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MODELING AND ANALYSIS OF ENERGY CONVERSION SYSTEMS

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ABSTRACT

An investigation was conducted to assess the need for and the feasibility of developing a computer code that could model thermodynamic systems and predict the performance of energy conversion systems. To assess the market need for this code, representatives of a few industrial organizations were contacted, including manufacturers, system and component designers, and research personnel. Researchers and small manufacturers, designers, and installers were very interested in the possibility of using the proposed code. However, large companies were satisfied with the existing codes that they have developed for their own use.

Also, a survey was conducted of available codes that could be used or possibly modified for the desired purpose. The codes were evaluated with respect to a list of desirable features, which was prepared as a result of the survey. A few publicly available codes were found that might be suitable. The development, verification, and maintenance of such a code would require a substantial, ongoing effort.

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SUMMARY

Recent events, including increasing energy efficiency and environmental concerns, have increased the demands on industry to respond quickly to improve their equipment and products. Such a response requires them to evaluate existing alternatives and explore new ones as rapidly as possible. To aid in this effort, we investigated whether or not there is a need for developing a code that could be used to predict the performance of thermodynamic and thermal-hydraulic systems such as heat pumps, refrigerators, and power cycles. For this study, we contacted appropriate representatives of industrial organizations, including system and component designers, manufacturers, and installers of heating and refrigeration equipment. We also contacted various research personnel in national laboratories. As a result of this limited survey, we found that researchers and small manufacturers, designers, and installers, were very interested in using the code, but that large companies were not. Several small companies indicated that many calculations are still done by hand, which is quite slow and tedious. The large companies are primarily satisfied with the codes that they have developed for their own use. These codes are specific to their own product line, and shared with their marketers and installers. However, they would be interested in a code that is better than what they are currently using.

In addition to contacting people in industry, we conducted a survey of available software that could be used in a large code of this type or possibly modified for the purpose. We considered both commercially available codes and codes that were developed by the Department of Energy (DOE) and are essentially free to the public. To evaluate these codes, we developed a list of criteria from our discussions with various software users in industry, research laboratories, and universities. The result is a list of attributes that an "ideal" thermodynamic system modeling code would possess. Among the most important attributes in this list are

- The capability to accurately model thermodynamic systems
- Flexibility

- The capability to be learned and used easily.

The existing codes we surveyed for this work are basically of four types:

- Chemical process simulators
- Computational fluid dynamics codes
- System simulators
- Equation solvers.

The features of each of these codes are discussed in this report.

We evaluated the codes based on the list of desirable attributes, and found a few publicly available codes that could possibly be modified. However, most of these codes lack the flexibility to model a variety of thermodynamic systems and are difficult to use.

As a result of this study, we made the following conclusions:

- Codes that could be used to model any thermodynamic system would be of great value to small industrial companies, including component and system manufacturers, designers, and installers. It would also be useful to researchers and to universities as a research tool.
- The proposed code would be of far less interest to large industrial companies because most already have in-house codes to model their products.
- In our survey of codes available to the public, we found none that meets all the given criteria for modeling thermodynamic systems. Most of these codes are either too specialized or too difficult to use, or both. One code fits the requirements very well, but is only commercially available.

- Several of the publicly available codes we looked at could be modified and used as a basis for this type of code. A more indepth analysis of these codes is needed to determine which would be the most suitable.
- Developing, verifying, and maintaining such a large thermodynamic systems modeling code properly would be a significant endeavor. A collaborative effort between potential users, equipment and system engineers, and programmers would be required to develop a code that is flexible, easy to use, accurate, and well-supported.

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ACRONYMS

ACSL	Advanced Continuous Simulation Language
ASPEN	Advanced System for Process Engineering
ANL	Argonne National Laboratory
COP	coefficient of performance
CFD	computational fluid dynamics
GEMS	General Energy and Material-Balance System
DOE	Department of Energy
GSMP	General System Modeling Program
EPRI	Electric Power Research Institute
HVAC	heating, ventilating, and air conditioning
INEL	Idaho National Engineering Laboratory
IRF	Idaho Research Foundation
LWR	light water reactor
ORNL	Oak Ridge National Laboratory
NESC	National Energy Software Center
NIST	National Institute of Standards and Technology
PHOENICS	Parabolic, Hyperbolic or Elliptic Numerical Integration Code Series
PWR	pressurized water reactor
SALT-ANL	Systems Analysis Language Translator

1. INTRODUCTION

Recent events have forced a re-examination of the processes used by industry in the research, design, and analysis of energy conversion systems. Public concerns such as global warming and ozone depletion, and recent governmental energy efficiency requirements have made it necessary for industry to respond quickly with improved equipment designs and improved thermodynamic system cycles. Rapid and accurate analysis of new components and thermodynamic systems is necessary if industry is to answer these concerns.

To this end, we investigated the need for and the feasibility of developing a code to be used in the design and analysis of thermodynamic and thermal-hydraulic energy conversion systems. This code would be applied to a variety of thermodynamic systems such as heat pumps, refrigerators, and power cycles. Figure 1 shows a diagram of a simple heat pump. Using a computer model, a designer or analyzer could observe the impact of changing system parameters or any of the components. For example, the heat exchanger area of the condenser could be optimized or the effects of using a smaller compressor could be evaluated without physically changing the components. Output from a computer model of the heat pump would need to include parameters such as the following:

- Power to the compressor
- Heat transfer and pressure drop in the condenser and evaporator
- Changes in working fluid-state parameters
- Exergy losses
- System efficiency or coefficient of performance (COP).

To determine the need for a computer code that could handle the heat-pump system described above, as well as any other type of thermodynamic system, we first conducted a limited and informal survey of possible users of such a code. The participants in the survey included energy component and

VAPOR COMPRESSION HEAT PUMP

Figure 1. Heat pump diagram.

system manufacturers, system designers and installers, and researchers in national laboratories and universities.

In addition, we surveyed codes that already exist and might be useful in this type of design work. This evaluation included both commercially available products and those that are publicly available through the DOE National Energy Software Center (NESC) in Argonne, Illinois. Based on discussions with users of various software packages, we compiled a list of desirable characteristics that an ideal code should possess. The potential usefulness of available codes was then judged based on these criteria (see Appendix A for detailed descriptions of the available codes).

2. INDUSTRIAL NEEDS

To determine the need for this type of tool for research and design, we contacted a number of potential users. This informal survey included personnel involved in component and system design and manufacture, system installers, and researchers in national laboratories and universities.

2.1 DESIGNERS AND MANUFACTURERS

Responses to the survey depended primarily on the size of the company. The companies we contacted included heating and air conditioning firms, an appliance manufacturer, and an architecture and engineering (A/E) firm. Most of those we surveyed expressed great interest in the code.

The firms we contacted include Trane, Carrier, Copeland, Command-Aire, Admiral, Johnson Control, and Stone & Webster. Trane is the largest U.S. manufacturer of industrial and commercial heating, ventilating, and air conditioning (HVAC) systems, while Carrier (now owned by United Technologies) is the largest in the residential air-conditioning market. Copeland is a smaller firm that is primarily involved in component design and manufacture. Command-Aire designs and installs mostly water-source heat pump systems. Admiral designs and manufactures household appliances, while Johnson Control mostly is responsible for control systems in commercial and industrial HVAC systems. Stone & Webster is a large A/E firm that builds power plants.

2.1.1 Large Firms

Technical personnel at Trane^a and Carrier^b were only mildly interested in a general thermodynamic system modeling code, stating that they already

a. Private communication with Mick Schwedler, Application Engineer, The Trane Company, June 1990.

b. Private communication with Bruce Bucholz (Director of Advanced Manufacturing and CAE CIM Systems) and Daryl Erbs (Systems Engineer), Carrier Corporation, August 1990.

have proprietary, in-house codes that meet their current needs. Trane has developed their proprietary simulation code TRACE (Trane Air Conditioning Evaluation) for marketing. TRACE is commercially available to contractors, electrical utilities, etc., and it contains many of the features applicable to their in-house product.

Although generally satisfied with their own code, one systems engineer at Carrier stated that the codes could be improved.^a For example, the system modeling codes he uses are not applicable to transient conditions. However, he felt that in order for Carrier to benefit from a DOE code, it would not only need to be a better code, but it would also need to be worth the cost of the time to learn it. He recommended a user-friendly code with a menu-driven interface and graphics.

Personnel at the other large companies we contacted, Johnson Control and Stone & Webster, were also not very interested in a thermodynamic modeling code. A systems engineering manager at Johnson Control told us that his company would probably find little use for this type of code. Johnson Control does some trouble-shooting of existing systems, but does not design new hardware.^b Computer codes are used to model systems at Stone & Webster, but according to a principal engineer in process computer modeling, they are very satisfied with the commercially available codes they are presently using.^c

2.1.2 Small Firms

Small firms were much more interested than the large firms in using a new energy conversion system model. The Vice-President of Residential Products at Command-Aire regarded the codes presently used by his firm as

a. Private communication with Daryl Erbs, Systems Engineer, Carrier Corporation, August, 1990.

b. Private communication with Peter Brothers, Systems Engineer, Johnson Controls Inc., June 1990.

c. Private communication with Bill Murray, Principal Engineer, Process Computer Modeling, Stone & Webster, August 1990.

narrow-based and felt that too much was being done by hand.^a

A design engineer at Admiral also expressed great interest in a system modeling code. Admiral developed their own set of finite difference codes when they were unable to find a single code that would adequately model their refrigerators. The designers use these codes and a few commercial ones to model the individual components of the refrigerators, but they are not able to model entire systems or transients. The design engineer was very interested in a code that could do these tasks, and felt that a good interactive, graphical front-end would be very useful. He was also interested in an economic analyses option.^b

Engineers at Copeland were also interested in the code. Copeland is involved specifically with individual component development, and the company's interest in system design lies primarily in the performance of their components in systems.^c Companies that design components for thermodynamic systems, such as Admiral and Copeland, need a very flexible code in order to examine the ramifications of a new component design on overall system performance.

2.2 RESPONSES FROM INSTALLERS

People who install and maintain equipment that could be modeled by this computer code had opinions similar to those of the manufacturers, depending on their affiliation. Independent distributors and installers and those from small firms expressed interest in a code that would help them size equipment. Those who are directly affiliated with large design and manufacturing companies indicated that they are well supported by their parent companies.

a. Private communication with Clarence Oscarson, Vice President of Residential Products and Ground-Coupled Heat Pumps, Command-Aire, July 1990.

b. Private communication with Ed Rockhold, Senior Advanced Design Engineer, Admiral Corp., August 1990.

c. Private communication with Stan Schumann, Senior Project Engineer of Applied Mechanics, Copeland Corporation, July 1990.

For example, a regional distributor and installer for Trane has sufficient software available to install and service Trane equipment.^a However, an independent system designer and installer in Coeur d'Alene, Idaho, who is currently using very little software to design and size systems, would be very interested in the proposed code.^b

2.3 RESEARCHERS IN NATIONAL LABORATORIES AND UNIVERSITIES

Most of those we contacted at national laboratories and universities were in favor of developing the proposed code. Research personnel at the National Institute of Standards and Technology (NIST),^c in Boulder, Colorado and at Oak Ridge National Laboratory (ORNL)^d expressed great interest in the potential assistance this code could give to ongoing energy conversion work. They agreed that development of such a code would be a substantial effort, and would require a significant ongoing support effort after completion. Those we talked with at universities were interested in the research and teaching assistance that this code could provide.^e One university researcher doubted that such a code could be sufficiently flexible to model the great variety of energy conversion systems that are presently under investigation.^f However, most were excited about the idea.

a. Private communication with Cal Dent, distributor and installer, Trane Company, July 1990.

b. Private communication with Art Fall, Owner, E-Con-Tech, July 1990.

c. Private communication with Mark McLinden, Chemical Engineer, NIST, July 1990.

d. Private communication with Fang Chen, Research Engineer, Oak Ridge National Laboratory, June 1990.

e. Private communication with Dave Drown, Associate Professor of Chemical Engineering, University of Idaho, June 1990; Bob Scaringe, Engineer, Mainstream Engineering and Instructor, Florida Institute of Technology, June 1990; Steven Beyerlein, Assistant Professor of Mechanical Engineering, University of Idaho, June 1990; and Richard T Jacobsen, Director of the Center for Applied Thermodynamic Studies and Dean of Engineering, University of Idaho, July 1990.

f. Private communication with Keith Herold, Assistant Professor of Mechanical Engineering, University of Maryland, June 1990.

3. AVAILABLE COMPUTER CODES FOR ENERGY CONVERSION SYSTEMS

We conducted a limited survey of the codes that are already available for thermodynamic cycle and thermal-hydraulic system modeling. These packages included both commercially and publicly available codes. The latter may be obtained from the National Energy Software Center (NESC) at Argonne National Laboratory (ANL). The following codes were similar to the proposed code but they were not closely related enough to modeling energy conversion systems and thermodynamic cycles to be surveyed:

- Codes that model a single system component, such as a turbine or a heat exchanger
- Codes that determine only building heating and cooling loads
- Codes that model only a single cycle (e.g., a diesel engine)
- Piping network codes
- HVAC design codes.

The codes we examined basically fit into four categories. The first category is chemical processing codes, or process simulators (L. T. Biegler, 1989). These codes contain many of the features that are useful for thermodynamic system modeling and many already perform thermodynamic analyses. It is possible that one of these codes could be modified for energy conversion. This alternative is discussed later in Section 4.2.

The next category is computational fluid dynamics (CFD) codes. These typically use either finite difference or finite-element numerical techniques to solve the constitutive equations. They often have easy to use input structures, and excellent solution techniques. Some features of the CFD codes would be useful in a thermodynamic system model.

The third category consists of system simulators. Many of these codes were written for only one type of system, such as a nuclear power plant or a solar energy system, but most of these may be easily modified for different

thermodynamic components. One commercial code was developed specifically to model thermodynamic systems and another to model any system. It is possible that one of these codes could be used to develop the desired type of thermodynamics modeling code.

The last category is rather distinct. The codes in this category are simply equation solvers, and may be used with any sort of program. The user must write the entire input/output structure and system model to use these solvers. While these codes presently have no thermodynamic system modeling capabilities, they are the more flexible ones.

The four categories of software packages and the individual computer codes examined in each category are discussed below. There are numerous codes available in each category, however, a thorough survey is beyond the scope of this investigation. Those discussed below are representative of the many available codes.

3.1 PROCESS SIMULATORS

3.1.1 ASPEN

The Advanced System for Process Engineering (ASPEN) is a publicly available code that was developed at the Massachusetts Institute of Technology with funding from DOE. Designed for fossil fuel conversion processes, ASPEN can handle chemical compounds, mixtures, multiphase fluids, and even solids. The code's capabilities include calculating steady-state material and energy balances, determining equipment size and cost, and evaluating preliminary economics (NESC, 1986a).

Private companies like Aspen Technology and JSD Simulation Service have further developed the code and have produced the commercial versions, ASPEN PLUS and ASPEN/SP, respectively. These companies have made various improvements to the code including the creation of a version for personal computers that makes it easier to use. Although not designed primarily for

thermodynamic system modeling, ASPEN and its commercial versions are capable of and have been used very successfully for this purpose. For example, one of the earliest applications of ASPEN was a thermodynamic analysis of an energy recovery system (Fish et al., 1982) at the Idaho National Engineering Laboratory (INEL). Engineers at the INEL used ASPEN to perform a preliminary analysis of a low-temperature binary Rankine cycle that would recover energy discarded during the operation of the Advanced Test Reactor. After using ASPEN, engineers concluded that ASPEN is a useful tool for this type of analysis.^a

3.1.2 ChemShare

One of the leading commercial sources of process simulation codes is the ChemShare Corporation. ChemShare produces three codes to model fossil energy conversion processes: DESIGN/2000, REFINE, and CHEMTRAN. DESIGN/2000 is a flow-sheet simulator that contains almost all standard unit operations. REFINE is a specialized subroutine designed for crude-oil distillation and CHEMTRAN is a multipurpose code that supplies physical property data.

ChemShare is easy to learn and use. Because input preparation is designed to be logical and is entirely in free-form English, the user is not required to have programming knowledge to begin using the code (Matulsky, 1982).

3.1.3 PROCESS and PRO/II

PROCESS is another excellent, commercially available process simulation code. PROCESS was developed by Simulation Sciences Inc. and calculates steady-state mass and energy balances in chemical, petroleum, and synfuels process plants. Because of the flexibility of the code, the user may add subroutines for components that are not included (or not adequately modeled) and fluid property subroutines. A few of the strong points of the code include

a. Private communication with Larry W. Fish, EG&G Idaho, Inc., July 1990.

- An extensive thermodynamic property package
- Gas, liquid, and solid modeling
- Numerous calculational blocks
- The ability to perform sensitivity analyses
- Optimization capabilities
- The ability to perform exergy analyses
- An option for equipment sizing and cost analysis.

Although the code was designed specifically for the petroleum industry, thermodynamic systems can also be modeled (Brannock et al., 1982). Recently, Simulation Sciences purchased one of the commercial versions of ASPEN-- ASPEN/SP. The company is currently working on combining PROCESS with ASPEN/SP. The resulting code is titled PRO/II, and Simulation Sciences is already supplying the first versions to its customers.^a

3.1.4 GEMS

The General Energy and Material-Balance System (GEMS) is a process simulator developed at the University of Idaho for the pulp and paper industry. As with ASPEN and PROCESS, the user can model fluids and solids with GEMS. The University of Idaho has also recently developed a version of GEMS for the food processing industry (Petersen and Drown, 1985).

GEMS does not have the capability to model thermodynamic systems and cannot be practically modified for this purpose. The code contains very limited thermodynamic property data and, more importantly, it is very inflexible. Only limited thermodynamic properties are included in the two versions because the need for thermodynamic properties in the pulp and paper industry is minimal and the food processing version of the code is relatively new. GEMS is inflexible because the code is supplied only in compiled form to the user. The Idaho Research Foundation (IRF), which markets GEMS, will license the code, provide listings of the specific equipment model source

a. Private communication with Lucien Jones, Simulation Sciences, Inc., June 1990.

code, help the user add subroutines, but at a cost. This operation is not practical and IRF does not recommend it.^a

3.2 COMPUTATIONAL FLUID DYNAMICS CODES

The number of publicly available fluid dynamics codes is relatively high. These codes are a direct result of DOE involvement in the nuclear power industry and the resulting need for accurate prediction methods for reactor cooling systems, among others. The three public codes discussed, TAP-LOOP, SOLA-LOOP, and COMMIX-1B, were developed specifically to analyze thermal-hydraulic processes in a nuclear reactor, but may be used for other applications involving heat transfer and fluid flow. These codes provide solutions to transient thermal-hydraulic problems by solving the governing momentum, continuity, and energy equations with variations of the finite-difference method.

The commercial computational fluid dynamics (CFD) codes, FLUENT and PHOENICS, are two of the more popular and more powerful codes available. Many other CFD codes are sold commercially, but FLUENT and PHOENICS are the most popular of this type of code.

3.2.1 TAP-LOOP

TAP-LOOP was created in the late 1960's from an older code, TAP, which was developed under the sponsorship of the Atomic Energy Commission (Leach and Kelley, 1970). The code was produced by Battelle Pacific Northwest Laboratories to perform scoping and conceptual design analyses in the Fast Flux Test Facility. TAP-LOOP was designed specifically for analyzing recirculating fluid loops and the associated heat transfer, but can handle a number of other problems, including studies of potential fluid flow,

a. Private communication with Louis Edwards, Professor of Chemical Engineering, IRF, University of Idaho, June 1990.

electrical networks, and stress analysis. There are no fluid property routines included; all properties must be supplied by the user (NESC, 1990).

3.2.2 SOLA-LOOP

SOLA-LOOP was developed at Los Alamos National Laboratory for nuclear reactor safety analysis. It models one-dimensional, two-phase flow in networks of one-dimensional components. Network systems of this type often contain low-speed flow with slowly varying properties in one region, and high-speed flow with rapidly varying properties in another region. To improve the calculation of properties in this type of system, the code has provisions for different time-steps inside the components (NESC, 1986b). SOLA-LOOP was designed for nuclear reactors, but can be used for other types of network analysis. The code can be used for almost any set of constitutive relations, property table, or other feature that may be required for different applications.

3.2.3 COMMIX-1B

COMMIX-1B was developed at ANL (ANL, 1985) for single-phase, three-dimensional analysis of compressible or incompressible fluid flow in a single-component or multicomponent system. Some important features of the code are

- A new formulation for modeling an anisotropic flow domain with stationary structures
- A special package for modeling any complex geometry in the most storage efficient way using either a Cartesian or a cylindrical coordinate system
- A generalized resistance model to allow for the resistance due to internal structures
- A generalized thermal structure formulation for modeling thermal interactions between structures and the surrounding fluid
- A semi-implicit solution procedure for fast transient analysis, as well as a fully implicit procedure for normal and slow transients and the ability to switch from one to another during simulation

- Four turbulence model options
- Built-in sodium and water properties with an option permitting the use of simplified property correlations for almost any fluid.

COMMIX-1B uses a proprietary cubic-spline, data-smoothing subroutine that is not included in the code. This subroutine (the International Mathematical and Statistical Library subroutine, ICSSCU) or a suitable alternative must be supplied to use the code (NESC, 1988).

3.2.4 FLUENT

FLUENT is a commercial CFD code from Create.x. The following features make FLUENT more user friendly and marketable than publicly available codes:

- An interactive and menu driven interface to set up the problem and perform computation
- 3-D color graphics
- The ability to interface with CAD/CAE software.

Features of the code that are particular to fluids problems include the ability to model

- Steady and transient flow
- Laminar and turbulent flow
- Internal and external flows
- Flows with a dispersed second phase (particles, droplets, or bubbles)
- Non-Newtonian flow
- Heat transfer
- Chemical reactions.

In addition, FLUENT can determine local and overall heat transfer coefficients and pressure losses through heat exchangers and other flow passages, and provide the detailed velocity field, pressures, temperatures, and other flow variables needed.

Creare.x also supplies the complete source code so the user can incorporate specialized subroutines. The company also provides training classes and extensive user support by telephone, documentation, quality assurance, user group meetings, and newsletters.

3.2.5 PHOENICS

CHAM of North America, Inc. has developed the Parabolic, Hyperbolic or Elliptic Numerical Integration Code Series (PHOENICS), a fluid dynamics code. User-friendly features of this code include

- A menu-driven, graphical interface to set up the problem and display it as it is defined
- The ability to use a cartesian, cylindrical, spherical, or curvilinear coordinate system
- An easy-to-use format that eliminates the need for extensive knowledge of fluid dynamics
- The ability to interface with other CAD/CAM programs.

The modeling capabilities of the PHOENICS code are very similar to those of FLUENT and include the following:

- Steady and transient flow
- Laminar and turbulent flow (with five alternative turbulence models)
- One-, two-, and three-dimensional flow
- Chemically reacting flow
- Heat transfer
- Two-phase flow
- Swirling flow
- Non-Newtonian fluid
- Subsonic, transonic, and supersonic flow
- Compressible and incompressible flow
- Viscous and inviscid fluid.

In addition, the user can write and add subroutines for special applications or have a CHAM consulting team build the models. The solvers used by the code can also be modified or replaced. CHAM holds training courses for PHOENICS users and offers full services for installation, updates, enhancements, and general user support, as well as conferences and publications.

CHAM has recently developed a new CFD code based on PHOENICS and designed specifically for 386-equipped personal computers. The code, EasyFlow, has the computational capabilities of codes designed for larger, more powerful processors, but is available on a PC.

3.3 SYSTEM SIMULATORS

All of the system simulation codes we reviewed model some type of thermodynamic or thermal-hydraulic system. Some of the codes, such as ATHENA, are designed for very specific applications, while others, like SimTool, are capable of modeling a number of different systems.

3.3.1 ATHENA

The Advanced Thermal Hydraulic Energy Network Analyzer (ATHENA) was developed at INEL to analyze a light water reactor (LWR). ATHENA is the result of previous work performed at INEL on the thermal-hydraulic code, RELAP5. RELAP5 simulates nonequilibrium conditions encountered in a pressurized water reactor (PWR) under normal or accident conditions. ATHENA is an extension of this project and the methods developed in the project for analyzing LWRs can be extended through ATHENA to any thermal-hydraulic system or component. The primary improvement of ATHENA over RELAP5 is that not only steam, but any two-phase, two-component working fluid can be used in the simulation. Modules developed for the code include hydrodynamic systems and components, heat structures, and control components. An experienced user may easily add new component models and modify existing ones.

The main difficulty with using ATHENA is its complexity. Extensive experience is required to become an expert user of the code and developing a system model can take a great deal of time. In addition, assembling the data necessary for describing a system and analyzing the output can be very complicated and time consuming (Ransom, 1986). The difficulties involved in using the code are great enough that ATHENA developers seriously considered developing an expert system to aid the user. This development has not been pursued, however, because of a lack of funding.^a

3.3.2 SALT-ANL

The Systems Analysis Language Translator (SALT-ANL) is a systems-analysis and process-simulation code developed at ANL (Geyer and Berry, 1985a). SALT-ANL will model steady-state and dynamic systems and has been used for various thermodynamic and power-producing systems. The code contains 34 precompiled modules, several flow types, and a number of thermodynamic and transport property routines (NESC, 1987). Although the code has been used primarily for process simulation, it is very flexible and can be used for other applications, including pure economics, electrical circuits, and transportation. SALT-ANL can also be used for optimization and sensitivity studies, which are valuable capabilities.

ANL has published a programmer's guide that provides the information needed to modify the SALT-ANL code (Geyer and Berry, 1985b). New models or property routines can be added to allow different systems to be modeled. The code is written in PL/I, but subroutines can be written in either PL/I or FORTRAN.

3.3.3 SOLTES 1

The Simulator of Large Thermal Energy Systems (SOLTES 1) was developed at Sandia National Laboratory to model the steady-state response of thermal energy systems to time-varying data such as weather and thermal loads (Fewell

a. Private communication with Kenneth Carlson, EG&G Idaho, Inc., June 1990.

and Grandjean, 1980). The code has a modular construction, with a library of routines that model components such as solar collectors, pumps, switches, and heat exchangers. The user can also add subroutines to the library, if necessary. These modules can be combined to model a number of simple and complex thermal energy systems, including Rankine power-generation systems. The code contains a preprocessor to help the user construct and edit system models.

Some systems that have been analyzed using SOLTES 1 include the following:

- Solar power
- Fossil-fired power plants
- Nuclear-fired power plants
- Solar energy heating and cooling
- Geothermal energy
- Solar heater water.

The code contains hourly weather data on typical meteorological years for 26 U.S. locations, or the user can supply weather data with any time increment. A quasi-transient method predicts the response of the system to time-varying data with steady-state calculations at successive time intervals (NESC, 1981).

3.3.4 TRNSYS

TRNSYS was designed at the University of Wisconsin-Madison for evaluating the transient behavior of various solar heating and cooling systems. To solve for the transient behavior, the user specifies time steps, and the code solves time-dependent differential equations and carries out any necessary numerical integration. TRNSYS is also capable of performing optimization and economic calculations.

Although designed initially for solar energy and HVAC systems, TRNSYS is now used for a number of other applications. These expanded capabilities are

possible because of the modular structure of the code and the ease with which the user may add new subroutines. This modular structure allows the user to connect individual components such as heat exchangers and pumps together by linking the output of one to the input of another.

3.3.5 MMS

The Modular Modeling System (MMS) is a commercial code marketed by Babcock & Wilcox and designed to analyze conventional and nuclear plant operations. The systems are built from separate modules contained in the component library. The library contains over 120 modules that represent most components used in pressurized- and boiling-water reactors.

MMS is designed for applications of plant analysis that do not require codes as complex as large thermal-hydraulics codes like RELAP5, discussed earlier. Developed under the sponsorship of the Electric Power Research Institute (EPRI), MMS uses the Advanced Continuous Simulation Language (ACSL), a FORTRAN based simulation language, for studying dynamic systems. ACSL is discussed further in Section 3.4.

Babcock & Wilcox has also organized a user support group. The B&W/MMS User's Group supports the code by providing a means for exchange of information, direction for future improvements, maintenance of the code, training for new users, and consultation for all users.

3.3.6 SimTool

SimTool, from Mainstream Engineering Corporation, is a commercially available, system simulation code designed specifically for advanced thermal systems (Buckman et al., 1990). SimTool will model both steady-state conditions and transients with user-specified time steps. The user can model fluids a number of different ways from ideal gas to multi-component, two-phase mixtures. Several models are available for modeling multi-component mixtures, and chemical reaction is allowed within specified components.

SimTool is considered a user-friendly, fluid-thermal systems simulation code. The many different component and device models contained in the library will model most thermodynamic systems, but user-defined models, property routines, and user-controls may be added without much difficulty. These subroutines can be added in FORTRAN or C, and the system model input file is in an English-like format.

3.4 EQUATION SOLVERS

The Advanced Continuous Simulation Language (ACSL) and the General System Modeling Program (GSMP) do not fit into the categories of computer codes already discussed. Both are designed to be used as a basis in developing system and process modeling codes, and are probably best classified as equation solvers.

3.4.1 ACSL

ACSL is a commercial FORTRAN-based simulation language available through Mitchell & Gauthier Associates. It is designed to help the user study dynamic systems without detailed programming knowledge. With ACSL, the user can model continuous systems described by time-dependent, nonlinear differential equations or transfer functions. Applications of ACSL have been very diverse. Some of the present applications include

- Power plants
- Nuclear reactors
- Chemical processing plants
- Instruments and computers
- Petroleum industry
- Robotics
- Biology and physiology.

ACSL uses a command-driven environment that permits the user to change input parameters while the code runs. Other features that make ACSL

attractive include graphics capabilities and the availability of optimizing software.

Dow Chemical has used ACSL to develop their own code [Dow Advanced Continuous Simulation Language (DACSL)] for analyzing the dynamic behavior of chemical processes (Agin and Blau, 1982). It was designed to be more user-friendly than ACSL and has the ability to estimate parameters from experimental data. From this research, Dow has also developed the code SIMUSOLV. SIMUSOLV has been used to study the kinetic behavior of chemical reactions, pharmacological systems, ecosystems, and engineering processes.

3.4.2 GSMP

GSMP was developed at ANL primarily for systems analysis teams to model advanced energy conversion systems (Cook, 1979). The code is basically an equation solver and an optimizer, and is designed to be versatile enough to model "any object satisfying the most general definition of the word 'system'" (NESC-882, 1982). Component models and fluid properties for specific applications are not included in the code and must be supplied by the user. GSMP users may write subroutines in PL/I, FORTRAN, COBOL, or OS Assembler Language. The code itself is written mostly in PL/I (90%), with some FORTRAN IV (9%) and assembly language (1%), and programming experience is necessary to add a component model into the interface.

4. JUDGMENT CRITERIA AND CODE EVALUATION

4.1 DESIRABLE CHARACTERISTICS OF SYSTEM MODELING CODES

To judge the available codes, we established appropriate judgment criteria. We compiled a list of desirable characteristics from those we contacted in industry and research laboratories. We added other requirements to the list because of their relevance to this particular project. For example, a code that is only available commercially is automatically disqualified. However, the desirable attributes of the commercial codes included in this study were added to the list of criteria. The basic criteria, desirable characteristics, and requirements used to judge available codes are as follows:

- Public availability through NESC or another government agency is required.
- Flexibility is necessary. The code should be easily adaptable to a particular application.
- The system should be user-friendly, especially in problem set-up, troubleshooting, and interpretation of the output.
- Steady-state and transient analyses should be possible.
- Accurate thermophysical properties for many working fluids should be available.
- The code should be well-validated to ensure its accuracy in system predictions.
- A support system for maintenance of the code and user assistance is necessary.
- The code should run on many different computer systems.
- Required software should be commonly available (possibly FORTRAN 77).

These are the most important requirements that must be considered to develop the type of thermodynamics system modeling code discussed here. Other useful characteristics would include the ability to do economic evaluations,

optimizations, unit conversion, graphical output, and controls.

4.2 EVALUATION OF AVAILABLE CODES

Bases on our discussions with personnel at industrial companies, national laboratories, and universities, we determined that the four most important requirements of a useful thermodynamic system modeling package are public availability, flexibility to model a variety of systems, the capability to be learned quickly and easily used, and good customer support.

4.2.1 Public Availability

Only a few of the codes in each category of software are publicly available. Publicly available codes are as follows:

- Process Simulators-- ASPEN
- CFD Codes-- SOLA-LOOP, TAP-LOOP, and COMMIX-1B
- System Simulators-- RELAP5, SOLTES 1, and SALT-ANL
- Solvers-- GSMP.

4.2.2 Flexibility

Of the eight public codes, only a few are flexible enough to be modified easily for different systems and new components. ASPEN, the only public process simulator, already contains many thermodynamic system component models. However, it also has a great deal of other capabilities that would be useless in software intended solely for thermodynamic systems. To use ASPEN in this type of code, subroutines extraneous to a thermodynamic system modeling code would need to be removed and the thermodynamic system modeling capabilities would need to be increased. Although this is possible, there are other options that appear more promising.

The CFD codes are designed to analyze fluid flow, not system performance. It would be very difficult or impossible to modify one of these

for modeling generalized systems. However, the accomplishments that have been made in fluid dynamics calculations could be very useful to the thermal-hydraulic aspect of the code and should be used if possible.

The system simulators ATHENA, SOLTES 1, and SALT-ANL may also be useful for developing a thermodynamic system model. ATHENA is a very precise code that was developed primarily to simulate accidents in nuclear reactors and solves the basic time-dependent fluid and heat transfer equations. Like ASPEN, this code could be modified for thermodynamic systems. However, ATHENA is a very large and powerful code that was designed for a specific application, and modifying it would be even more difficult than modifying ASPEN. SOLTES 1 was developed for solar energy systems and can also be modified for use in modeling other types of systems, again with some difficulty. Of the system simulators, SALT-ANL shows the most flexibility and the greatest promise for use in this project. SALT-ANL has a structure that could be modified for almost any thermodynamic or thermal-hydraulic system.

GSMP is the most flexible of the public codes. The user can model any desired system by supplying the code with compiled subroutines that define the system and instructions to connect the subroutines. While the superstructure of a general thermodynamic system modeling code that would use the GSMP solver would require a large effort to develop, this option is very promising.

After considering the flexibility of the public codes, five codes in three categories remain as possible starting points for a system modeling code:

- Process Simulators-- ASPEN
- System Simulators-- ATHENA or RELAP5, SOLTES 1, and SALT-ANL
- Solvers-- GSMP.

4.2.3 Ability to be Learned and Used Easily

Making a large, powerful code user-friendly can be a very difficult task for a developer. Often, the more powerful a code is, the more time a user

must spend learning to use it. While commercial software companies invest a great deal to make their codes user-friendly, public code developers are not concerned marketability and consequently, the codes tend to be more difficult to learn and use. For this reason, none of the five public codes listed above are particularly easy to use, and we have not eliminated any of these from the list based on their usability. From discussions with possible users of the type of code being considered (see Section 2), it is apparent that for the code to be widely used by industry, it must be made user-friendly. Engineers at Carrier and Admiral suggested using an interactive, menu-driven front-end with graphics as one way of increasing the usability of and interest in the code.

4.2.4 Customer Support

Lack of user support is often a problem with public codes. In many cases, funding for the projects that develop the codes is terminated, and it becomes difficult not only to learn to use a particular code, but even to locate the individuals who initially developed it. Again, while we are unable to remove any of the codes from the list because of this criterion, it is important to recognize the role of customer support in developing a useful and productive code.

5. CONCLUSION

SALT-ANL and GSMP appear to be the most promising candidates for forming the basis for a large thermodynamic system modeling code. Both were developed with DOE funding and are available for further public or private development. Both codes are also very flexible.

At present, the large companies are basically satisfied with the code they have developed for modeling their particular components and systems. However, if a modeling code were sufficiently powerful, easy to learn and use, and had proper customer support, large companies might also become interested. Small industrial companies and the majority of those involved in basic research expressed interest in using the code to model thermodynamic systems and believe it would be a very useful tool. Development of such a code would, of course, be a substantial effort requiring collaboration between potential users, programmers, and researchers. This effort should also include ongoing support for code validation, maintenance, and upgrades. With that type of commitment, such a code would be quite useful to the industrial and research communities.

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APPENDIX A
CODE DESCRIPTIONS

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Table 1. ACSL description

ADDRESS	Mitchell & Gauthier Associates (MGA, INC) 73 Junction Square Drive Concord, MA 01742
PHONE FAX	(508) 369-5115 (508) 369-0013
PRICE	\$2300 for one PC copy Mainframe and workstation versions are \$5,000- \$40,000/yr
AVAILABILITY	Commercial
TRANSIENT OR STEADY STATE ANALYSIS	Transient--solves the systems of nonlinear ordinary differential equations with known initial conditions
BASIC UNIT	N/A--program is an equation solver
SYSTEMS MODELED	Designed to model a system described by time- dependent non-linear differential equations or transfer functions. Primarily designed for control systems
HARDWARE/SOFTWARE REQUIREMENTS	IBM PC or compatible 512K of main memory DOS 2.0 or higher or OS2 Microsoft or Ryan-McFarland FORTRAN
FLUIDS	N/A
HOW CONTROLS ARE SPECIFIED	Controls are described as part of the system of equations A command driven environment permits the user to change values of model data while the program runs
OUTPUT	User-specified Graphics capabilities are included
OTHER COMMENTS	ACSL is a FORTRAN based simulation language designed to help the user study dynamic systems without detailed programming knowledge. Optimizing software is available. Dow Chemical has developed a more user-friendly version which estimates model parameters from experimental data--DACSL (Dow Advanced Continuous Simulation Language)

Table 2. ASPEN description

ADDRESS	Available through NESC Argonne National Lab 9700 South Cass Ave. Argonne, IL 60439	Author R.A. Bajura METC Process Technology and Engineering Branch P.O. Box 880 Morgantown, WV 26507-0880
PHONE	(312) 972-7250 (FTS) 972-7250	(FTS) 923-4764
PRICE	\$2400	
AVAILABILITY	Public	
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state only	
BASIC UNIT	Components	
	Information streams which connect components and material streams representing the flow of matter throughout the process must also be defined.	
SYSTEMS MODELED	Chemical processes, thermal systems	
	May include user-written components	
HARDWARE/SOFTWARE REQUIREMENTS	IBM mainframe or VAX	
	FORTRAN	
FLUIDS	Over 700 pure fluids available	
	Can also operate with multiphase streams (including solids) and mixtures	
HOW CONTROLS ARE SPECIFIED	N/A--Model is only for steady-state	
OUTPUT	Includes a "system report writer" for user to produce reports from the output file	
OTHER COMMENTS	Original version of ASPEN--developed by MIT for DoE	
	Includes economic calculation capabilities	

Table 3. ASPEN/SP description

ADDRESS	JSD Simulation Service Company 6000 East Evans Avenue Building 1 Denver, CO 80222
PHONE FAX	(303) 758-6862
PRICE	\$15,000
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE ANALYSIS	Steady state only
BASIC UNIT	Components Information streams which connect components and material streams which represent the flow of matter throughout the process must also be defined.
SYSTEMS MODELED	Chemical processes, thermal systems May include user-written components
HARDWARE/SOFTWARE REQUIREMENTS	IBM mainframe, IBM compatible PC with OS or 4MB extended memory, VAX, or UNIVAC FORTRAN
FLUIDS	Over 700 pure fluids available Can also operate with multi-phase streams (including solids) and mixtures User can alter the method of property calculations. Different equations or data banks may be used.
HOW CONTROLS ARE SPECIFIED	N/A--Model is only for steady state
OUTPUT	User-specified
OTHER COMMENTS	Does economic calculations Has optimization capabilities Can be used to model fluids and solids ASPEN/SP has been bought by Simulated Sciences, Inc. They are incorporating it into their PRO2 code, and plan to convert their customers to PRO2 and discontinue selling ASPEN by late December, 1990.

Table 4. ATHENA description

ADDRESS	Kenneth E. Carlson Mail Stop 2404 EG&G Idaho Inc. P.O. Box 1625 Idaho Falls, ID 83415
PHONE	(208) 526-9361 (FTS) 583-9361
PRICE	N/A
AVAILABILITY	Public domain
TRANSIENT OR STEADY STATE ANALYSIS	Transient--solves the governing time-dependent equations.
BASIC UNIT	Fluid volume (or loop) Connecting components are "heat structures" or "controls".
SYSTEMS MODELED	Any thermal/hydraulic system Program was specifically developed for light water nuclear reactors.
HARDWARE/SOFTWARE REQUIREMENTS	Presently requires a mainframe, but versions for workstations are in progress. FORTRAN 77
FLUIDS	liquid metals cryogenics water a few refrigerants
HOW CONTROLS ARE SPECIFIED	controllers are system components
OUTPUT	Specified by user
OTHER COMMENTS	Model presently includes heat pipe heat transfer, boiling heat transfer, reactor kinetics, and magnetic effects (MHD). Fluid model is one-dimensional.

Table 5. ChemShare description

ADDRESS	ChemShare Corp. Houston, Texas
PHONE FAX	(713) 627-8945
PRICE	
AVAILABILITY	Commercial codes
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state
BASIC UNIT	Components
SYSTEMS MODELED	Gas processing and transmission
	Crude-oil refining
	Chemical and petrochemical production and purification
	Coal-conversion processes
HARDWARE/SOFTWARE REQUIREMENTS	
FLUIDS	Includes over 900 organic and inorganic compounds
	Can include up to 20 components in a mixture
HOW CONTROLS ARE SPECIFIED	
OUTPUT	User-specified
OTHER COMMENTS	No programming language knowledge is necessary-- input files are free-form English
	There are three ChemShare programs designed for specific needs--DESIGN/2000, REFINE, and ChemTran.
	User can supply properties if not in database. Contains a Physical Properties Generator which can estimate properties if full property data are unknown.

Table 6. COMMIX-1B description

ADDRESS	Available through NESC Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439	Author W.T. Sha Components Tech. Div. Argonne Natl. Lab.
PHONE	(312) 972-7250 (FTS) 972-7250	
PRICE	\$310	
AVAILABILITY	Public	
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state, or	
	Transient--uses a finite difference method to solve the conservation and transport equations	
BASIC UNIT	Component	
SYSTEMS MODELED	Designed for nuclear reactor systems, but can be applied to non-nuclear systems requiring heat transfer and/or fluid flow analysis	
	Performs single-phase, 3-d analysis of fluid flow with heat transfer	
HARDWARE/SOFTWARE REQUIREMENTS	IBM3033 mainframe with MVS/SP1 operating system, or IBM4331 with VM/CMS operating system	
	Written in FORTRAN-77	
	Also uses the proprietary IMSL cubic spline data smoothing subroutine ICSSCU	
FLUIDS	Can be used for any fluid through the simplified property correlations	
	Detailed sodium and water properties are included	
HOW CONTROLS ARE SPECIFIED	Not given	
OUTPUT	Not given	
OTHER COMMENTS	Performs a 3-d analysis (for single-phase fluids only)	
	Can require a large amount of computer time	
	Includes turbulence models	
	Can be used to analyze fast transients	

Table 7. FLOWTRAN description

ADDRESS	Monsanto Co. St. Louis, Missouri
PHONE FAX	
PRICE	
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state only
BASIC UNIT	Components
SYSTEMS MODELED	Process simulator
	Can be used to model nearly all steady-state vapor-liquid and liquid-liquid processes
HARDWARE/SOFTWARE REQUIREMENTS	
FLUIDS	Hydrocarbons and petrochemicals, among others
HOW CONTROLS ARE SPECIFIED	
OUTPUT	User-specified
OTHER COMMENTS	FLOWTRAN was licensed by MIT as the basis for ASPEN.
	Includes economic analysis

Table 8. FLUENT description

ADDRESS	create.x Etna Road P.O. Box 71 Hanover, New Hampshire 03755
PHONE	(603) 643-3800 (800) 521-0282
FAX	(603) 643-4657
PRICE	
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE ANALYSIS	Steady state and transient
	Solves the governing Navier-Stokes equations
BASIC UNIT	Fluid volume
SYSTEMS MODELED	Fluid systems
	Can include user-written subroutines
HARDWARE/SOFTWARE REQUIREMENTS	IBM AT (or compatible), workstation, or supercomputer
FLUIDS	
HOW CONTROLS ARE SPECIFIED	
OUTPUT	
OTHER COMMENTS	User needs a sound knowledge of fluid dynamics.
	Can be interfaced with CAD/CAE software
	Can model heat transfer and chemical reactions
	Can model laminar and turbulent flow
	Updates are free and occur about once a year.

Table 9. GEMS and PCGEMS description

ADDRESS	Idaho Research Foundation University of Idaho Moscow, ID 83843 ATTN: FOOD GEMS/PC
PHONE FAX	(208) 885-6793 (208) 885-7462
PRICE	\$7500 for first copy price is less for subsequent copies
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state only
BASIC UNIT	Component
SYSTEMS MODELED	Process simulator
	Designed for food processing and pulp/paper applications
HARDWARE/SOFTWARE REQUIREMENTS	IBM-PC or compatible with 640K RAM, 8087 Math coprocessor, and 1-1.2M disk drive or a 360K floppy and a hard disk
	MS-DOS 2.0 or higher, and an editor or a word processor
FLUIDS	Includes physical properties for steam, air, fluegas, and food
HOW CONTROLS ARE SPECIFIED	A "Key Trap Update" is available to allow the user to change parameters as the program runs
OUTPUT	User-specified
	May be linked with Lotus 1-2-3 or AUTOCAD
OTHER COMMENTS	Extra options include: \$ 495 - input file builder \$ 385 - BASIC Report Writer \$ 495 - Key Trap Update \$ 500 - GEMSCR to build a spread- sheet of input and output \$1500 - link with AUTOCAD \$3500 - optimizer
	Can be used to model fluids and solids
	A demo disk and manual are available.

Table 10. GSMP description

ADDRESS	Available through NESC Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439	Author J.M. Cook Computing Services Div. Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439
PHONE	(312) 972-7250 (FTS) 972-7250	
PRICE	\$1100 through NESC	
AVAILABILITY	Public code	
TRANSIENT OR STEADY STATE ANALYSIS	Steady state, or	
	Cyclic time-dependence	
BASIC UNIT	Components	
SYSTEMS MODELED	Though developed primarily for the modeling of advanced energy conversion systems, it is designed to model any "system".	
	Program is basically a solver and an optimizer	
	Subroutines for specific applications are not included--user must supply component subroutines	
HARDWARE/SOFTWARE REQUIREMENTS	IBM 370 mainframe	
	Can use PL/1, FORTRAN, COBOL, or OS assembler for user-written subroutines	
FLUIDS	User must supply fluid properties	
HOW CONTROLS ARE SPECIFIED	User-specified	
OUTPUT	User-specified	
OTHER COMMENTS	Programmed in PL/1 (90%), FORTRAN IV (9%), and assembly language (1%), and executed in OS/370.	
	Programming experience is needed to insert a component model into the interface.	

Table 11. MMS description

ADDRESS	P.S. Bartells Babcock & Wilcox 3315 Old Forest Road P.O. Box 10935 Lynchburg, VA 24506-0935
PHONE FAX	
PRICE	
AVAILABILITY	Both a public and a commercial version are available
TRANSIENT OR STEADY STATE ANALYSIS	Transient
BASIC UNIT	Component
SYSTEMS MODELED	Designed for nuclear power reactors (BWRs and PWRs), but modules may be used for other systems
	Not designed to add user-written subroutines
HARDWARE/SOFTWARE REQUIREMENTS	IBM or CDC mainframe DEC-VAX or HP 9000 minicomputer IBM or compatible PC
	ACSL (Advanced Continuous Simulation Language)
	FORTTRAN
FLUIDS	Steam--single-phase and two-phase
HOW CONTROLS ARE SPECIFIED	Part of input
OUTPUT	Specified by user
OTHER COMMENTS	MMS is basically an application of ACSL (Advanced Continuous Simulation Language)
	Designed to analyze power plant operations which do not require codes as complex as Trac, Relap, or Retran
	Program has been extensively tested and validated

Table 12. NPA with RELAP5 description

ADDRESS	Ron Beelman Mail Stop 2403 EG&G Idaho, Inc. P.O. Box 1625 Idaho Falls, ID 83415
PHONE	(208) 526-9703 (FTS) 583-9703
PRICE	N/A
AVAILABILITY	Public domain (RELAP5 is also available from NESC)
TRANSIENT OR STEADY STATE ANALYSIS	Transient analysis with variable time steps
BASIC UNIT	Fluid volume (or loop)
SYSTEMS MODELED	Designed for nuclear power plant systems
HARDWARE/SOFTWARE REQUIREMENTS	Presently requires a DEC or IBM workstation, or VAX, or CRAY mainframe
	FORTRAN
FLUIDS	liquid metals
	cryogenics
	water
HOW CONTROLS ARE SPECIFIED	Controllers are system components.
OUTPUT	Specified by the user
OTHER COMMENTS	NPA is the graphical interface to the RELAP5 code.
	NPA assists in construction of the system description and in the actual analysis.

Table 13. PHOENICS description

ADDRESS	CHAM of North America 1525-A Spardman Drive Huntsville, Alabama 35816
PHONE FAX	(205) 830-2620 (205) 830-2628
PRICE	Licenses are available on an annual or perpetual basis and fees vary according to the code capabilities required and user's computer system.
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE ANALYSIS	Steady state, and
	Transient--solves the governing Navier-Stokes equations
BASIC UNIT	Fluid volume
SYSTEMS MODELED	Fluid systems
	Can include user-written subroutines
HARDWARE/SOFTWARE REQUIREMENTS	Designed to operate on a wide range of computers, from an IBM AT to a supercomputer
	At least 1.0 MB of main memory, 10 MB disk storage, and 5-10 MB disk storage for each user
	FORTRAN-77 compiler and link editor
FLUIDS	
HOW CONTROLS ARE SPECIFIED	
OUTPUT	User-specified--can solve for up to 50 dependent variables
OTHER COMMENTS	General knowledge of fluid dynamics is helpful, but not essential.
	Can use PATRAN or Supertab interfaces to set up the geometry for a problem
	Can model heat transfer and chemical reactions
	Can model laminar and turbulent flow, and compressible and incompressible fluids
	A new version, EasyFlow, has been designed specifically for 80386-equipped PCs and has greater capabilities than the previous PC version.

Table 14. PRO2 description

ADDRESS	Simulation Sciences, Inc. 1051 W. Bastanchury Fullerton, CA 92633
PHONE	(714) 879-9180
FAX	(800) 854-3198
PRICE	Lease--preferably for 3 years \$2000/month for one copy
AVAILABILITY	
TRANSIENT OR STEADY STATE ANALYSIS	
BASIC UNIT	
SYSTEMS MODELED	Process simulator
HARDWARE/SOFTWARE REQUIREMENTS	
FLUIDS	
HOW CONTROLS ARE SPECIFIED	
OUTPUT	
OTHER COMMENTS	Simulated Sciences recently bought ASPEN/SP and assimilated the code into PRO2
	They expect most of their customers to convert to PRO2 by late December, 1990

Table 15. PROCESS description

ADDRESS	Simulation Sciences, Inc. 1051 W. Bastanchury Fullerton, CA 92633
PHONE	(713) 683-1710 (800) 854-3198
PRICE	Lease \$2000/mo
AVAILABILITY	Commercial code
TRANSIENT OR STEADY STATE	Steady-state
BASIC UNIT	Modular
SYSTEMS MODELED	Designed for chemical, petroleum, refining and synfuels process plants
	Contains over 1000 components in its library
	Can include user-written component subroutines
HARDWARE/SOFTWARE REQUIREMENTS	Written in FORTRAN IV
	There is a PC version
FLUIDS	Over 1300 organic and inorganic compounds
	User may add, delete, or modify any of the fluid property data provided, and a private databank may be used.
	Contains the world's largest thermodynamics property package
HOW CONTROLS ARE SPECIFIED	User-specified
OUTPUT	Standard output module is constructed, but may be altered
OTHER COMMENTS	Includes optimization capabilities
	Can perform sensitivity and exergy analyses
	Can calculate restart and equipment costing & sizing
	Can be used to model fluids and solids.
	Program executes in batch mode
	PROCESS is being incorporated into PRO2 (along with ASPEN/SP), but will still be available for a few more years.

Table 16. SALT-ANL description

ADDRESS	Available through NESC Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439	Authors H.K. Geyer & G.F. Berry Energy and Environmental Systems Division Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439
PHONE	(312) 972-7250 (FTS) 972-7250	
PRICE	\$1300	
AVAILABILITY	Public	
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state	
	Transient--solves the governing time-dependent equations	
BASIC UNIT	Component	
SYSTEMS MODELED	Program is a process simulator and a system analyzer	
	Contains 34 precompiled component models and several flow types	
	May include user-written subroutines in PL/I or FORTRAN	
	Includes various thermodynamic and power-producing systems	
HARDWARE/SOFTWARE REQUIREMENTS	IBM3033 mainframe	
	Written in PL/I	
FLUIDS	Includes a number of thermodynamic and transport property routines	
	Can handle more than 400 different chemical species--mostly light hydrocarbons and gases such as steam, CO ₂ , N ₂ , and O ₂	
HOW CONTROLS ARE SPECIFIED	Specified by user in input files	
OUTPUT		
OTHER COMMENTS	Can do optimization and sensitivity analyses	
	Contains a non-linear equation solver and integration methods for systems of differential equations	

Table 17. SimTool description

ADDRESS	Mainstream Engineering Corporation Software Systems Division Pines Industrial Center 200 Yellow Place Rockledge, FL 32955-5327
PHONE	(407) 631-3550
FAX	(800) 866-3550 (407) 631-3552
PRICE	From \$ 270 for 25 components to \$15,000 for 1000 components
AVAILABILITY	Commercial product
TRANSIENT OR STEADY STATE ANALYSIS	Steady state Transient with user-specified time steps
BASIC UNIT	Component
SYSTEMS MODELED	Fluid/thermal systems
	Standard components and devices are included
	May include user-written components
	User can supply variable property routines (VARs).
HARDWARE/SOFTWARE REQUIREMENTS	IBM-AT compatible microcomputer, or DEC VAX series minicomputer Mainframe versions available upon request.
	A hard disk is required. A math coprocessor is recommended.
	Microsoft FORTRAN, and MS-DOS/PC-DOS 3.0 or higher are required.
FLUIDS	Over 1000 fluids are available.
	Ideal gases, single-phase liquids, two-phase fluids, or multicomponent two-phase mixtures
HOW CONTROLS ARE SPECIFIED	User chooses a "device" from the Component Toolkit
OUTPUT	Any system variables or parameters
OTHER COMMENTS	Space applications (microgravity)
	Chemical reaction of one fluid component is allowed within specified components.
	A demo version is available for microcomputers.

Table 18. SOLA-LOOP description

ADDRESS	Available from NESC Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439	Author to Contact M.D. Torrey Los Alamos Nat. Lab. P.O. Box 1663 Los Alamos, NM 87185
PHONE	(312) 972-7250 (FTS) 972-7250	
PRICE	\$230	
AVAILABILITY	Public property	
TRANSIENT OR STEADY STATE ANALYSIS	Transient	
BASIC UNIT	Component	
SYSTEMS MODELED	Two-phase flow networks--developed for nuclear reactor analysis	
HARDWARE/SOFTWARE REQUIREMENTS	CDC mainframe	
	Written in FORTRAN IV	
	SCOPE operating system	
FLUIDS	Not given--but does two phase flow	
HOW CONTROLS ARE SPECIFIED		
OUTPUT	User-specified	
OTHER COMMENTS		

Table 19. SOLTES1 description

ADDRESS	Available through NESC Argonne National Lab. 9700 South Cass Ave. Argonne, IL 60439	Author to Contact N.R. Grandjean Component and Subsystem Development Div. Sandia National Lab. P.O. Box 5800 Albuquerque, NM 87185
PHONE	(312) 972-7250 (FTS) 972-7250	(505) 844-5678 (info) (FTS) 844-5678 (info)
PRICE	\$1300	
AVAILABILITY	Public	
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state response to time-varying data such as weather and loads	
	Transient with user-specified time steps and steady- state calculations	
BASIC UNIT	Components	
SYSTEMS MODELED	Solar, geothermal, nuclear, and fossil fuel systems	
	Contains many basic thermal energy system components, including boilers, heat exchangers, pipes, and pumps	
	Can include user-written component subroutines	
HARDWARE/SOFTWARE REQUIREMENTS	CDC6600 or CDC7600 mainframe	
	NOS or SCOPE operating system	
	FORTRAN IV	
FLUIDS	Alcohols, water, hydrocarbons, ethers, and a few Freons, among other organic and inorganic compounds	
	Thermodynamic properties are calculated with the HBMS generalized equation of state for real gases.	
	Calculation of heat transfer fluid properties (density, specific heat, etc.) is based on polynomial fits of published data.	
HOW CONTROLS ARE SPECIFIED	As time-dependent input	
	Open control routines	
OUTPUT	User-specified	
OTHER COMMENTS	Includes weather data for 26 locations in the U.S.	

Table 20. TAP-LOOP description

ADDRESS	Available through NESC Argonne National Lab 9700 South Cass Ave. Argonne IL 60439	Author C.E. Leach and E.L. Kelly, Jr. Battelle Memorial Inst. Pacific Northwest Lab. Battelle Boulevard P.O. Box 999 Richland, WA 99352
PHONE	(312) 972-7250 (FTS) 972-7250	
PRICE	\$700	
AVAILABILITY	Public	
TRANSIENT OR STEADY STATE ANALYSIS	Steady-state	
	Transient--uses a finite-difference method	
BASIC UNIT	Fluid loop	
SYSTEMS MODELED	Developed to perform scoping and conceptual design analyses for closed test loops in the Fast Flux Test Facility	
	Designed for thermal analysis of recirculating fluid loops and associated heat transfer equipment	
	Handles heat transfer problems, studies of potential fluid flow, electrical networks, and stress analysis	
HARDWARE/SOFTWARE REQUIREMENTS	UNIVAC with EXEC8 operating system	
	Written in FORTRAN IV	
FLUIDS	Properties must be supplied	
HOW CONTROLS ARE SPECIFIED		
OUTPUT	Output format is set by the program	
OTHER COMMENTS	Written circa 1970	

Table 21. TRACE description

ADDRESS	Trane Company Commercial Systems Group 3600 Pammel Creek Rd. LaCrosse, WI 54601-7599
PHONE FAX	
PRICE	\$2400
AVAILABILITY	Commercial--designed for Trane, but available to the public
TRANSIENT OR STEADY STATE ANALYSIS	Transient
BASIC UNIT	System
SYSTEMS MODELED	Building loads, fans/ducts, Trane systems, piping
HARDWARE/SOFTWARE REQUIREMENTS	IBM PC's and compatibles
FLUIDS	Not given
HOW CONTROLS ARE SPECIFIED	
OUTPUT	
OTHER COMMENTS	Program only includes Trane equipment--not clear whether the program could be modified to be more general

Table 22. TRNSYS description

ADDRESS	TRNSYS Coordinator Solar Energy Laboratory 1500 Johnson Dr. University of Wisconsin Madison, WI 53706
PRICE	(608) 263-1589
FAX	(608) 262-6707 BITNET: TRNSYS @ WISCMACC
PRICE	\$1000
AVAILABILITY	Commercial product
TRANSIENT OR STEADY STATE ANALYSIS	Transient: User-specified time steps
BASIC UNIT	Components; plus controls, inputs, etc.
SYSTEMS MODELED	Solar energy systems
	HVAC systems
	User written components are very easily added.
HARDWARE/SOFTWARE REQUIREMENTS	IBM compatible microcomputer, or Mainframe
	FORTRAN-77 compiler
FLUIDS	Properties are specified by the user.
HOW CONTROLS ARE SPECIFIED	Controls are either internal to a component or are specified in an external subroutine.
OUTPUT	Specified by the user
OTHER COMMENTS	Can perform economic calculations
	Has optimization capabilities
	A user-friendly front-end is being tested.
	Version 13.1 and a Macintosh version will be available soon.

- END -

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