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# HYCSOS: HYDRIDE CONVERSION AND STORAGE SYSTEM SENSITIVITY ANALYSIS



by

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# 1 INTRODUCTION

The Hydride Conversion of Solar Energy System (HYCSOS) chemical heat pump has been under development at Argonne National Laboratory since 1975. As part of this work two design studies were performed by TRW (References 1 and 2). A major part of the more recent TRW study was the development of a computer program to design a HYCSOS system.

The work described in this report was to modify and use this program to perform HYCOS sensitivity studies. Although it is recognized that the program used is not entirely correct, it is felt that studies of this kind are valuable for determining the important parameters of the system design.

# 2 DESCRIPTION OF THE TRW DESIGN PROGRAM

The computer program used in this work was based on the program developed by TRW (Reference 2) to run on CDC Cyber 74 and Cyber 174 computers. The program was written in Fortran IV for use in an interactive mode, and its logic is shown schematically in Figure 1.

The program consists of a main program and several subroutines. A functional description of these routines as well as a description of the program's input and output is presented in Reference 2.

# 3 DESCRIPTION OF MODIFIED PROGRAM

The TRW program was considerably modified in the course of this investigation. First of all the program was modified to run in a batch mode on the ANL IBM 370/190 computer system. As part of this modification, a number of formatting changes in the output were made to provide more readable and useful output.

In addition to these changes, a number of more substantial changes were also made. These modifications will be discussed in the results sections below.

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*A copy of the program is available from the author of this report.

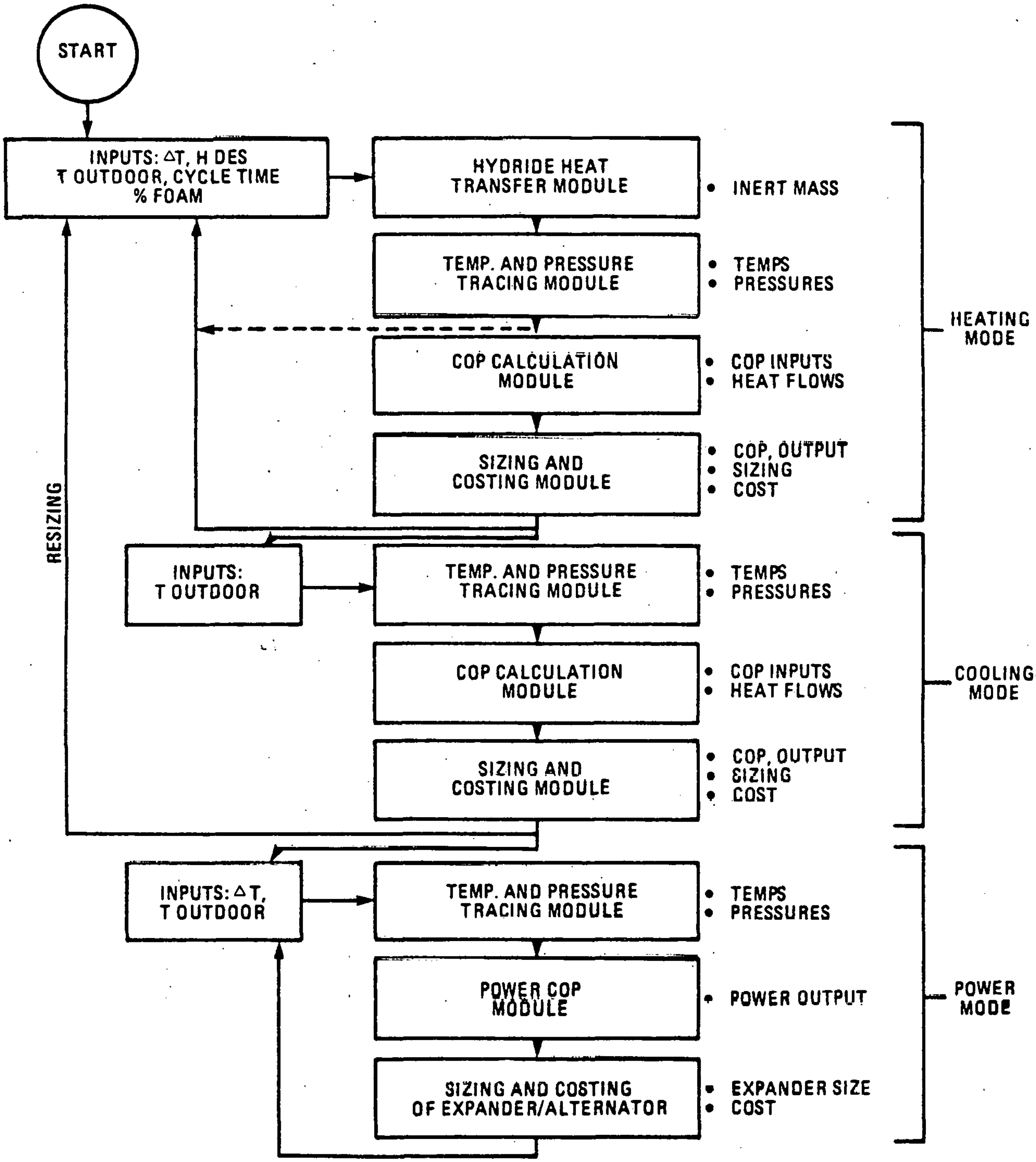


Fig. 1. Computer Logic Diagram (Ref. 2)

# 4 RESULTS

After the program was operational and checked out against the TRW sample case, several hundred test cases were run. This section will present a description of the test series, the results obtained, and the significance of these results to the overall system design.

## 4.1 ADSORPTION AND REGENERATION TIME

As used in the TRW study, the adsorption time (T) was equal to the desorption time and was input by the user. This time corresponds to the period that the system is operating as a heat pump. The regeneration time (RGT) is the time, input by the user, that beds are in a regenerative or nonoperating mode. Thus, the cycle time is the sum of these times (RGT + T), and the percent operational is given by:

$$\% = \frac{T}{RGT + T} \times 100 \tag{1}$$

Figure 2 shows the dependence of normalized system cost (NSC) and cooling coefficient of performance (COP) versus adsorption time. It should be noted at this point that the heating COP and the cooling COP were in general related by:

$$COP_h \simeq COP_c + 1 \tag{2}$$

Therefore, it is sufficient to consider only one of the COPs. Figure 3 presents $COP_c$ and NSC as a function of the regeneration time. From these two figures several conclusions can be drawn.

The adsorption time strongly influences the system cost - linear increase with increase in T - and the COP reaches a plateau. This clearly indicates a compromise between the cost and performance of the unit. The influence of regeneration time on NSC is not as pronounced as the adsorption time, but it exhibits the same behavior. The COP apparently reaches a maximum at RGT ≃ 0.2, but the curve here is very flat.

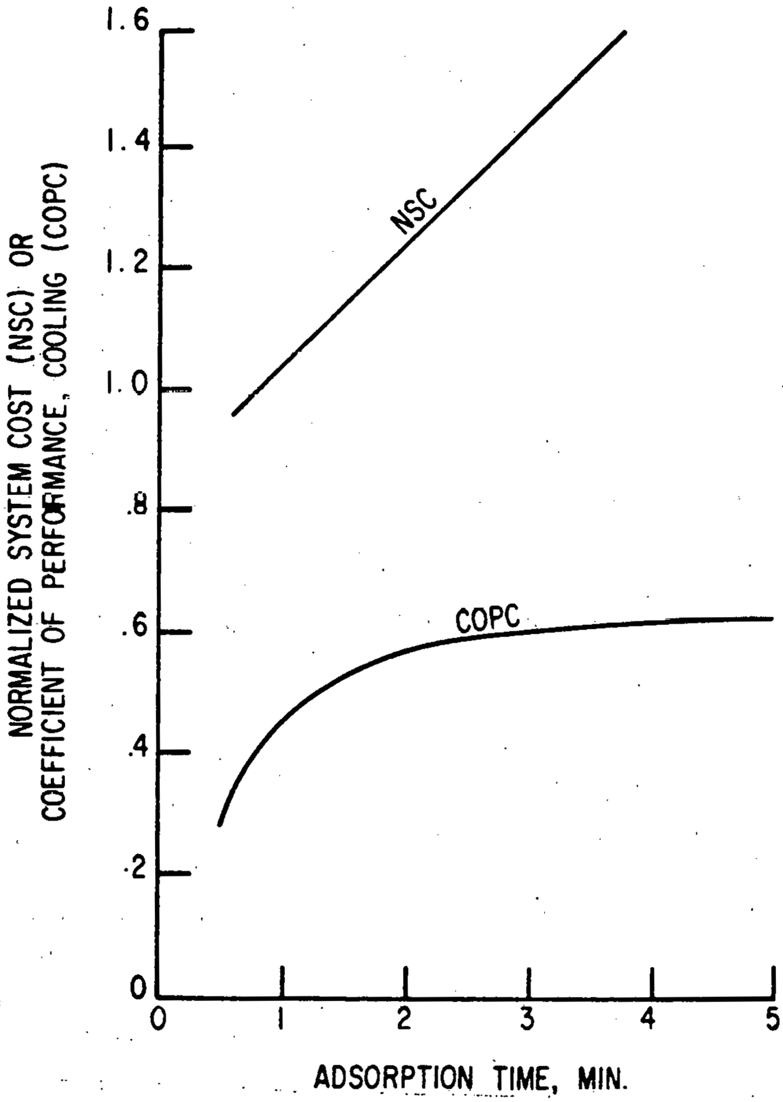


Fig. 2. Effect of Adsorption Time on Cost and Performance

The significance of these results on the system design is that, as the cycle time increases, more hydride material and hence heat-exchanger area are required. Thus, the cost increases but the COP also increases, so the designer must make a tradeoff between added cost and added performance.

It should be noted that the performance of the unit is not directly related to the cycle time. If the cost and performance of the unit were plotted against the cycle there would not be a smooth curve. Rather, there is an optimum regeneration time at any given adsorption time.

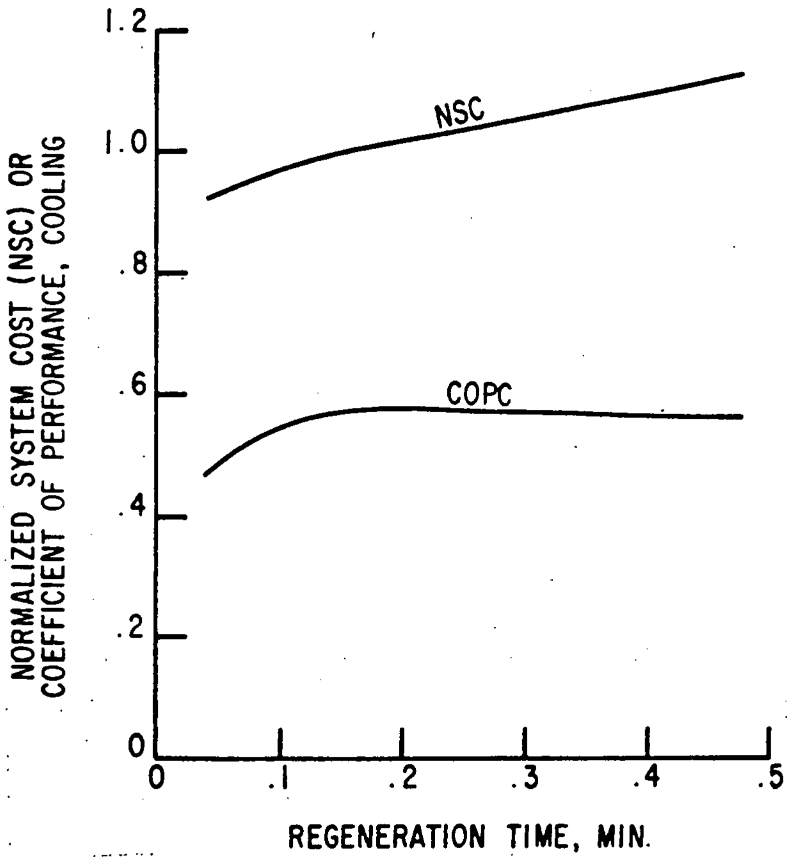


Fig. 3. Effect of Regeneration Time on Cost and Performance

4.2 DESIGN HEAT FLUX

The design heat flux (HDES) is the rate of heat flow per unit area per unit time in the hydride heat exchanger. HDES is specified by the user, and the program will either print a message that the heat flux is too high or it will continue with the calculations.

Figure 4 presents the effect of HDES on $COP_c$ and NSC. The cost is decreased and the performance increased by higher values of heat flux. This occurs because less inert (nonhydride) material is required as the area of the heat exchangers is more effectively utilized.

From this result, it appears that higher heat fluxes are desirable; however, this conclusion ignores the fact that the heat flux must also be sustained in the coolant (R-114 in this case)*. The coolant temperature

*R-114 is the ASHRAE designation of dichlorotetrafluoroethane ($Cl_2F_4C_2$).

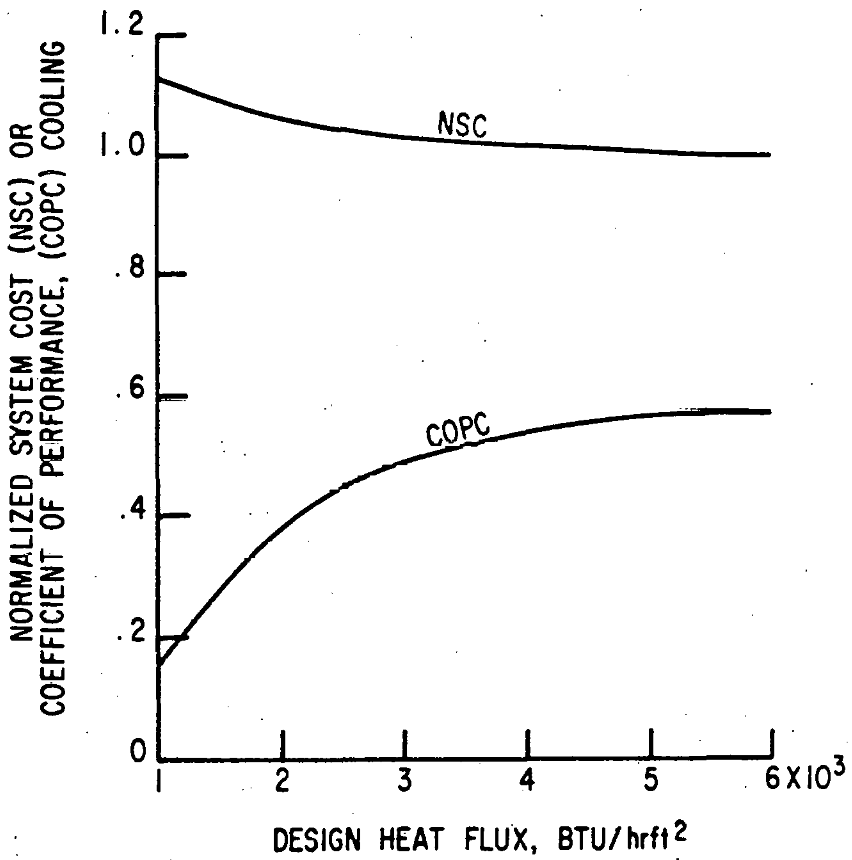


Fig. 4. Effect of Design Heat Flux on Cost and Performance

difference is assumed in all cases to be 1°F. Thus, at the same temperature difference and at increasing heat flux, the heat transfer coefficient between the coolant and the surface must also increase. The sensitivity of the result to the coolant surface temperature difference will be examined below.

## 4.3 HYDRIDE MATERIAL

The performance of the system with different hydride materials was examined within the program limitations. The program uses, as the default case, $LaNi_5$ for the high-temperature material, and $CaNi_5$ for the low-temperature material. The composition of the low-temperature bed can be changed to one of the substituted tertiary alloys of the form $LaNi_{5-x}Al_x$. The program uses the input value to specify the composition of the low-temperature bed. A value of zero or no input value means that the default $CaNi_5$ material is used.

The results of runs with several different compositions are presented in Figure 5 as the COP versus the NSC. From these curves the substitute alloys have a slightly lower cost and a lower performance.

The results of these tests alone cannot be used to select the hydride pairs, as the usable temperature range of the heat pump also depends on the alloys used. The alloys selected have several influences on the temperature range of operation. They affect the amount of output available at low temperature and also the source temperatures required for both heating and cooling.

Figure 6 presents the normalized heating output for four different alloys. All four designs were for an ambient temperature of 47°F. As can be seen, the larger amount of aluminum substituted, the better the low-temperature heating performance. On the other hand, this performance is at the expense of requiring a higher source temperature. Figure 7 presents the source temperature versus the ambient temperature for the four cases con-

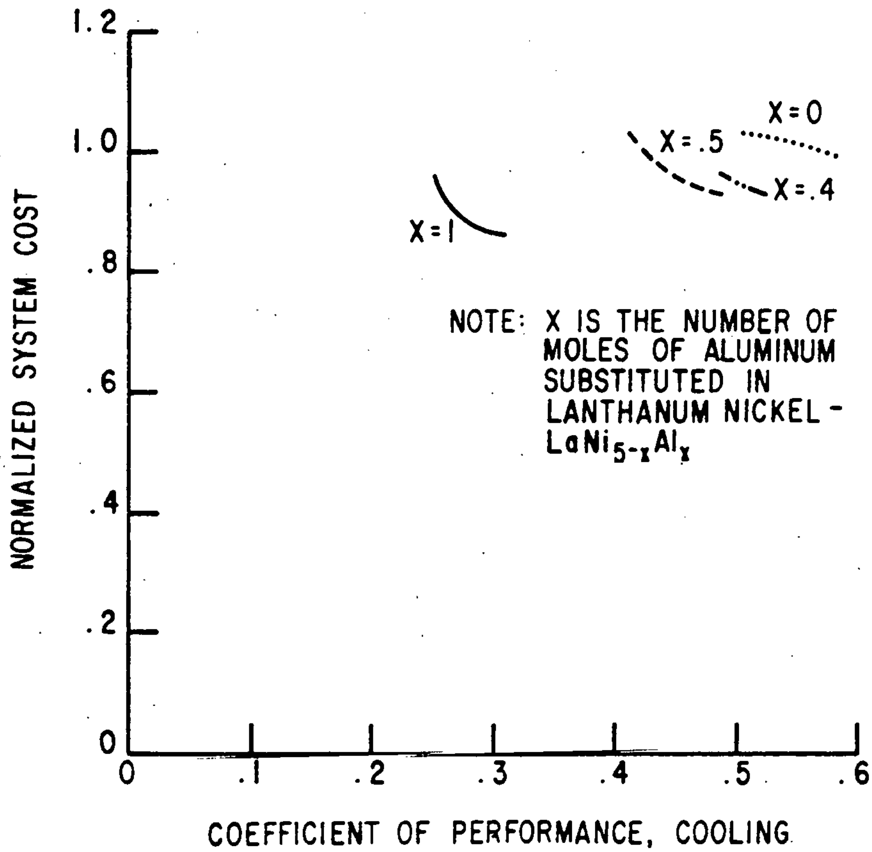


Fig. 5. Effect of Alloy Composition on Cost and Performance

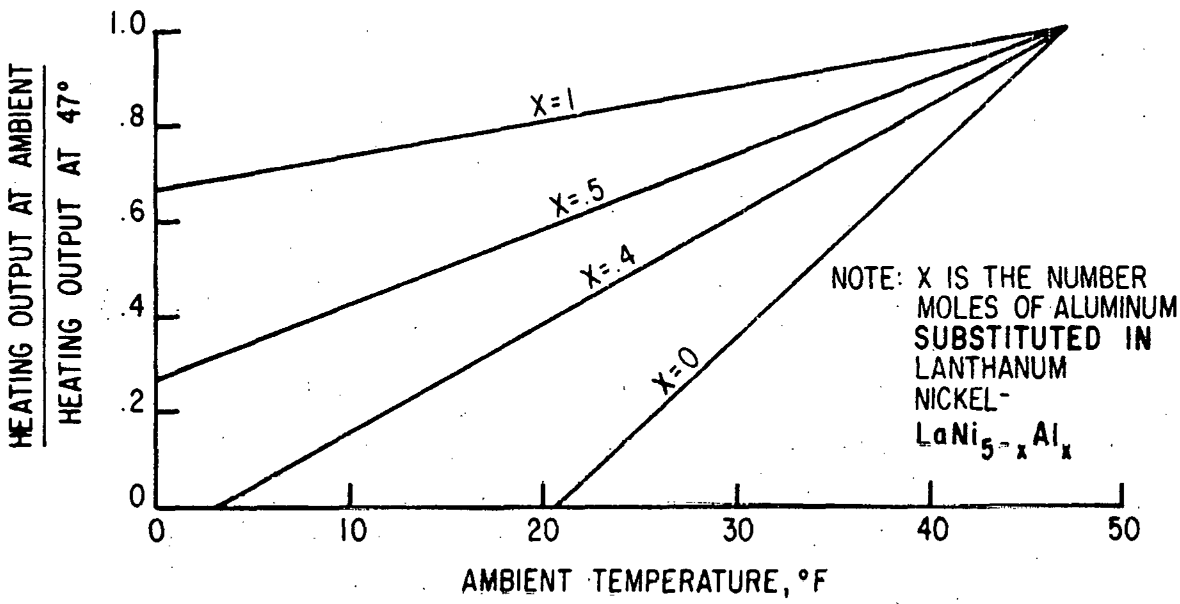


Fig. 6. Effect of Alloy Composition on Heating Output

sidered. As can be seen, there is a substantial increase in source temperature required to obtain low-temperature performance.

Figure 8 presents the source temperature versus the cooling output. As before, the ternary alloys require a higher source temperature.

The purpose of this section has been to point out some of the tradeoffs which must be made in order to select the appropriate alloy pair for a given application.

## 4.4 DESIGN HEAT LOAD

The design heat load (DESOUT) is the heating capacity of the unit at the design conditions. The sensitivity of system size (heating load) to cost was investigated. Figure 9 presents the NSC against the design heat load. As can be seen, the system exhibits a large economy of scale, i.e., the larger the system, the lower the per unit cost.

This conclusion is probably true, but it is also sensitive to the costing algorithm built into the program. Therefore, this conclusion should be used with a due amount of caution.

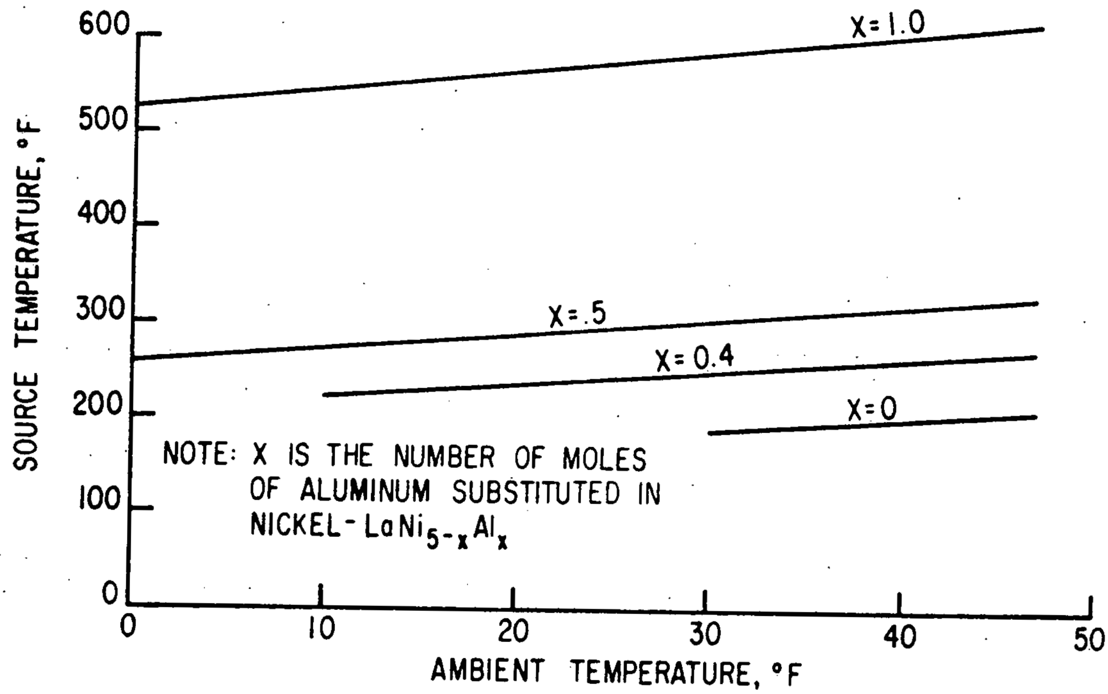


Fig. 7. Effect of Alloy Composition on Source Temperature for Heating Mode

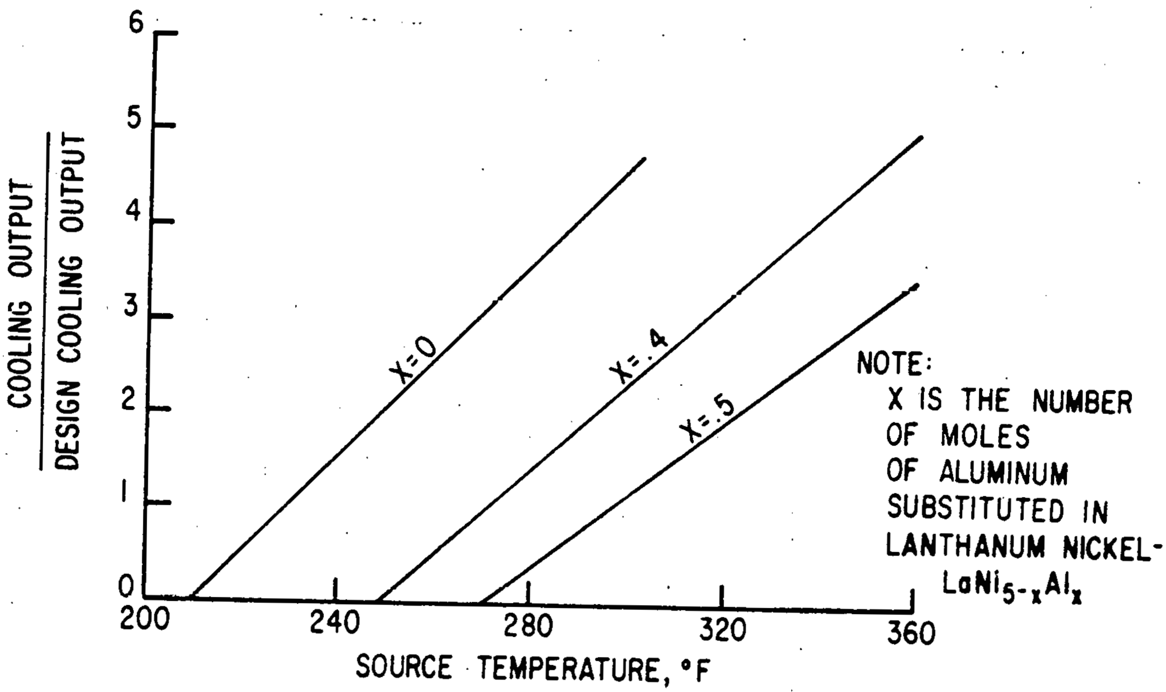


Fig. 8. Effect of Alloy Composition on Source Temperature for Cooling Mode

### 4.5. COOLANT TEMPERATURE DIFFERENCE

As mentioned earlier, the program assumes for all cases that there is a 1°F temperature difference between the R-114 and the surface temperature. This assumption is made in both the hydride and nonhydride heat exchangers. This assumption was examined by varying this temperature difference. Table 1 presents the results of the tests conducted. As can be seen, there is little change in either the cost or the COP as the temperature difference is increased. The only observed change is that the program will not operate at high values of heat flux and R-114 temperature difference. This is due to the program logic and is probably not significant.

### 4.6 FINS

As written, the TRW program calculates the heat transfer properties of the hydride heat exchangers in the subroutine HEAT. This routine calculates the performance of a finned bed and a plain bed (no fins). The performance of the two beds is compared and the one with the lower conductance is selected. In virtually every case, the finned case is chosen. The influence of this result was examined by making a program change to force the selection of

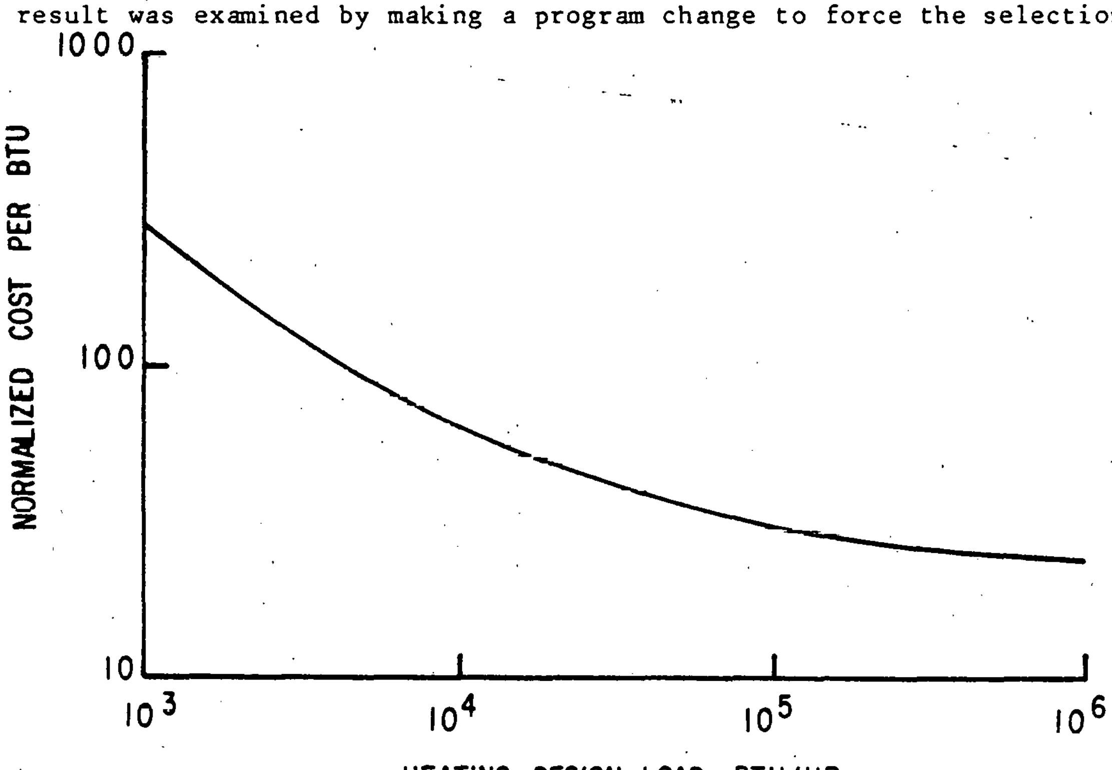


Fig. 9. Effect of Heating Design Load on Unit Cost

Table 1. Effect of Coolant Temperature Difference on Cost and Performance

| Heat Flux Btu/hr ft$^2$ | Coolant Temperature Difference °F | Normalized System Cost | Cooling COP |
|---|---|---|---|
| 5350 | 1 | 1 | 0.574 |
| 5350 | 2 | 1 | 0.571 |
| 5350 | 5 | a | |
| 5350 | 10 | a | |
| 2500 | 1 | 1.047 | 0.475 |
| 2500 | 2 | 1.047 | 0.470 |
| 2500 | 3 | 1.047 | 0.466 |
| 2500 | 5 | 1.048 | 0.458 |
| 2500 | 10 | a | |
| 1000 | 1 | 1.114 | 0.154 |
| 1000 | 2 | 1.114 | 0.142 |
| 1000 | 3 | 1.115 | 0.129 |
| 1000 | 5 | 1.117 | 0.103 |
| 1000 | 10 | a | |

[a]Program could not satisfy the condition.

the nonfinned bed. The results of these tests were that the addition of fins gave some improvement in the COP, and also resulted in a very slight cost savings. However, it is felt that both of these results were within the inaccuracies of the conduction model used.

## 4.7 INERT MASS

In a HYCSOS heat exchanger any material that is not a hydrogen adsorber/desorber causes a parasitic loss in the system because this material must be heated or cooled as the beds are regenerated. In order to examine this effect quantitatively, a programming change was made to vary the amount of inert mass present. The results of several tests are presented in Figure 10 as the cooling COP versus the active mass ratio (AMR). AMR is defined as the thermal mass of the hydride divided by the sum of the thermal mass of the heat exchanger. In particular, the denominator is the sum of the hydride thermal mass, the structural thermal mass, and the thermal mass of the coolant. As shown in the figure, the COP is a very strong function of the AMR. This illustrates the importance of minimizing the inert materials present in the heat exchanger, and also the importance of regeneration on the process.

Another observation drawn from this figure is the fact that points for two different heat fluxes fall on the same curve. This suggests that this curve may be of general use in predicting the performance of systems of this type. Knowing the physical arrangement of the heat exchanger, the performance could be obtained from a curve similar to Figure 10.

4.8 BED CONDUCTANCE

The program uses a very simple model to compute the conduction heat transfer through the hydride bed. The model used solves the steady, one-dimensional conduction equation in a homogeneous material. As this model is very simplistic, the sensitivity of the program output to the results of this model was determined. The output of this model, namely the bed conductance, was reduced by arbitrary amounts and the results on the system were noted. In

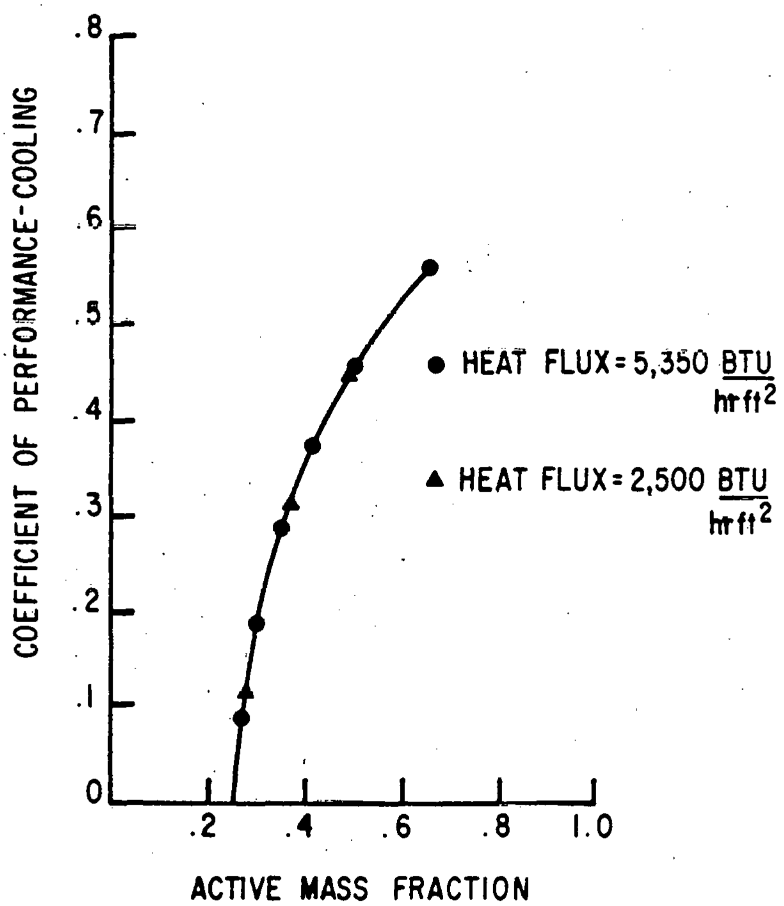


Fig. 10. Influence of Active Mass Fraction on Cooling Coefficient of Performance

general, reducing the bed conductance had very little influence on the results. In fact, the results obtained were very similar to the results obtained by varying the fluid surface temperature difference.

## 4.9 SINGLE-PHASE COOLANT

The program was designed to use a coolant, R-114, that transfers heat to and from the hydride by boiling or condensing. This allowed the coolant flow to be determined only on the basis of the heat load and the latent heat. The use of a two-phase coolant has certain advantages, such as a more uniform temperature distribution in the heat exchangers and a high heat transfer coefficient, but it has certain disadvantages. The chief disadvantage is the necessity of having additional heat exchangers to interface with the solar/storage system.

Several program modifications were performed to permit the use of single-phase coolants. These changes permit the use of either a 50% ethylene-glycol/water mixture or air. These modifications were successful to the point that the program would run but the results obtained were not deemed to be satisfactory.

The results obtained for ethylene glycol were very strongly influenced by the mass of the coolant within the heat exchanger. In the unmodified program, it was assumed that the coolant occupied 1/533 the volume of the heat exchanger. This assumption was not rationalized in any way. This assumption might be based on the fact that aluminum foam occupied the coolant passages. In any event, the results of the glycol runs were extremely sensitive to the fraction of glycol in the heat exchanger. Since this fraction appears to be an arbitrary constant until a glycol-hydride heat exchanger is designed for this application, no results are presented here.

For the cases run with air as the working fluid, there was a different problem. As part of the design process, the program sized the pumps driving the coolant in the various circuits. With air as a working fluid, the parasitic power caused by pumping the large amount of low-density material caused the program to yield unreasonable results.

Either of the above problems could be corrected with some amount of additional work, but these changes were not felt to be warranted at this time.

## 5 CONCLUSIONS

A computer program has been used to investigate the design parameters of a four-bed HYCSOS heat pump. The results of this study were presented in the previous section.

Although several useful results have been obtained, further use of this program should be delayed until a better definition of the heat pump system becomes available. Particularly, data are required to establish the design and performance of the hydride heat exchangers.

## REFERENCES

1. Gorman, R., *Performance and Cost Analysis of a Hydride Air Conditioning System*, prepared by TRW Energy Systems Group for Argonne, Argonne Report ANL/EES-TM-65 (April 1977).

2. Gorman, R., and P. Moritz, *Hydride Heat Pump, Vol. I: Users Manual for HYCSOS System Design Program* and *Vol. II: Cost, Performance, and Cost Effectiveness*, prepared by TRW Energy Systems Group for Argonne, Argonne Report ANL/EES-TM-66, Vols. I and II (May 1978).

3. *Handbook of Fundamentals*, American Society of Heating, Ventilating and Air Conditioning Engineers, New York (1972).

4. Kreith, F., *Principles of Heat Transfer*, International Textbook Company, Scranton, Pa. (1965).