unit, the two processes are essentially the same. Note that in effect the second compression stage is doing very little work and thus might well be deleted. Finally it is quite apparent from a comparison of Cases II and III as well as V and VI that the constant pressure ratio rule is far from optimal if all of the costs are taken into account. Although the costs themselves are not dramatically effected, the values of the design variables are. In both pairs the optimization forced a reduction in exchange area at the cost of some increase in the required horse power. The effect of the reduction in water costs from 10¢ to 2¢ per M gals. could have been anticipated: at lower water cost a lower interstage temperature and higher flow rates are economical and hence exchange areas can be reduced. In addition, the duty of the second compressor stage is low suggesting that two stages might suffice. In general the cost of power and fixed costs for compression are balanced against the cost of cooling water and fixed costs for heat exchangers. An increase in water costs shifts the balance toward higher interstage temperatures and higher fixed costs for compression.

Table 2 summarizes the details of the design of Case III, the base case. Note that both the heat exchange area and the stage compressor duty decrease with successive stages. Most of the condensation takes place in the first condenser. At each subsequent condenser further condensate can be removed after each compression stage, but this diminishes until essentially no moisture remains.

CONCLUSIONS

From the study it can be concluded that:

1) deviation from non-ideal behavior must be taken into account in compressor design
2) in the presence of condensibles, cooling costs significantly influence the optimal design
3) when all cost factors are taken into account the constant pressure ratio rule of thumb does not yield an optimal design.

The DYSYM library combined with the Complex direct search method provides a flexible and convenient vehicle for undertaking an optimal design study of modular flow systems.

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APPENDIX

Details of design optimization criterion.

The installed cost of a staged centrifugal compressor including electric driver and speed reducer over the range of 2×10^4 to 350 hp (Walker, 1974) is given by

$$6960\ (BHP)^{0.57}$$

The installed cost of a single shell aluminum tube floating head condenser is estimated (Walker, 1974) as

$$2750\ (A/100)^{0.823} \qquad A \text{ is } ft^2$$

This cost assumes 20 ft long, 3/4" tubes, arranged on a one inch square pitch with an operating pressure of 150 psig. To correct the cost for other operating pressures, the value at 150 psig is multiplied by the relative cost factor correlation (Peters and Timmerhaus, 1968)

$$[0.92 + 0.052\ (P/150) + 0.028\ (P/150)^2]$$

If the area of the exchanger exceeds 9000 ft^2 then multiple parallel shells must be used.

The installed cost of the separating drums is based on pressure vessel costs,

$$4,840\ \left(\frac{w}{10^3}\right)^{0.71}$$

where w is the weight of steel required to construct the vessel. The diameter, D, of the vessel is obtained by using an empirical entrainment velocity relation (Walker, 1974)

$$V = 0.27 \sqrt{\left(\frac{\rho_1 - \rho_v}{\rho_v}\right)} = \frac{Q}{\Pi/4D^2}$$

where ρ_1 and ρ_v are the densities of the vapor and liquid under process conditions, V is the maximum linear vapor velocity in ft/sec, and Q is the volumetric flow rate of the gas. The above relationship is valid for vertical drums with demisters. The height of the vessel is obtained by assuming a 15 minute residence time for the liquid, positioning the inlet one foot above the liquid level; locating the demister pad a distance of 0.75 times the vessel diameter or six feet above the inlet, whichever is the smaller; and, allowing one foot of space above the demister.

Hence, the height will be

$$H = \frac{\text{Flow of Liquid } (ft^3/min) \times 15 \text{ min}}{\Pi/4D^2} + 2 + \min\ (0.75D,\ 6')$$

The vessel thickness is calculated by using a modified hoop stress formula with a 1/4" corrosion allowance:

$$t = \frac{P_D\ D/2}{12,000 - 0.6\ P_D} + 0.25$$

where P_D is the design pressure and is equal to the larger of (P + 25) psig, or 1.1 times P.

The weight of the vessel is then calculated by using a density of $40.8\#/ft^2$ -in for steel and a correction factor of 1.5 to account for eliptical heads, flanges, and fittings. Hence,

$$\text{weight} = Dxt \times 1.5 \times 40.8 \times (H + 0.75D)$$

The cost of a 4 inch thick stainless steel (316) demister pad is given by

$$10 + 22D + 15.4D^2$$ where D is the vessel diameter in feet.

By using the above relationships to size and cost the equipment items, the total fixed investment can be obtained.

Annual cost is then equal to

$$\text{Annual cost } (\$/yr) = C_1\ F_w + C_2\ BHP + d\ I_F$$

where F_w is the total flow of cooling water required

BHP is the total power required

I_F is the total fixed investment

The cost of cooling water is taken to be $10¢/10^3$ gal with the water available at 25°C and returned at a maximum of 50°C. The power costs are taken to be 1¢/KWH and delivery efficiency is assumed to be 75%. Investment cost is converted to fixed annual cost by multiplying by a factor d = 0.2 which includes depreciation and interest. The system operates 8400 hours/year.

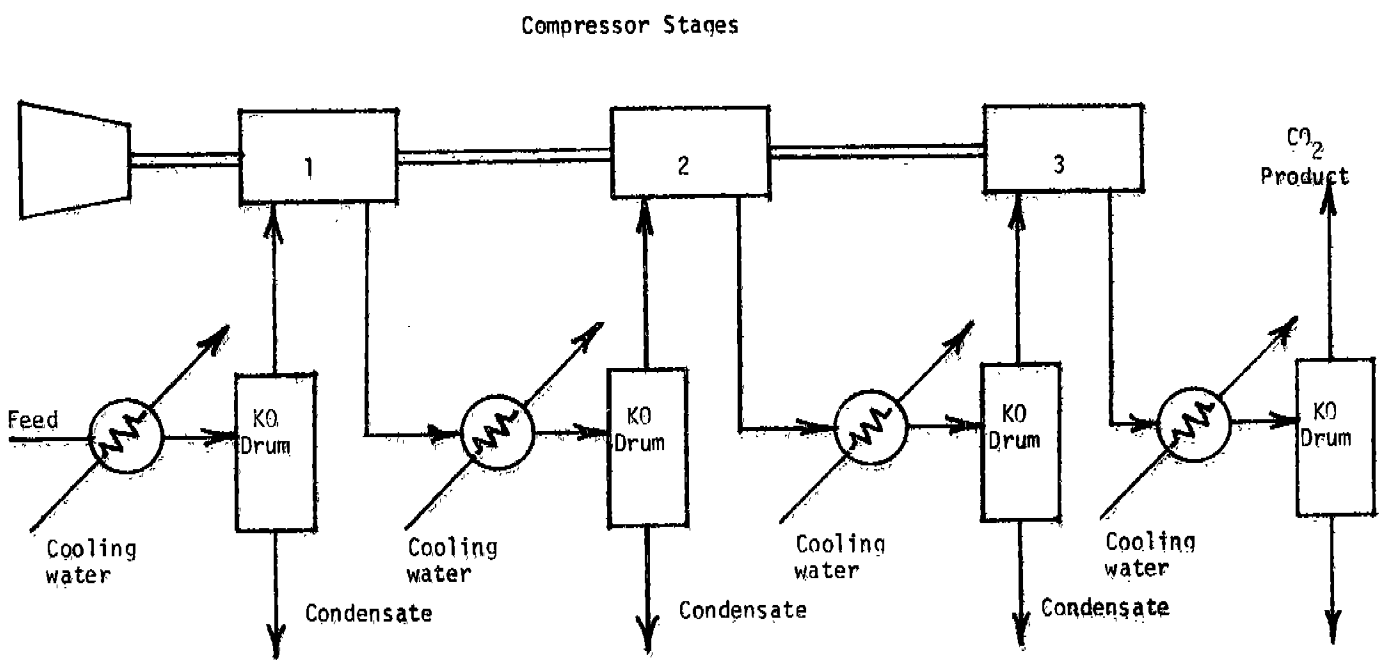

Fig. 1: Wet CO_2 Compression Facility

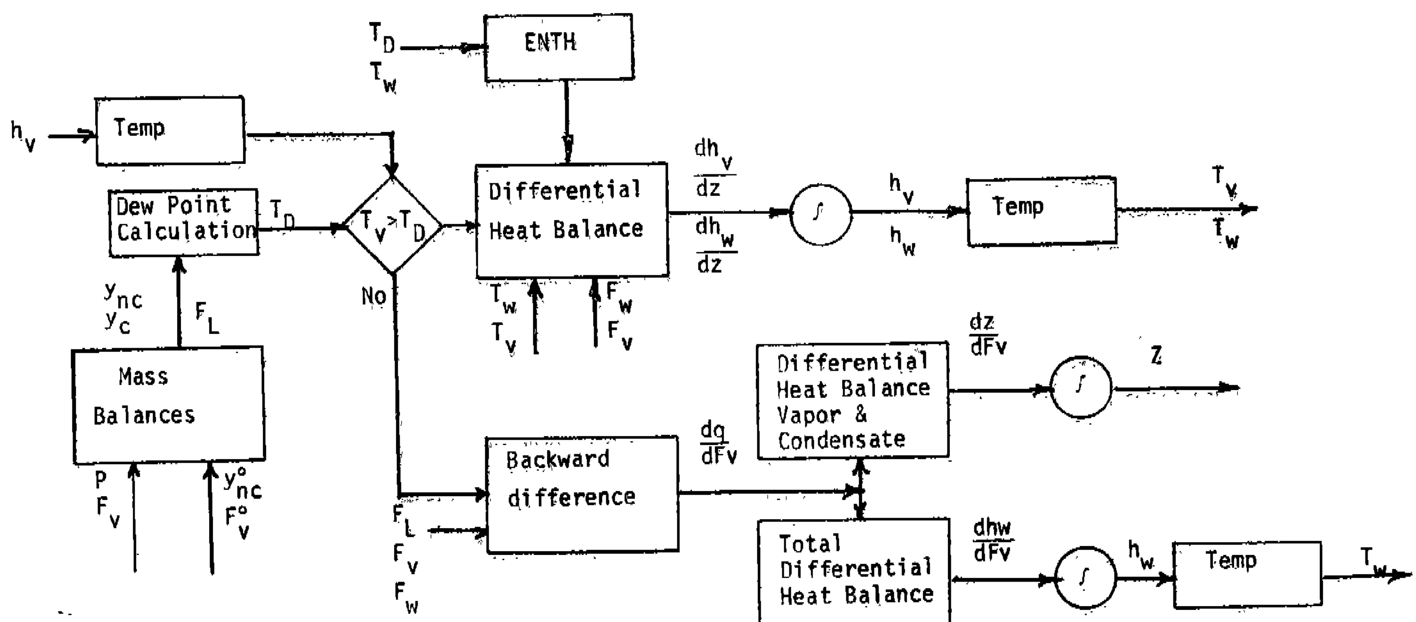

Fig. 2: Information Flow, VVCON2B

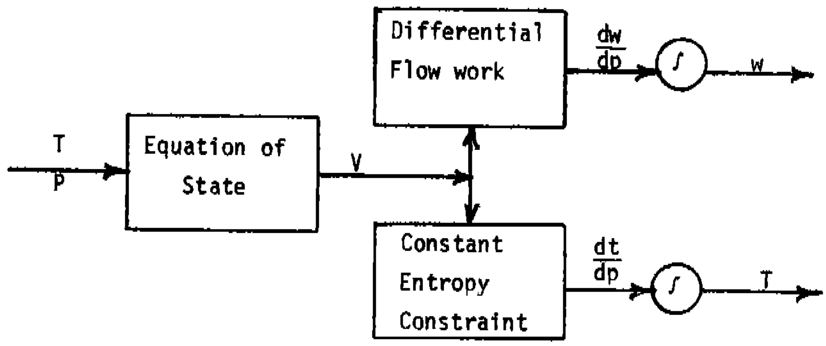

Fig. 3: Information Flow, COMP2S

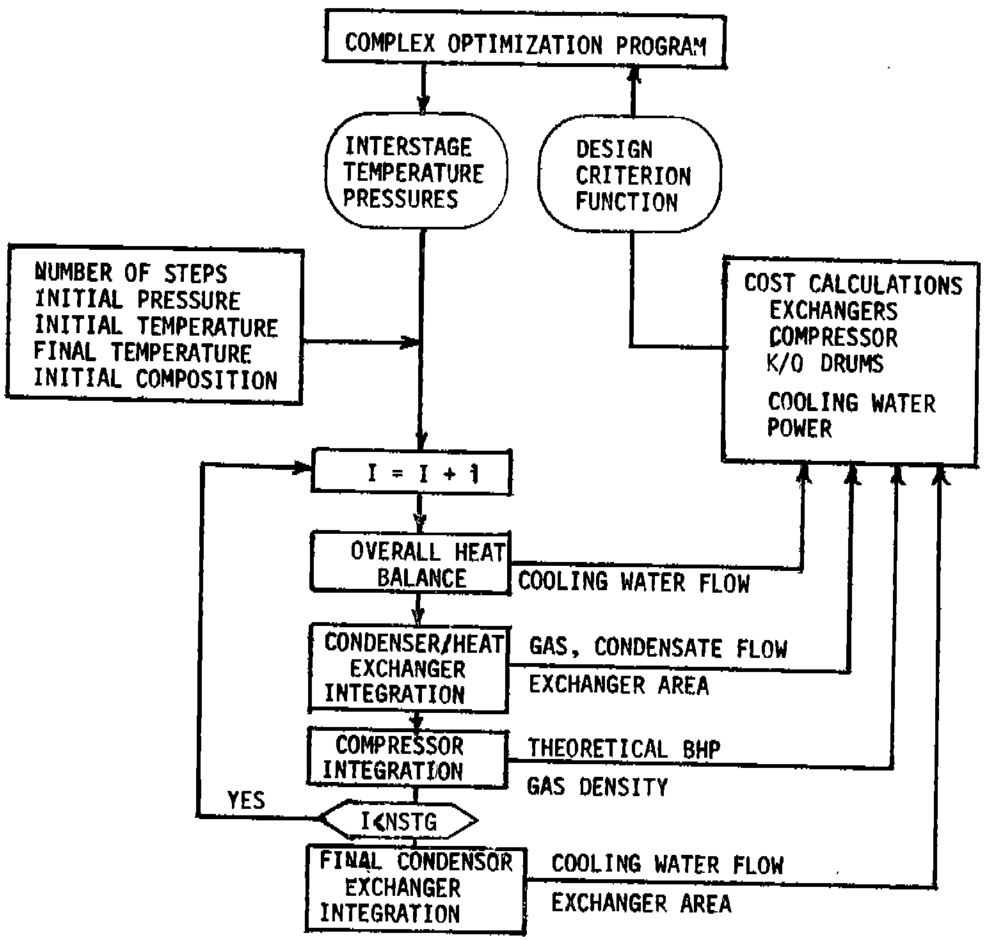

Fig. 4: SIMULATOR ORGANIZATION

Table 1. Summary of Optimization Results

CASE	Interstage Pressures, Atm P_2	P_3	P_4	Exch. Exit Temp. °C	Total Comp. Power, BHP	Total Exch. Area, Sq.ft.	Cooling Water MMM gal/yr	Total Cost $M/yr
I. Ideal gas	5.00	5.22	---	30.8	3298	6391	1.239	506
II. Constant pressure ratio	3.73	11.43	---	28.0	3073	11022	1.238	499
III.*Base Case	4.48	12.26	---	31.4	3121	8320	1.233	496
IV. Cooling water at 2¢/M gal	6.97	8.79	---	28.2	3132	7714	1.282	397
V. 4 stage, constant pressure ratio	2.82	6.54	15.13	28.0	3009	17100	1.251	513
VI. 4 stages	3.17	9.15	10.62	34.3	3101	7990	1.236	498
VII. 30% water vapor in feed	4.82	5.53	---	26.01	3114	8333	0.273	398
VIII. 15% water vapor in feed	5.32	5.88	---	26.01	3114	7907	0.306	400

*Conditions of base case: 60 vol % water vapor in feed, feed pressure=1.22 atm, feed temperature=92°C, cooling water cost=10¢/M gal, final pressure=35 atm, 3 compressor stages used, real gas equation of state used in the computations, dry gas rate=1600 lb moles/hr. All other cases are variations from base case.

Table 2: Base Case Design Details
Compressor Stage Inlet Temperatures are all 31.4°C

Condenser Inlet Stream: Flow (moles/hr)	Condenser Inlet Stream: H_2O mole fraction	Cooling water flow MM gal/yr	Exchanger Area (ft^2)	Separator: Condensate Flow (moles/hr)	Separator: Drum Dimensions (ft) H	Separator: Drum Dimensions (ft) D	Compressor: Pressures atm in	Compressor: Pressures atm out	Compressor: Outlet Temp. °C	Compressor: Horse Power
				Stage 1						
4000	0.6	1060	2249	2340	13.0	5.75	1.22	4.48	69.8	1276
				Stage 2						
1660	0.036	72.5	2230	45	5.25	4.10	4.48	12.25	61.1	931
				Stage 3						
1615	0.0097	46.2	1945	10.2	4.45	3.13	12.25	35.0	65.6	915
				Final Cooler						
1605	0.0035	51.9	1896	4.2	3.85	2.38	---	---	---	---