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MARTIN MARIETTA

**Assessment of Thermal Analysis
Software for the DOE Office of
Civilian Radioactive
Waste Management**

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Chemical Technology Division

**ASSESSMENT OF THERMAL ANALYSIS SOFTWARE FOR THE DOE
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT**

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ABSTRACT

This assessment uses several recent assessments and the more general code compilations that have been completed to produce a list of 116 codes that can be used for thermal analysis. This list is then compared with criteria prepared especially for the Department of Energy Office of Civilian Radioactive Waste Management (DOE/OCRWM). Based on these criteria, fifteen codes are narrowed to three primary codes and four secondary codes for use by the OCRWM thermal analyst. The analyst is cautioned that since no single code is sufficient for all applications, a code must be selected based upon the predominate heat transfer mode of the problem to be solved, but the codes suggested in this report have been used successfully for a range of OCRWM applications. The report concludes with a series of recommendations for additional work of which the major points include the following:

- The codes suggested by this report must be benchmarked with the existing U.S. and international problems and validated when possible.
- An interactive code selection tool could be developed or, perhaps even more useful, a users group could be supported to ensure the proper selection of thermal codes and dissemination of information on the latest version.
- The status of the 116 codes identified by this report should be verified, and methods for maintaining the still active codes must be established.
- Special capabilities of each code in phase change, convection and radiation should be improved to better enable the thermal analyst to model OCRWM applications.

1. INTRODUCTION

The purpose of this study is to provide an assessment of the current thermal analysis computer codes that are usable by the multiple program elements (i.e., monitored retrievable storage, transportation and cask design, and repository) of the Department of Energy (DOE) Office of Civilian Radioactive Waste Management (DOE/OCRWM). The criteria used for the assessment are based on guidelines given by the U.S. Nuclear Regulatory Commission (NRC)¹ and other requirements discussed in the report.

1.1 DOE/OCRWM MISSION

OCRWM has been established, in accordance with the Nuclear Waste Policy Act of 1982 (NWPA), to serve as the lead office for siting, constructing, and operating nuclear waste repositories; transporting commercial spent fuel and high-level radioactive wastes (HLW); developing a proposal to construct a monitored retrievable storage (MRS) facility; and aiding utilities in solving spent fuel storage problems.

For NWPA activities, DOE will comply with all Department of Transportation (DOT) and NRC requirements for transportation of commercial spent fuel and HLW. DOE has initiated procedures to provide for the technical development of the transportation system including, but not limited to, engineering development and certification of the shipping casks. OCRWM has committed to using NRC standards for the design and development of casks used for shipment to a repository.

1.2 NEED FOR THERMAL ANALYSIS

NRC regulations² provide that a shipping cask must prevent the loss or dispersion of its radioactive contents, provide adequate shielding against radiation and sufficient dissipation of heat, and prevent nuclear criticality under both normal and accident conditions of transportation.

Licensing requirements³ for the storage of spent nuclear fuel and HLW include design criteria to provide criticality safety, protection against fire, explosions, and excessive accumulation of radiation and heat. To comply with the requirement of regulatory guidelines, the designer must demonstrate that the structural integrity of the storage cask can be maintained during the conditions described above. The structural integrity must include the prevention of cladding degradation and gross rupture of the spent fuels and the melting of radiation shielding.

The most critical structural requirement for a cask is to keep the thermally induced stress below the allowable stress specified in the ASME Boiler and Pressure Vessel Codes. The allowable stress for a material is temperature dependent. Thermal history information in the structure also affects the analysis of material fatigue, creep, and cracking. The temperature distribution and history within the structure are necessary information for the stress analyst to perform an accurate structural analysis. The critical temperature history needed for the design of cask in transit may be 30 min under fire, but if a dual-purpose cask is used, the temperature history needed for repository application may be years. The cost of material, manpower, and time to obtain accurate thermal information through actual testing is usually very high. Therefore, it is an established practice by the engineering community to use computerized heat transfer programs and modeling techniques to simulate the design conditions and predict the temperature distribution and thermal history.

1.3 COMPUTATIONAL TOOLS

In 1971 Shuker⁴ identified "more than a dozen general-purpose heat conduction programs" and noted that nearly all of them reduce the conservation of energy equation to a set of algebraic equations by replacing the space and time derivatives with their finite-difference approximations. Fifteen years later, Noor^{5,6} presented an overview of 33 computer programs that can be used to solve heat transfer problems. Two-thirds of these programs recast the conservation of energy equation

to an integral equation that is solved with finite-element approximations. The fundamental difference between the finite-difference and finite-element method is explained in Sect. 2 of this report, but it is evident that over the past 15 years the finite-element technique has become increasingly popular for heat transfer. Although the finite-element method requires considerably more programming effort and computer core storage, the use of this method for structural analysis has greatly increased. This dramatic change in mathematical technique is evidence of how computer technology has altered the computation of heat conduction and has given the analyst greater flexibility.

1.4 EVALUATION CRITERIA

Budden⁷ has presented a comparison and evaluation of several heat conduction computer programs for use in the design of shipping casks, and Claiborne et al.⁸ and Graham⁹ have compared several heat conduction computer programs for use in the design of repositories.

Analysis capabilities and user features vary considerably from one code to another and, therefore, it is often difficult to identify a code that meets a specific need. A number of factors that affect the selection have been enumerated by Noor⁵ as follows:

1. Analysis capabilities. These capabilities include the range of applications and limitations of the code.
2. Adequacy of user-oriented features. These features include automatic (or semi-automatic) mesh (or model) generation, error checks, displays of original model and of various intermediate results, and mechanisms for data transfer to other program packages.
3. Maintainability. This feature includes updating the computational modules, extending the capabilities of the code, and improving its performance.
4. Adequacy of user support facilities. In addition to the printed documentation (user manuals, training manuals, programming manuals, sample problems, and test cases), the following services are desirable: training courses, users meetings, hotline consultation, assistance by data centers, and consulting organizations.

5. Portability. Although many of the heat transfer codes are written in standard FORTRAN 77 language, a code developed on one computer system may not be entirely compatible with another system due to differences such as I/O facilities, operating system, and precision of the machine.
6. Experience of other users. This factor can be invaluable if the users are objective in their evaluation and are familiar with some of the other software packages.

1.5 ASSESSMENT CRITERIA

The criteria established for this report in order of importance are the following:

1. Used by an OCRWM contractor. A large number of thermal analysis programs have been developed commercially or through DOE funding. The user groups within OCRWM contractors and several technical publications have already performed qualified screening processes to select the applicable thermal analysis codes based on their individual merits. The user's acceptance and familiarity with the programs are good indications about the code's applicability and credibility.
2. Code suitability and modeling capabilities. It is important that the computer codes that meet OCRWM needs yield sufficiently accurate results for the physical system and phenomena they are to simulate. The codes must be capable of modeling the latest engineering concepts evolved in the design of shipping casks and repositories.
3. Verification and benchmarking. The computer programs appropriate for NRC acceptance must be thoroughly verified and benchmarked for a wide range of applications and the assessments properly documented, maintained, and supported according to NRC guidelines.¹
4. Availability, ease of use, cost to use. In order for an OCRWM contractor to use a thermal analysis code for a particular application, the resources required to run the program must be considered. These resources include license or membership fee to acquire the program, computer hardware required to run, and manpower investment needed to learn and effectively use the analysis tool.
5. Mathematics modeling technique. The modeling capability of a computer code depends on the numerical solution technique used to solve the governing equations. The techniques include finite element, finite difference, boundary integral,

perturbation, or other hybrid methods. As can be seen from the rest of the report, no single code satisfies all problems. The intricacy of the engineering systems and phenomena will affect the selection of computer codes. For example, if natural convection is the predominant heat transfer mechanism, then a thermo/hydraulic code is preferred over a solid/conduction code. A companion structural analysis code is important if a sufficiently detailed temperature gradient is required by the stress analyst. In this case, the finite-element codes are preferred because structural codes may utilize the same modeling mesh to facilitate data transfer between thermal and structural models.

6. Documentation and quality assurance. To provide the code user and the NRC reviewer with confidence and convenience, a computer code should be well documented according to NRC guidelines¹ in terms of the mathematical theory, numerical method, program flow chart, input/output utilities, sample problems and results, capabilities and incapacities, error interpretation, modeling optimization technique and, most importantly, the quality assurance record, and current program updates and revisions. The commitment from the code developer to meet these requirements must be credible.
7. Computer compatibility (type and language). A wide variety of computer hardware is available and in use throughout the engineering community. The thermal analysis program will gain popular acceptance and prolong its use, provided the program can be transferred easily between different computer configurations. As the proliferation of personal computers or workstations increase, the availability of thermal programs for advanced microcomputers will be another attractive option. The acceptance and popularity within the DOE/OCRWM community will also encourage and enable continuous support and improvement of the thermal computer programs.

After a discussion of methodology in Sect. 2, an overview of all thermal analysis codes is presented in Sect. 3. The NRC regulations are presented in Sect. 4. A discussion of shipping cask and repository applications are presented in Sect. 5. The code assessment is given in Sect. 6, and the conclusions and recommendations for future work are given in Sect. 7. The references are listed in Sect. 8.

2. METHODOLOGY

2.1 DESCRIPTION

Many levels of sophistication exist in thermal analysis codes that have been used to analyze various aspects of the waste isolation program. The level of detail necessary for a particular analysis depends on the purpose of the analysis and the scope of the system being analyzed. In general, the more detailed the analysis possible with a code, the more computer memory and computing time required. For an entire geologic repository, the details of heat transfer in the waste containers may be of lesser importance, whereas for a fuel transport cask the details of heat transfer throughout the cask is important. Since the class of problems is so broad, the solution techniques utilized also include a broad range.

General solution methods include finite element, finite difference, boundary integral, perturbation technique, hybrid, and other methods. A detailed discussion of each technique is beyond the scope of this report and can be found in various textbooks. The most common numerical techniques found in the more general purpose codes utilize either the finite-difference method (FDM) or the finite-element method (FEM). The other solution techniques have only limited applications due to many special restraints and, therefore, are not considered further. The codes of primary interest in this study use either finite-difference (FD) or finite-element (FE) formulations of the energy-conservation equations with various approximations. A general description of these two techniques follows in the next section. More detailed descriptions can be found in the cited references.

A basic difference between the FDM and FEM is that the FEM is based on the solution of an integral formulation whereas the FDM is based on differential formulation of the conservative equations. Consequently, some of the inherent instability in evaluation of derivatives numerically in the FDM are alleviated in the FEM.

2.1.1 Finite-Difference Method

The FDM¹⁰ for the solution of the partial differential equations arising from the energy conservation equations for heat conduction problems is based on the use of special difference approximations for the resulting set of equations.

The model is constructed as follows:

1. The solution domain is first divided into a group of "n" node points.
2. For each node or grid point, the partial differential equation at the node is transformed into a FD approximation of the derivatives involved. This FD approximation relates nearby nodes to each other. Backward, central, or forward FD approximations can be used.
3. The resulting set of "n" equations in "n" unknowns is solved to obtain the approximate solution values at each node point.

One inconvenience with the FDM is that physical models must be divided into a set of nodes parallel to the coordinate axes and thus modeling of complex geometries may be difficult. This negative aspect can be a significant consideration in code selection.

2.1.2 Finite-Element Method

The FEM¹⁰ is a numerical procedure for use in the solution of differential equations in physics and engineering. The method had its beginning in the 1950s. The FEM is a variation of the Raleigh-Ritz procedure and utilizes a set of linearized equilibrium equations minimizing the potential energy of the system.

Any continuous quantity such as temperature, pressure, or displacement can be approximated by a discrete model composed of a set of piecewise continuous functions defined over a finite number of subdomains.

The model is constructed as follows:

1. A finite number of points in the domain are identified. These points are called nodal points or nodes.
2. The value of the continuous quantity at each nodal point is denoted as a variable that is to be determined.
3. The domain is divided into a finite number of subdomains called elements. These elements are connected at common nodal points and approximate the shape of the domain.
4. The continuous quantity is approximated over each element by a polynomial that is defined using the nodal values of the continuous quantity. A different polynomial may be defined for each element, but the element polynomials are selected in such a way that the heat flux and temperature remain compatible along the element boundaries.

Some advantages of the FEM that have contributed to its extensive use are the following:

1. Irregularly shaped boundaries can be approximated using elements with straight or curved boundaries. The boundaries need not be parallel to the coordinate axes. The method, therefore, may allow complex geometries to be modeled relatively easily.
2. Boundary conditions such as discontinuous surface loadings present no difficulties for the method. Mixed boundary conditions can be easily handled.
3. Extensive pre- and post-processors have been written for the major FE codes that provide a great deal of convenience for the user in input preparation and output processing. In general, the same level of user interaction has not been built into the FD codes.

A significant disadvantage of the FE technique may be an increased requirement for computer resources, particularly memory. However, with the advent of virtual memory machines and the rapidly increasing performance and large memory size of computing hardware, the efficiency of FE methods is competitive with more traditional methods.

2.2 SELECTION OF METHODOLOGY

Both FDM and FEM have their advantages and disadvantages. Both can yield accurate results. There is, in general, no "best" method, although that point is often debated. Familiarity with the particular method and/or code, code availability, ease of use, verification/benchmarking, and other criteria ultimately determine the user's choice of codes and thus, numerical solution method.

2.3 FUTURE TRENDS

There is an increased demand to develop computer programs that have combined capabilities of thermal/structural or thermal/fluids. The majority of the structural analysis computer programs in use today utilize FEM. Most general-purpose fluid dynamic computer codes under development today use the FEM to handle complicated geometry and mass transfer. When incorporating thermal capabilities in the structural programs, the same modeling mesh can be used for both heat transfer and stress analysis. This results in great simplification of mapping the nodal thermal solution onto the stress calculation. The code developer familiar with the FEM used in the stress analysis programs most likely will implement the heat transfer solution using the same numerical solution techniques.

The thermal analysis capabilities of these structural or fluid dynamics programs are not yet as versatile or general as the thermal analysis programs using FDMs developed solely for the purpose of solving heat transfer problems. The following factors can be expected to favor FEM in the future:

1. the rapidly evolving computer technology,
2. the increasing popularity of PCs and workstations with power approaching that of the minicomputers,
3. the constant demand for better and more general analysis tools for design engineers and scientists, and
4. the availability of computer programs as "turnkey systems" that can handle more versatile thermal analysis for the structural analyst.

These factors require the program input stage to have sufficiently intelligent preprocessor and postprocessor to prevent erroneous input and output interpretation. A thermal program that is compatible with the structural/fluid code can avoid confusion for the thermal, structural, and fluid analysts.

The following future developments on thermal analysis computer codes are still needed:

1. automatic mesh generation,
2. self-adaptive mesh refinement,
3. error-bounding prediction,
4. flexible user interface, and
5. the integration of engineering analysis procedures in the computer-aided-design software.

Such integration also means that the analysis tool must be reliable and user-friendly so that a nonspecialist can apply it to a wide range of applications.

3. CODE DESCRIPTION

A total of 116 thermal analysis codes have been identified and are listed in Table 1. These codes have been assigned to one of the following five categories:

1. Special-Purpose Thermal Analysis Codes for Specialized Geometries, Heat Transfer Mechanisms, etc.,
2. Simplistic Thermal Models Primarily Intended for Scoping/Parametric Studies,
3. General-Purpose, Finite Difference Heat Transfer Codes,
4. General-Purpose, Finite Element Heat Transfer Codes, and
5. Foreign Codes Not Extensively Utilized in the United States.

Each of these categories is listed in a table with the name of the code, the source of the code for this report, and a reference or contact where more information can be obtained on the code. The sources of the codes can be grouped into five areas:

1. Previous code compilations [i.e., the work sponsored by the Office of Nuclear Waste Isolation,¹¹ the Commission of the European Communities,¹² and the Office of Civilian Radioactive Waste Management (DOE/OCRWM)].
2. Previous thermal code assessments [i.e., the Pacific Northwest Laboratory comparison and evaluation,⁷ the survey done at George Washington University,^{5,6} and the survey completed at Bettis Atomic Power Laboratory⁴].
3. Personal communication with various workers in the waste management field [i.e., Jeff Arbital (ARBITAL, FLUOR SOURCE INDEX), David Korns (ONWI DRAFT PAP), Bob Prindle (PRINDLE), Doug Vogt (VOGT), and Jim Creer (CREER)].
4. The software collection centers [i.e., the National Energy Software Center (NESC) and the Computer Software Management and Information Center (COSMIC)].
5. Other reports and references [i.e., the Office of Nuclear Waste Isolation,¹³ Sandia National Laboratories,¹⁴⁻¹⁶ the Argonne National Laboratory,¹⁷ and the Nuclear Regulatory Commission.¹⁸

Because of the length, all the tables referenced in this section are attached at the end of this section.

3.1 SPECIAL-PURPOSE THERMAL ANALYSIS CODES

Thirty-five codes have been identified in Table 2 that are for special-purpose thermal calculations. The CHESS and TEMP codes are good examples of this type of code. They are finite source codes for repository design calculations. Many of the other codes such as CONFAC2, CONRAD, COX, HEX, RAD, and VIEW are special purpose radiation codes. A number of the codes in this section such as LONAC, RETRAN, SODEMME, and HYDRO-ACE are one-dimensional codes and may not be useful for general calculation.

3.2 SIMPLISTIC THERMAL MODELS

Ten codes have been identified in Table 3 as primarily intended for scoping/parametric studies. This category of codes could overlap with many of the codes in the previous section, but these codes appear to be more general in scope.

3.3 GENERAL-PURPOSE FINITE-DIFFERENCE CODES

Twenty-four codes have been identified in Table 4 as general-purpose FD codes. Each major laboratory or contractor has developed a code within this category. Oak Ridge National Laboratory has the HEATING series and the ORTHIS/ORTHAT and MORSE codes; Pacific Northwest Laboratories uses TEMPEST, COBRA, and HYDRA; Idaho National Engineering Laboratory uses SIMIR/6; Lawrence Livermore National Laboratory developed TRUMP; and MITASII, SINDA, TAC, and THT are examples of codes developed by contractors. The most widely available of these codes appear to be the HEATING series, SINDA, TAC, TEMPEST, and TRUMP.

3.4 GENERAL-PURPOSE FINITE-ELEMENT CODES

Twenty-five general-purpose FE codes have been identified in Table 5. Similar to the FD codes, each major laboratory or contractor has developed a FE code with thermal capabilities. For example, Lawrence Livermore National Laboratory developed TACO and TOPAZ, but the emphasis for these codes has been the commercial vendor. ABAQUS, ADINAT, ANSYS-THERMAL, BEASY, CONCEPT, MARC-HEAT, MSC-NASTRAN, and WECAN are proprietary codes available from the vendors. Computer codes APACHE, COYOTE, DOT, NACHOS, SPECTROM-41, TACO, and TOPAZ were all developed using government funding and are available from various government clearinghouses. ADINAT, COYOTE, DOT, MARC-HEAT, SPECTROM-41, and TACO appear to be widely used and available to the waste management community.

3.5 FOREIGN THERMAL ANALYSIS CODES

Table 6 presents a list of 22 foreign codes that are not extensively utilized in the United States. These codes will not be considered further in this report.

3.6 SUMMARY

Because of the limited resources and time available to compile this report, the status of each code listed in Tables 2 through 6 have not been thoroughly verified. Further information can be obtained from the listed reference or contact for each code. The authors have selected a few codes to obtain more information for the purpose of code evaluation. The response from each contact has been very courteous and cooperative. The tables in this section can be used as a reliable data base for further investigation, with additional updating recommended for code status to complete and augment the information in this section.

Table 1. List of thermal analysis codes

Code name	Table where referenced	Category
ABAQUS	5	Finite-Element Methods Codes
ADINAT/ADINA	5	Finite-Element Methods Codes
ANDES	2	Special Geometries, Mechanism
ANSALT	5	Finite-Element Methods Codes
ANSYS/ANSYS-THERMAL	5	Finite-Element Methods Codes
APACHE/MATUS	5	Finite-Element Methods Codes
ARRAYF	2	Special Geometries, Mechanism
ASAS-HEAT	6	Foreign Codes
ASTREA/ASTHER	6	Foreign Codes
BASFEH	5	Finite-Element Methods Codes
BEASY	5	Finite-Element Methods Codes
BEH2D	3	Simplistic Scoping/Parametric
CAVE I, II, III	2	Special Geometries, Mechanism
CHES	2	Special Geometries, Mechanism
CLUHET	6	Foreign Codes
COBRA-SFS	4	Finite-Difference Methods Codes
COMMIX-1A, B/-2	4	Finite-Difference Methods Codes
CONCEPT	5	Finite-Element Methods Codes
CONFAC2	2	Special Geometries, Mechanism
CONRAD	2	Special Geometries, Mechanism
COX	2	Special Geometries, Mechanism
COYOTE	5	Finite-Element Methods Codes
CYNDER	3	Simplistic Scoping/Parametric
DAMBIT	2	Special Geometries, Mechanism
DAMSEL	4	Finite-Difference Methods Codes
DIFFUS2	3	Simplistic Scoping/Parametric
DOT	5	Finite-Element Methods Codes
EAL	5	Finite-Element Methods Codes
EASE2	5	Finite-Element Methods Codes
EDITH/ESTHER	6	Foreign Codes
EXPAR	3	Simplistic Scoping/Parametric
FAST	6	Foreign Codes
FIESTA	5	Finite-Element Methods Codes
FILINE	3	Simplistic Scoping/Parametric
FLLSSM	3	Simplistic Scoping/Parametric
FLUXT	2	Special Geometries, Mechanism
FLUX2	2	Special Geometries, Mechanism
GOLIA-RK	6	Foreign Codes
GTA	4	Finite-Difference Methods Codes
HEAT	6	Foreign Codes
HEATING6, 5, 3	4	Finite-Difference Methods Codes
HEATP1	2	Special Geometries, Mechanism
HEATRAN	6	Foreign Codes
HEX	2	Special Geometries, Mechanism
HOT-2	2	Special Geometries, Mechanism

Table 1. (Continued)

Code name	Table where referenced	Category
HYDRA-I/-II	4	Finite-Difference Methods Codes
HYDRO-ACE	2	Special Geometries, Mechanism
INCA/DELFIN	5	Finite-Element Methods Codes
KO/NEMP	4	Finite-Difference Methods Codes
LION4, LION	2	Special Geometries, Mechanism
LONAC	2	Special Geometries, Mechanism
MARC-HEAT	5	Finite-Element Methods Codes
MITASII	4	Finite-Difference Methods Codes
MORSE-SGC, -L	4	Finite-Difference Methods Codes
MOTIF	6	Foreign Codes
MOXY	2	Special Geometries, Mechanism
MPGST	6	Foreign Codes
MSC/NASTRAN	5	Finite-Element Methods Codes
NACHOS	5	Finite-Element Methods Codes
NAMMU	6	Foreign Codes
NASTRAN	5	Finite-Element Methods Codes
ORTHIS/ORTHAT	4	Finite-Difference Methods Codes
PAFEC	5	Finite-Element Methods Codes
PISCES	4	Finite-Difference Methods Codes
PLUS FAMILY	2	Special Geometries, Mechanism
Q/TRAN	4	Finite-Difference Methods Codes
RAD	2	Special Geometries, Mechanism
RAGRAF	2	Special Geometries, Mechanism
RAT-3D	4	Finite-Difference Methods Codes
REFLUX	2	Special Geometries, Mechanism
REPOS(2)	2	Special Geometries, Mechanism
RETRAN	2	Special Geometries, Mechanism
SAMCEF	6	Foreign Codes
SAP, SAP4	5	Finite-Element Methods Codes
SARFIN	2	Special Geometries, Mechanism
SIM	3	Simplistic Scoping/Parametric
SIMIR/6	4	Finite-Difference Methods Codes
SIMMER	2	Special Geometries, Mechanism
SINDA/CINDA-3G	4	Finite-Difference Methods Codes
SODEMME	2	Special Geometries, Mechanism
SPECTROM-341	5	Finite-Element Methods Codes
SPECTROM-349	3	Simplistic Scoping/Parametric
SPECTROM-41/TRANCO	5	Finite-Element Methods Codes
SSPTA	2	Special Geometries, Mechanism
STAFF-5	2	Special Geometries, Mechanism
SYM3D	3	Simplistic Scoping/Parametric
T14	2	Special Geometries, Mechanism
TAC-3D/TAC-2D	4	Finite-Difference Methods Codes
TACO2D/TACO3D	5	Finite-Element Methods Codes
TAP-A	4	Finite-Difference Methods Codes

Table 1. (Continued)

Code name	Table where referenced	Category
TASTE	6	Foreign Codes
TAU	6	Foreign Codes
TEFELD	6	Foreign Codes
TEMP	2	Special Geometries, Mechanism
TEMP/NTEMP	5	Finite-Element Methods Codes
TEMPEST	4	Finite-Difference Methods Codes
TEPSA	6	Foreign Codes
THAC-SIP-3D	4	Finite-Difference Methods Codes
THAP	2	Special Geometries, Mechanism
THTD-THTE	4	Finite-Difference Methods Codes
TOODEE	4	Finite-Difference Methods Codes
TOPAZ2D/TOPAZ3D	5	Finite-Element Methods Codes
TOSS	4	Finite-Difference Methods Codes
TRAD	6	Foreign Codes
TRAITEME	6	Foreign Codes
TRASYS II	2	Special Geometries, Mechanism
TROUGH	6	Foreign Codes
TRUMP	4	Finite-Difference Methods Codes
UNNAMED (THUNVIK)	6	Foreign Codes
UNSAT2	6	Foreign Codes
VARR2	2	Special Geometries, Mechanism
VIEW	2	Special Geometries, Mechanism
VIPLEF/CHEF	6	Foreign Codes
WATSON	2	Special Geometries, Mechanism
WECAN	5	Finite-Element Methods Codes
WONDY/TOODY	4	Finite-Difference Methods Codes

Table 2. Special-purpose thermal analysis codes for specialized geometries, heat transfer mechanisms, etc.

Code	Source	References/contacts
1. ANDES	NOOR	Contact R. F. Emery Department of Mechanical Engineering University of Washington Seattle, WA 98195
2. ARRAYF	PRINDLE, SAND80-0440	Contact Sandia National Laboratories Albuquerque, NM 87185
3. CAVEI, CAVEII, CAVEIII	NOOR	Contact John G. Roukis, MS B22/35 Grumman Aerospace Corporation Bethpage, NY 11714
4. CHESS	ARBITAL	Contact Bill Yeung Science Applications International Corporation 160 Spear Street, Suite 1250 San Francisco, CA 94105
5. CONFAC2	NOOR, COSMIC	Contact John G. Roukis MS B22/35 Grumman Aerospace Corporation Bethpage, NY 11714
6. CONRAD	BUDDEN	Reference J. A. Fillo, R. Benenati, J. R. Powell, <u>CONRAD - Heat Conduction Radiation Code</u> , Brookhaven National Laboratory, 1976.
7. COX	ONWI-78, EUR.8669	Reference R. L. Cox, 1977. <u>Radiative Heat Transfer in Arrays of Parallel Cylinders</u> . Contact R. L. Cox Oak Ridge National Laboratory Oak Ridge, TN 37831
8. DAMBIT	ONWI-98	Contact Grant Hocking, Dames and Moore 44 Mall Road Burlington, MA 01803

Table 2. (Continued)

Code	Source	References/contacts
9. FLUXT	FLUOR SOURCE, INDEX	Contact Fred Su Science Applications Int. Co. 10210 Campus Point Drive San Diego, CA 92121
10. FLUX2	NOOR	Contact John G. Roukis, MS B22/35 Grumman Aerospace Corporation Bethpage, NY 11714
11. HEATP1	FLUOR SOURCE, INDEX	Contact Bruce Kirstein Science Applications Int. Co. 10210 Campus Point Drive San Diego, CA 92121
12. HEX	BUDDEN	Reference R. L. Cox, <u>A Computer Program for Calculating the Temperatures Attained by LMFBR Fuels for Decay Heat Emission</u> , ORNL-TM-3773, Union Carbide Corp. Nuclear Div., Oak Ridge Natl. Lab., 1973.
13. HOT-2	BUDDEN, NESC-286	Reference W. D. Petersen, J. Spanier, <u>HOT-2: A Two-Dimensional Transient Heat Conduction Program for the CDC-6600</u> , USAEC Report WAPD-TM-669, Westinghouse Electric Corporation, 1967.
14. HYDRO-ACE	CREER	Contact K. Abe Japan Atomic Energy Research Institute Tokyo, Japan
15. LION4, LION	NESC-299	UNKNOWN
16. LONAC	CREER	Contact R. J. Ribando ORNL/TM-6228 Oak Ridge National Laboratory Oak Ridge, TN 37830

Table 2. (Continued)

Code	Source	References/contacts
17. MOXY	BUDDEN, NESC-551	Reference D. R. Evans, <u>MOXY. A Digital Computer Code for Core Heat Transfer Analysis</u> , IN-1392, August 1970; <u>MOXY Core Heat Transfer Code: Model Description and User's Guide</u> , PG-R-76-003, 1976.
18. PLUS, CELERY, MIDNITE DAYLITE, STALKS, TWIGS	OCRWM	Contact D. N. Montan Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94550
19. RAD	FLUOR SOURCE, INDEX	Contact Fred Su Science Applications International Corporation 10210 Campus Point Drive San Diego, CA 92121
20. RAGRAF	CREER	Contact A. Eastham UKAEA Risley Nuclear Power Development Establishment United Kingdom
21. REFLUX	NESC-763	Contact National Energy Software Center Argonne National Laboratory 9700 South Cass Ave. Argonne, IL 60539
22. REPOS (2)	EUR.8669	Reference J. S. Y. Wang, <u>Program Repos - User's Guide</u> , Lawrence Berkeley Laboratory, University of California, Berkeley, 1982. Contact J. S. Y. Wang Earth Sciences Division Lawrence Berkeley Laboratory University of California Berkeley, CA 94720

Table 2. (Continued)

Code	Source	References/contacts
23. RETRAN	CREER	Contact J. H. McFadden Energy Inc. Idaho Falls, ID 83415
24. SARFIN	BUDDEN	Reference A. J. Brook, P. M. Shaw, <u>Calculations of Heat Transfer into Finned Surfaces, and the SARFIN Code</u> , 1974.
25. SIMMER	CREER, NESC-9965	Contact L. L. Smith Los Alamos National Laboratory Los Alamos, NM
26. SODEMME	CREER	Contact L. G. Epel Brookhaven National Laboratory Upton, NY
27. SSPTA	NOOR, COSMIC	Contact Arthur D. Little Acorn Park Cambridge, MA 02140
28. STAFF-5	CREER	Contact S. R. Fields Hanford Engineering Development Laboratory Richland, WA 99352
29. T14	NOOR	Contact John G. Roukis MS B22/35 Grumman Aerospace Corporation Bethpage, NY 11714
30. TEMP	EUR.8669, ANL/EES-TM- -356 ONWI DRAFT, PAP	Reference K. J. Wurm, S. G. Bloom, W. C. Atterbury, TEMP: A Finite-Line Heat Transfer Code for Geologic Repositories for Nuclear Waste, Battelle Memorial Institute, Office of Nuclear Waste Isolation, 1985.
31. THAP	COSMIC	

Table 2. (Continued)

Code	Source	References/contacts
32. TRASYSII	COSMIC	
33. VARR2	NESC-755	Contact J. L. Cook Westinghouse Electric Corp Waltz Mill, PA
34. VIEW	COSMIC	
35. WATSON	CREER	Contact M. Chandrashekar Univeristy of Waterloo Ontario, CANADA

**Table 3. Simplistic thermal models primarily intended
for scoping/parametric studies**

Code	Source	References/contacts
1. BEH2D	ONWI-98, EUR.8669, ONWI-78	Contact Grant Hocking Advanced Technology Group 44 Mall Road Burlington, MA 01803
2. CYNDER	ONWI-78, EUR.8669	Reference T. Chan, N. G. W. Cook and C. F. Tsang, <u>Theoretical Temperature Fields for the Stripa Heater Project</u> , LBL-7082-1, Lawrence Berkeley Laboratory, 1978. Contact T. Chan Atomic Energy of Canada Ltd. Whiteshell Nuclear Research Establishment Pinawa, Manitoba, ROE ILO, Canada
3. DIFFUS2	ONWI-78, EUR.8669, ONWI-98	Reference C. M. St. John, <u>DIFFUS2 - A Computer Model to Approximate the Thermal Response of a Rock Mass to Heat Generating Waste</u> , Report Prepared for Rockwell Hanford Operations, Energy Systems Group, University of Minnesota, 1979. Contact C. M. St. John Agbabian Associates 250 North Nash Street El Segundo, CA 90245
4. EXPAR	ONWI-98	Contact Dept. of Civil and Mineral Engineering University of Minnesota Minneapolis, MN 55455
5. FILINE	ONWI-78, EUR.8669	Reference T. Chan, N. G. W. Cook, and C. F. Tsang, <u>Theoretical Temperature Fields for the Stripa Heater Project</u> , LBL-7082-1, Lawrence Berkeley Laboratory, 1978. Contact T. Chan Atomic Energy of Canada Ltd. Whiteshell Nuclear Research Establishment Pinawa, Manitoba, ROE ILO, Canada

Table 3. (Continued)

Code	Source	References/contacts
6. FLLSSM	ONWI-78	Reference Kaiser Engineers, Finite-Length Line Source Superposition Model (FLLSSM), ONWI-94, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, OH, 1980.
7. SIM	OCRWM	Contact Ahmad Badie Parson Brinkerhoff San Francisco, CA
8. SNEAKY	ONWI-78, EUR.8669	Contact R. Hart Department of Civil and Mineral Eng. University of Minnesota Minneapolis, MN 55455
9. SPECTROM 349	OCRWM	Contact D. K. Svalstad Re/SPEC P. O. Box 725 Rapid City, SD 57709
10. SYM3D	ONWI-78, EUR.8669	Reference Santich, J. et al., Numerical Modeling of Rock Stresses within a Basaltic Nuclear Waste Repository, RHO-BWI-C-47, Rockwell Hanford Operations, Richland, WA, 1979. Contact Department of Civil and Mineral Eng. University of Minnesota Minneapolis, MN 55455

Table 4. General-purpose finite-difference heat transfer codes

Code	Source	References/contacts
1. COBRA-SFS	CREER, NESC-9601	Reference D. R. Rector, C. L. Wheeler, N. J. Lombardo, <u>COBRA-SFS: A Thermal Hydraulic Analysis Computer Code</u> , PNL-6049, Vol. 1, Battelle, Pacific Northwest Laboratory, 1986.
2. COMMIX1A-1B, COMMIX-2	BUDDEN, CREER, NESC-1066	Reference H. M. Domanus, et al., <u>A Steady/Unsteady Single-Phase/Two-Phase Three-Dimensional Computer Program for Thermal-Hydraulic Analysis of Reactor Components</u> , NUREG/CR-1807, ANL-181-10, Argonne National Laboratory, 1980.
3. DAMSEL	ONWI-98	Contact Grant Hocking, Dames and Moore 44 Mall Road Burlington, MN 01803
4. GTA	COSMIC	UNKNOWN
5. HEATING6, HEATING5, HEATING3	EUR.8669 BUDDEN, NOOR, SAND84-1854, ONWI-78, NESC-517	Reference D. C. Elrod, W. D. Turner, G. E. Giles, <u>HEATING6: A Multidimensional Heat Conduction Analysis with Finite-Difference Formulation</u> , NUREG/CR-0200, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., 1981. Contact Radiation Shielding Information Center Oak Ridge National Laboratory Oak Ridge, TN 37831
6. HYDRA I, HYDRA II	CREER, BUDDEN, EUR.8669, ONWI-78	Reference R. A. McCann, <u>HYDRA I, A Three-Dimensional Finite Difference Code for Calculating the Thermal-Hydraulic Performance of a Fuel Assembly Contained within a Canister</u> , PNL-3367, Battelle, Pacific Northwest Laboratory, 1980.
7. KO/NEMP	ONWI-98	Contact Lawrence Livermore Laboratory P.O. Box 808 Livermore, CA 94550

Table 4. (Continued)

Code	Source	References/contacts
8. MITAS II	NOOR	Reference <u>Martin Marietta Interactive Thermal Analysis System Version 2.0 (MITAS II), User's Manual</u> , Report No. M-76-2, Eng. Dept. Tech. Manual, Martin Marietta Corp., Denver, CO, May 1976.
9. MORSE-SGC, MORSE-L	BUDDEN, NESC-9912	Reference S. Fraley, T. J. Hofman, P. N. Stevens, <u>Monte Carlo Method for Solving Heat Conduction Problems</u> , ORNL/NUREG/CSD-3.
10. ORTHIS, ORTHAT	BUDDEN, NESC-525	Reference R. C. Durfee, C. W. Nastor, Jr., <u>Two Computer Programs for Solving Two-Dimensional Steady-State and Transient Heat Conduction Problems</u> , ORNL-TM-3324, Union Carbide Corp., Nuclear Div., Oak Ridge Natl. Lab., 1971.
11. PISCES	ONWI-98	Contact Physics International International Atomic Energy Agency
12. Q/TRAN	SAND84-1854	Reference F. A. Rockenbach, Q/TRAN, Ver. 1.0 User's Manual, The ROCK, Los Alamos NM, 1984.
13. RAT-3D	BUDDEN	Reference S. S. Clark, M. Troost, <u>RAT-3D - A General Three-Dimensional Heat Transfer Code</u> , USAEC Report GAMD-7346, General Dynamics Corporation, 1966.
14. SIMIR/6	BUDDEN	Reference H. G. Kraus, <u>SIMIR/6 - A 2-D Heat Conduction Code for use on an IBM-360/75 Computer</u> , TREE-1127, Idaho National Eng. Lab., Idaho Falls, ID, 1977.

Table 4. (Continued)

Code	Source	References/contacts
15. SINDA, CINDA-3G, Sinda/1983/ ANSI, SINDA/ 1987/ANSI, Rel 1.30	ONWI-78, EUR.8669, SAND84-1854 NOOR, COSMIC	Reference National Aeronautics and Space Administration, <u>Systems Improved Numerical Differencing Analyzer (SINDA) - User's Manual</u> , NASA-CR-134271, 1971. Reference D. R. Lewis, J. D. Gaski, and L. R. Thompson, <u>Chrysler Improved Numerical Differencing Analyzer for Third Generation Computers</u> , Report NASA-CR- 99595, National Aeronautics and Space Administration, 1967. Contact J. D. Gaski Network Analysis Associates 17165 Newhope Fountain Valley, CA 92728
16. TAC-3D, TAC-2D	BUDDEN, SAND84-1854 NOOR, NESC-408, NESC-414	Reference J. F. Petersen, <u>TAC3D: A General Purpose Three-Dimensional Heat Transfer Computer Code - User's Manual</u> , USAEC Report GA-9263, Gulf General Atomic, (TAC-2D, GA-8868), 1969. Contact General Atomic Corporation P.O. Box 81608 San Diego, CA 92138
17. TAP-A	COSMIC	Reference B. L. Pierce, H. J. Stumpf, <u>TAP-A - A Program for Computing Transient or Steady-State Temperature Distributions</u> , WANL-TME-1872, Westinghouse Astronuclear Laboratory, 1969.
18. TEMPEST	BUDDEN, SAND84-1854, NESC-9808	Reference D. S. Trent, M. J. Budden, L. L. Eyler, <u>TEMPEST: A Three-Dimensional Time- Dependent Computer Program for Hydrothermal Analysis</u> , PNL-4348, Vols. 1- 4, Battelle, Pacific Northwest Laboratory, 1981.

Table 4. (Continued)

Code	Source	References/contacts
19. THAC-SIP-3D	ONWI-78, ANL/EES-TM- 256 EUR.8669	Reference W. D. Turner, <u>THAC-SIP-3D. A Three-Dimensional, Transient Heat Analysis Code Using the Strongly Implicit Procedure</u> , K/CSD/TM-24, Union Carbide Corp., Nuclear Div., Oak Ridge Gaseous Diffusion Plant, 1978.
20. THTD, THTE	BUDDEN, NOOR	Reference S. C. Skirvin, <u>User's Manual for the THTD Computer Program (Transient Heat Transfer, Version D)</u> , Report 69-C-205, General Electric, 1969.
21. TOODEE	SHUKER	Reference J. A. McClure, <u>TOODEE - A Two-Dimensional, Time-Dependent, Heat Conduction Program</u> , USAEC Report IDO-17277, Phillips Petroleum Co., 1967.
22. TOSS	BUDDEN	Reference D. Bagwell, <u>TOSS - An IBM-7090 Code for Computing Transient or Steady-State Temperature Distributions</u> , USAEC Report K-1494, Union Carbide Corp., Nuclear Div., Oak Ridge Gaseous Diffusion Plant, 1961.
23. TRUMP	ONWI-78, EUR.8669, BUDDEN, SAND84-1854, PRINDLE, VOGT, NOOR, NESC-771, NESC-37	Reference A. L. Edwards, <u>TRUMP: A Computer Program for Transient and Steady-State Temperature Distribution in Multidimensional Systems</u> , UCRL-14754, Rev. 3, Lawrence Livermore Laboratory, 1972. Contact J. Parlagreco Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94550
24. WONDY, TOODY, TOODY2	ONWI-98 NESC-627	Contact Sandia National Laboratories Albuquerque, NM 87185

Table 5. General-purpose finite-element heat transfer codes

Code	Source	References/contacts
1. ABAQUS	EUR.8669, NOOR	Contact Hibbitt, Karlsson and Sorensen, Inc. 35 South Angell Street Providence, RI 02906
2. ADINAT	EUR.8669, BUDDEN, PRINDLE, VOGT, NOOR, ONWI-78	Reference K. J. Bathe, <u>Finite Element Procedures in Engineering Analysis</u> , Prentice-Hall, Inc., Englewood Cliffs, NJ, 1982. Contact Adina Engineering 71 Elton Avenue Watertown, MA 02172
3. ANSALT	EUR.8669, SAND81- 1293C	Reference M. Wallner and A. Wulf, <u>Thermo-mechanical Calculations Concerning the Design of a Radioactive Waste Repository in Rock Salt</u> , Proc. Int. Symp. Rock Mechanics: Caverns and Pressure Shafts, ISRM AACHEN, 1982. Contact A. Wallner, BGR Alfred-Benz Haus Stilleweg 2 3000 Hanover 51 W. Germany
4. ANSYS-THERMAL	EUR.8669, NOOR, ONWI-78	Reference <u>ANSYS User's Manual (Revision 4)</u> , Swanson Analysis Systems, Inc., 1982. Contact Swanson Analysis Systems, Inc. P.O. Box 65 Houston, PA 15342
5. APACHE/MATUS	BUDDEN, NESC-858	Reference D. N. Hutula, B. E. Wianco, S. M. Zeiler, <u>APACHE: A Three-Dimensional Finite Element Program for Steady-State or Transient Heat Conduction Analysis</u> , WAPD-TM-1080, Bettis Atomic Power Laboratory, Pittsburgh, PA, 1973.

Table 5. (Continued)

Code	Source	References/contacts
6. BASFEH	ONWI-98, ONWI-78	Contact Dept. of Civil and Mineral Eng. University of Minnesota Minneapolis, MN 55455
7. BEASY	-	Contact Computational Mechanics 400 West Cummings Park Suite 6200 Woburn, MA 01801
8. CONCEPT	-	Contact Concept Analysis 9145 General Court Plymouth, MI 48170
9. COYOTE	EUR.8669, ONWI-78, BUDDEN, SAND84-1854 PRINDLE, FLUOR SOURCE, INDEX, VOGT	Reference D. F. Gartling, <u>COYOTE - A Finite Element Program for Nonlinear Heat Conduction Problems</u> , SAND-77-1332, Sandia National Laboratories, Albuquerque, NM, 1987. Contact David Gartling Sandia National Laboratories, Albuquerque, NM 87185
10. DOT	EUR.8669, FLUOR SOURCE, INDEX, ANL/EES-TM 256, ONWI DRAFT PAP, ONWI-78, NESC-9833	Reference Intera Environment Consultants, Inc., <u>DOT - A Nonlinear Heat Transfer Code for Analysis of Two-Dimensional Planar and Axisymmetric Representation of Structures</u> , ONWI-420, Battelle, Office of Nuclear Waste Isolation, 1983. Contact
11. EAL	NOOR	Contact W. D. Whetstone Engineering Information Systems, Inc. 5120 West Campbell Avenue, Suite 240 San Jose, CA 95130
12. EASE2	-	Contact Engineering Analysis Corporation 24050 Madison Street Torrance, CA 90505

Table 5. (Continued)

Code	Source	References/contacts
13. FIESTA	BUDDEN	Reference E. Spreeuw, <u>FIESTA: Finite Elements Stress and Temperature Analysis</u> , RCN-L49, 1971.
14. INCA/DELFINE	EUR.8669	Reference H. S. Morgan, R. T. D. Krieg, R. V. Matalucci, <u>Comparative Analysis of Nine Structural Codes used in the Second WIPP Benchmark Problem</u> , SAND81-1389, Sandia National Laboratories, 1982. Contact Alain Combecure C.E.A.-Cen/Saclaytat Berlin Instdent/Smts/Lamsechnik Marcf-91191 Gif Sur Yvette Cedex, France
15. MARC-HEAT	BUDDEN, NOOR, SAND81-1293C, EUR.8669	Contact MARC Analysis Research Corporation 260 Sheridan Avenue, Suite 200 Palo Alto, CA 94306
16. MSC-NASTRAN	NOOR	Contact MacNeal - Schwendler Corp., 815 Colorado Boulevard, Los Angeles, CA 90041
17. NACHOS	BUDDEN	Reference D. K. Gartling, <u>NACHOS - A Finite Element Computer Program for Incompressible Flow Problems</u> , SAND77-1333/34, Sandia National Laboratories, 1977.
18. NASTRAN, COSMIC	BUDDEN, COSMIC	Reference NASA, <u>NASTRAN User's Manual</u> , NASA-SP-222(04), Washington, D.C., 1979.
19. PAFEC	ONWI-78, EUR.8669	Reference Hinshall, R. D., <u>PAFEC 75: Theory. Results. Easydata. Get Started. Data Preparation. Systems</u> , PAFEC, Ltd., Nottingham, England, 1977. Contact PAFEC Engineering Consultants, 6855 Jimmy Carter Blvd, Bldg. L, Suite 1200 Norcross, GA 30071

Table 5. (Continued)

Code	Source	References/contacts
20. SAP, SAP4, SAP5	ONWI-98, NESC-641	Contact University of California Berkeley, CA 94720
21. SPECTROM-41 (TRANCO), SPECTROM-341	ONWI-78, ONWI DRAFT PAP, ONWI-98, EUR.8669, VOGT, SAND81- 1293C, PRINDLE, BUDDEN	Reference D. K. Svalstad, <u>User's Manual for SPECTROM-41: A Finite Element Heat Transfer Program</u> , ONWI-326, Battelle Memorial Institute (RSI-0152), 1981. Contact D. K. Svalstad Re/SPEC, Inc. P.O. Box 725 Rapid City, SD 57709
22. TACO2D, TACO3D	BUDDEN, NOOR, NESC-562, NESC-9838	Reference W. E. Mason, Jr., <u>TACO. A Finite Element Heat Transfer Code</u> , Methods Development Group, Mechanical Engineering Dept., Lawrence Livermore Laboratory.
23. TEMP/NTEMP	BUDDEN, NOOR	Contact A. F. Emery Department of Mechanical Engineering University of Washington Seattle, WA 98195
24. TOPAZ2D, TOPAZ3D	OCRWM, NESC-9801	Contact A. Shapiro Lawrence Livermore Laboratory Livermore, CA 94550
25. WECAN	NOOR	Contact Albert H. Aarsch Westinghouse Engineering Service Bureau Advanced Mechanics Services P.O. Box 15230 Pittsburgh, PA 15230

Table 6. Foreign codes not extensively utilized in the United States

Code	Source	References/contacts
1. ASAS-HEAT	ONWI-78, EUR.8669	Contact Atkins Research and Development Woodcote Grove, Ashley Road Epsom Surrey KT18 5BW, England
2. ASTREA, ASTHER	EUR.8669	Contact H. Rolnik Laboratoire de Mecanique des Solides Ecole Polytechnique 91128 Palaiseau France
3. CLUHET	GREER	Contact P. Barroyer Swiss Fed. Institute of Reactor Research Eidgenoessisches Inst, fur Reaktor- forschung, Wuerenlingen, Switzerland
4. EDITH, ESTHER	EUR.8669	Reference J. P. Sauty, A. C. Gringarten, A. Menjoz, and P. A. Landel, "Sensible Energy Storage in Aquifers, Part 1: Theoretical Study. Part 2: Field Experiments and Comparison with Theoretical Results." Water Resour. Res., <u>18</u> (2), 245-265 (1982). Contact A.C. Gringartin, P.A. Landel, J.P. Sauty Departement Geothermie et Hydrogeologie Bureau de Recherches Geologiques et Minierse (BRGM) BP 6009-45018 Orleans Cedex France
5. FAST	EUR.8669	Contact Rwth-Aachen Institut fur Elektrische Analgen und Energiewirtschaft Lehrauftrag Leistungsreaktoren Aachen West Germany

Table 6. (Continued)

Code	Source	References/contacts
6. GOLIA-RK	EUR.8669	<p>Reference</p> <p>L. G. J. Janssen, J. Hamstra, <u>Further Design Work on a Repository in a Salt Dome</u>, Progress Report ECN-82-07, Netherlands Energy Research Foundation, Petten, 1982.</p> <p>Contact</p> <p>J. Prij, C. Beemsterboer, and C. Jong Applied Mechanics Group Netherlands Energy Research Foundation (ECN) 1755 Zg Petten, Netherlands</p>
7. HEAT	EUR.8669	<p>Reference</p> <p>E. L. Wilson and R. E. Nickell, <u>Application of Finite Element Method to Heat Conduction Analysis</u>, Nuclear Engineering and Design 4, North Holland Publishing Co., Amsterdam, 1966.</p> <p>Contact</p> <p>P. Gonze Foraky S.A., 13, Place de Barricades Brussels, Belgium</p>
8. HEATRAN	BUDDEN, NOOR	<p>Reference</p> <p>W. D. Collier, <u>HEATRAN: A Finite Element Code for Heat Transfer Problems</u>, British TRC Report 1807(R), 1969.</p>
9. MOTIF	EUR.8669	<p>Reference</p> <p>V. Guvanasen, <u>HEATRAN: A Finite-Element Three-Dimensional Model of Flow and Transport in Fracture/Porous Media: Formulation and User's Manual</u>, In Preparation, 1985.</p> <p>Contact</p> <p>V. Guvanasen Applied Geoscience Branch Atomic Energy of Canada Limited Whiteshell Nuclear Research Establishment Pinawa, Manitoba Canada R0E 1L0</p>

Table 6. (Continued)

Code	Source	References/contacts
10. MPGST	EUR.8669	Contact M. Put Cen/Sck Boeretang 200 B-2400 Mol, Belgium
11. NAMMU	EUR.8669	Reference J. Rae, P. C. Robinson, and L. M. Wickers, <u>A User's Guide for the Program NAMMU 1. General Information</u> , Harwell AERE-R10120, 1981. Contact J. Rae Theoretical Physics Division Aere Harwell Oxfordshire OX11 0RA England
12. SAMCEF	NOOR	Contact L. T. A. S. Aerospace Laboratory University of Liege Rue Ernest Solvay, 21 B-4000 Liege Belgium
13. TASTE	EUR.8669	Contact J. Kevenaar and C. Jong Applied Mechanics Group Netherlands Energy Research Foundation (ECN) 1755 Zg Petten Netherlands
14. TAU	NOOR	Contact J. A. Enderby JKA EA Risley Nuclear Power Development Establishment Warrington, Cheshire WA3 6AT England

Table 6. (Continued)

Code	Source	References/contacts
15. TEFELD	EUR.8669	Contact Rwth-Aachen Institut fur Elektrische Analgen und Energiewirtschaft Lehrauftrag Leistungsreaktoren Aachen W. Germany
16. TEPsa	NOOR	Contact T. R. Hsu Department of Mechanical Engineering University of Manitoba Winnipeg, Mannitoba R3T 2N2 Canada
17. TRAD	EUR.8669	Contact D. J. Gilby Polydynamics Ltd. Schaffhauserstrasse 24, CH 8006 Zurich, Switzerland
18. TRAITEME	EUR.8669	Reference M. Borsetto, G. Carradori and R. Ribacchi, "Coupled Seepage, Heat Transfer, and Stress Analysis with Application to Geothermal Problems", in <u>Numerical Methods in Thermal Problems</u> , Lewis, Morgan and Zienkiewicz, eds., John Wiley, London, 1980. Contact A. Peano ISMES Viale Giulio Cesare 29 2410 Bergamo Italy
19. TROUGH	EUR.8669	Reference R. S. Hopkirk, D. J. Gilby, I. Schwanner, and P. O. Gillis, <u>User's Manual TROUGH -</u> <u>1D, 2DP, 2DF</u> , Polydynamics, Zurich, 1983.

Table 6. (Continued)

Code	Source	References/contacts
20. UNNAMED (THUNVIK)	EUR.8669	<p>Reference R. Thunvik and C. Braester, <u>Hydrothermal Conditions Around a Radioactive Waste Repository. Parts 1, 2, and 3</u>, KBS Technical Reports 80-19 and 82-01, Stockholm, 1980.</p> <p>Contact R. Thunvik Department of Land Improvement and Drainage Royal Institute of Technology (KTH) S-100 44 Stockholm Sweden</p>
21. UNSAT2	EUR.8669	<p>Reference S. P. Neuman, R. A. Feddes and E. Bresler, <u>Finite Element Simulation of Flow in Saturated-Unsaturated Soils Considering Water Uptake by Plants</u>, Technion, Hydrodynamics and Hydraulic Engineering Laboratory Report, 1974.</p> <p>Contact S. P. Neuman Technion, Israel Institute of Technology Haifa, Israel</p>
22. VIPLEF/CHEF	EUR.8669	<p>Contact S. M. Tijani Centre de Mecaniques des Roches Ecole des Mines de Paris 35 Rue Saint-Honore 77305 Fontainebleau Cedex France</p>

4. NRC GOVERNING REGULATIONS

4.1 SHIPPING CASKS

DOE/OCRWM is required to use NRC standards for the design and development of casks used for the shipment of HLW to a repository. NRC regulations² provide that a shipping cask must prevent the loss or dispersion of its radioactive contents, provide for adequate shielding against radiation and for the dissipation of heat, and prevent nuclear criticality under both normal and accident conditions of transportation. Potential accident conditions include the following sequence:

- **Free drop** - 9.1 m (30 ft) onto a flat unyielding surface;
- **Puncture** - a free drop of a cask for a distance of 102 cm (40 in.) onto the end of a steel bar 10.2 cm (4 in.) in diameter and 20.3 cm (8 in.) in length;
- **Fire** - thermal exposure of casks to temperatures of 800°C (1475°F) for no less than 30 min;
- **Water immersion** - a cask must not leak when immersed in 1 m (3 ft) of water for a minimum of 8 h.

The primary purpose of most thermal analyses of shipping casks is to support the structural design of the cask. "Claims of adequacy of designs or design methods should be supported by technical bases, i.e., by an appropriate engineering evaluation or description of actual tests".¹⁹ Engineering evaluations using an acceptable method of analysis have typically been found to be more cost effective than carrying out full scale thermal tests on each new design. It must be demonstrated by the designer in the engineering evaluation that under normal transport conditions no radioactive material can escape from the cask, and that under the prescribed hypothetical accident conditions the amount of radioactive material allowed to escape cannot exceed the designated maximum. These structural design computations require as input the results of thermal analyses in order to calculate temperature dependent material properties, stresses caused by temperature gradients

and differential thermal expansions, and stress concentrations due to local thermal "hot spots."

4.1.1 Title 10, Code of Federal Regulations, Part 71

The principal instrument used by the U.S. Nuclear Regulatory Commission (NRC) to govern the design of shipping casks is Title 10, Code of Federal Regulations, Part 71 (10CFR71).² In 1987 the NRC issued its latest revision of 10CFR71 with the stated purpose of achieving compatibility with the transport regulations of the International Atomic Energy Agency (IAEA). In addition to the performance standards presented in 10CFR71, the NRC also provides the designer with more specific criteria for the structural analysis of shipping casks in NRC Regulatory Guides 7.6 (ref. 20) and 7.8 (ref. 21). The only explicit temperature limitation identified in 10CFR71 for the cask is in Sect. 71.43 where it is stated that a package should be designed in the following manner:

so that in still air at 38°C (100°F) and in the shade, no accessible surface of a package would have a temperature exceeding 50°C (122°F) in a non-exclusive use shipment or 82°C (180°F) in an exclusive use shipment.

Maximum temperatures, used to aid in determining allowable stress intensities, are given in Reg. Guide 7.6 for various classes of materials including low-alloy steel, martensitic stainless steel, carbon steel, austenitic stainless steel, and nickel-chromium-iron.

4.1.2 Normal Conditions of Transport

The "normal conditions of transport" are defined in 10CFR71, Sect. 71.71 for two ambient thermal states:

1. Hot environment - An ambient temperature in still air of 38°C (100°F) is to be assumed with the whole cask exposed to direct sunlight. The required maximum solar heating values are provided by 10CFR71 as adopted from IAEA standards.²² If the cask design has any auxiliary cooling capability for the neutron shield or containment

fluids, Reg. Guide 7.8 requires that such "systems should be considered to be inoperable during the hot environment condition." The maximum decay heat load is to be used for this case.

2. Cold environment - An ambient temperature of -40°C in still air is to be assumed with no solar heating. Two cases must be evaluated: (a) the maximum decay heat load is applied, and (b) no internal heat load is used. Reg. Guide 7.8 also requires that the possibility and effect of freezing of the neutron shield and/or containment fluids be considered.

Thermal analysis may also be required for the vibration condition in Sect. 71.71 in which thermal fatigue must be considered. Reg. Guide 7.8 specifies a review of the "thermal transients encountered in the loading and unloading of irradiated nuclear fuel." An ambient temperature range of from -29°C (-20°F) to $+38^{\circ}\text{C}$ (100°F), along with minimum-to-maximum values for decay heat and insulation, must be considered to determine the most unfavorable condition.

4.1.3 Accident Conditions

The "hypothetical accident conditions" that require thermal analysis are defined in Sect. 71.73, subsection c.3:

Thermal. Exposure of the whole specimen for not less than 30 minutes to a heat flux not less than that of a radiation environment of 800°C (1475°F) with an emissivity coefficient of at least 0.9. For purposes of calculation, the surface absorptivity must be either that value which the package may be expected to possess if exposed to a fire or 0.8, whichever is greater. In addition, when significant, convective heat input must be included on the basis of still, ambient air at 800°C (1475°F). Artificial cooling must not be applied after cessation of external heat input and any combustion of materials of construction must be allowed to proceed until it terminates naturally. The effects of solar radiation may be neglected prior to, during, and following the tests.

The above accident conditions were designed by the NRC to simulate the exposure of the cask to an enveloping fire. The initial condition for the fire transient is determined by assuming a steady-state, prefire

environment consisting of an ambient air temperature of 38°C (100°F) and maximum decay heat. At the start of the fire transient, any fluid in the neutron shield is assumed to be lost. During the 30-min fire, the cask is exposed to a radiant and possibly convective heat load calculated by assuming a heat source at 800°C (1475°F) with an emissivity of 0.9. The cask itself is assumed to have a surface absorptivity of 0.8 or higher. No convection film coefficients are explicitly given in 10CFR71 or in the Reg. Guides, but if an external convection load is applied in the analysis, the value used for the coefficient must be justified by the analyst. At the end of the 30-min transient, the ambient air temperature returns to 38°C (100°F), and the structural response of the cask is followed until it again returns to a steady-state condition.

4.2 REPOSITORIES - TITLE 10, CODE OF FEDERAL REGULATIONS, PART 72

In 1986 the NRC proposed an addition to the previously published instrument of Title 10, Code of Federal Regulations, Part 72 (10CFR72)³ that establishes the licensing requirement for the independent storage of spent nuclear fuel and HLW. In Section 72.92, as a part of the general design criteria requires the following:

- Structures, systems, and components important to safety. These components must be designed and located so that they can continue to perform their safety functions effectively under credible fire and explosion exposure conditions.
- Confinement barriers and systems. The spent fuel cladding must be protected during storage against degradation that leads to gross ruptures. The fuel must be otherwise confined so that degradation of the fuel during storage will not pose operational safety problems with respect to its removal from storage.

In Sect. 72.93, Criteria for Nuclear Criticality Safety, it states the design for criticality safety as

Spent fuel handling, packaging, transfer, and storage systems must be designed to be maintained subcritical and to prevent a

nuclear criticality accident. The design of handling, packaging, transfer, and storage systems must include margins of safety for the nuclear criticality parameters that are commensurate with the uncertainties in the handling, packaging, transfer, and storage conditions in the data and methods used in calculations, and in the nature of the immediate environment under accident conditions.

Section 72.105, Design Control, states the following:

The design control measures must provide for verifying or checking the adequacy of design, by methods such as design reviews, alternate or simplified calculational methods, or by a suitable testing program. ... The licensee shall apply design control measures to items such as the following: criticality physics, radiation, shielding, stress, thermal, hydraulic, and accident analyses.

When designing for the repository applications, NRC regulations are not well defined for the critical thermal requirements for the cask and storage structures. The accidental fire and explosion exposure can only be hypothesized through in-depth safety analysis to arrive at a reasonable design thermal condition.

5. APPLICATIONS OF THERMAL ANALYSIS PROGRAMS

5.1 NEEDS AND PROBLEM DESCRIPTION

As noted in the previous section on NRC regulations, the licensing requirements for repositories emphasize the controlling of criticality and credible fire and explosion accidents. No specific thermal conditions are given. At present, clearly defined thermal design and licensing requirements are to be found only in the application of nuclear waste packages for the transportation of spent nuclear fuel. A long design, regulatory, and operational history are available to draw upon when new designs for such packages are being considered. This is not the case for other nuclear waste management applications. However, all scenarios now under consideration require the transportation of spent nuclear fuel from the reactor to the storage site in NRC-licensed containers. In fact, it is expected that while under the control of DOE/OCRWM, the spent fuel may remain for a significant period of time in a licensed transport container. Thus, in seeking guidance with respect to thermal design issues and potential regulatory requirements for non-transportation storage packages, the designer must rely upon the experience gained in the design and licensing of transport containers commonly referred to as shipping casks.

In order to provide a rational basis upon which the cask designer can select heat transfer analysis tools and have confidence in their results, a significant effort is now under way to provide relevant benchmarks for the assessment of applicability of general purpose heat transfer codes.

Historically, there have been three accepted methods of evaluating computer codes: (1) "verification," which involves comparison of code results with problems having closed-form solutions, (2) "benchmarking," in which code results are compared with the results of other codes that have the ability to solve problems with similar physical phenomena and geometric properties, and (3) "validation," where the code is used to simulate actual integrated experiments with comparisons made between experimental data and code predictions. Of these three methods,

validation has the potential of inspiring the greatest confidence (limited only by the confidence one can place in the reliability of the experimental data) of a code's ability to provide accurate results for a given application. However, validation experiments that provide sufficiently accurate data can also prove to be very expensive to carry out and difficult to execute. Verification problems are able to demonstrate the reliability of the numerical algorithms used by a code to solve correctly the governing differential equations with applied boundary and initial conditions. These verification problems are typically limited in number and degree of complexity. As a result, benchmarking methods have been the most popular for code comparison studies.

As mentioned in the previous section, the primary purpose of the thermal analysis of a shipping cask is to provide temperature distribution data for normal and accident conditions. These data are used in a structural analysis of the cask to determine temperature-dependent material properties, thermally induced stresses, and areas of stress concentrations due to localized "hot spots." In ref. 23, emphasis is placed not only on stress, but also on ensuring that the maximum fuel temperature under accident conditions stays below a predicted fuel rupture temperature. This rupture temperature depends on "the cladding, the material of construction, the cladding thickness, the fuel material, the burnup, the cooling time, the specific power, the fuel damage caused by impact, etc."²³

5.2 SHIPPING CASK APPLICATIONS

Cask Geometry and Materials of Construction

Figure 1 presents a schematic of a longitudinal cross section of typical shipping casks. The specific design details of shipping casks can vary from one application to the next, but most are basically cylindrical with an internal cavity which contains the spent fuel assemblies. A fuel basket is employed to hold the fuel rods in place. Fuel basket designs using materials such as aluminum or copper with

water-filled borated stainless-steel tubes, inserted into the webbing of the basket to ensure subcriticality, have been reported in the literature.²⁴

A range of differing grades of carbon, low alloy, and stainless steels²³ have been used in the design of the inner and outer shells. These shells contain the gamma shielding, which can be made of lead, steel, depleted uranium, or combinations of these three. The neutron shield surrounds the outer shell and typically consists of water or borated water mixed with ethylene glycol contained by an outer water jacket. External fins are sometimes applied to assist in rejecting heat to the ambient, as well as providing additional protection from impact loads during a hypothetical dropping accident. Section 71.73 of 10CFR71 describes the 9-m (30-ft) mechanical drop test that requires the implementation of impact limiters, which usually are a crushable material such as balsa wood located on the top and bottom of the cask for protection of the package under drop conditions. Other design features might include: lifting trunnions, tie-down lugs, gaskets, drain plugs, relief valves, auxiliary cooling systems, piping, closure devices, expansion tanks, etc. Reg. Guide 7.9 (ref. 19) makes the following statement in its description of the standard format for 10CFR71 applications when the designer chooses to use an analytical model to demonstrate the adequacy of the cask thermal design: "the model should include gaskets, valves, fuel assemblies, and the overall package." For the normal conditions of transport, the maximum and minimum temperature distribution for the fuel assembly, containment vessel, shielding material, gaskets, valves, etc., must be included in the application. Under the accident condition, the transient temperature results are reported for critical items such as the fuel assembly, gaskets, valves, and shielding.

5.2.1 Heat Sources

Under normal conditions of transport, there are two sources of heat for a shipping cask: (1) internal heat generation in fuel rods caused by radioactive decay and (2) solar radiation incident on the outside of the

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Fig. 1. Schematic of longitudinal cross-section of a typical cask geometry.

cask. The level of decay heat for a fuel element is dependent upon its irradiation time (the time it spent in the reactor), the number of fissions occurring per unit time, and its cooling time (the time since discharge).²³ Maximum insulation data are provided in Reg. Guide 7.8 for flat and curved surfaces.²¹

In addition to decay heat and insulation, the accident condition provides for substantial heat gain from the assumed fire. The heat inputs from this 30-min fire are modeled as parallel, radiative, and convective sources at a constant temperature of 800°C (1475°F). The fire is assumed to have an emissivity of 0.9, and the exposed surface of the cask has an absorptivity of 0.8 or its actual value, whichever is higher.

5.2.2 Heat Transfer Mechanisms

The physical phenomena that an ideal thermal model should be able to simulate are (1) conduction, (2) internal or external, forced, or natural convection, (3) applied heat fluxes, (4) radiation to an ambient temperature, (5) radiation across gaps, (6) enclosure radiation, (7) internal heat generation, (8) contact resistances at part interfaces, (9) phase changes with consequent changes in mass redistribution and thermophysical properties, and (10) temperature and phase dependency of thermal properties and multiple materials within the cask. All three fundamental mechanisms of heat transfer (1) conduction, (2) convection, and (3) radiation are involved in the rejection of heat from a shipping cask. Conduction occurs through the fuel rod cladding, the solid sections of the fuel basket, the inner and outer shells, the gamma shielding, the impact limiters, the water jacket, any external fins, and other solid components such as gaskets, seals, lifting trunnions, valves, piping, etc. Convection can occur within fluids surrounding or flowing through the fuel basket, the neutron shield, and the outer surfaces of the cask. The solar heat load is applied to the model as a constant heat flux boundary condition. If the fuel bundle is not explicitly included in the model, then the decay heat is applied to the inner shell as a heat flux boundary condition. Thermal radiation from a fire is an

important mechanism during an accident condition and produces a heat load on the outside of the cask. At the beginning of the fire transient, if the fluids in the neutron shield and/or fuel cavity are assumed to be lost, radiation in parallel with natural convection in air can be significant. When computing radiant heat transfer within the fuel assembly or an empty neutron shield, it may also be necessary to include the effects of inter-reflections by means of a radiation enclosure model. The decay heat in the fuel assembly appears as an internal heat generation term in the model. Calculating the heat transfer across contiguous parts (e.g., gaskets, seals, bolted interfaces) typically requires the ability to include contact resistances in the model. If the gamma shielding is made of a material with a low melting point such as lead, then the capability of modeling phase changes can be important. If melting occurs, it may be advantageous to track the movement of the gamma shield if it is expected to change shape. During the fire transient, large temperature excursions can occur which may result in significant changes in thermal conductivity and specific heat, which should be taken into account by the model. All the above physical phenomena occur under both steady-state and transient conditions that require appropriate solution techniques in the model. The ideal model should have the capability of investigating three-dimensional, as well as two-dimensional effects.

5.3 INFORMATION SOURCES

The primary sources of information used by the authors of this report to select codes for review were: (1) a survey carried out and recently updated^{5,6} by A. K. Noor, George Washington University, of some 33 general heat transfer codes; (2) a report⁷ by M. J. Budden of Pacific Northwest Laboratory (PNL) describing an extensive study, performed in conjunction with a parallel effort by Sandia National Laboratories / Transportation Technology Center (SNL/TTC), of computerized thermal analysis methods for shipping casks; (3) workshops and information exchange meetings on analysis of shipping casks; (4) papers and reports available in the open literature describing benchmarking efforts by both

U.S. and international investigators; (5) a study⁸ by H. C. Claiborne et al., which compared several general heat transfer codes for use in the thermal analysis of a hypothetical nuclear waste repository; and (6) user's manuals of selected codes.

5.3.1 Noor Survey

In 1984, Dr. A. K. Noor of George Washington University published the results of an extensive survey of heat transfer codes.⁵ An update to this report was prepared in 1986 (ref. 6). The 1984 report reviewed some 38 codes using information obtained from a questionnaire; the 1986 report gives an overview of the capabilities of 33 codes. Tables are presented for each code, which offers information on such topics as

- goal of program system;
- method of analysis;
- space dimensionality;
- range of applications and phenomena;
- formulation;
- material properties and material models;
- initial conditions;
- boundary conditions and thermal loads;
- solution techniques;
- operational computers;
- documentation; and
- user interfaces (pre- and post-processors, input and output formats, etc.).

A number of codes surveyed by Noor appeared to have some potential in the analysis of shipping casks. The assumed potential was based on the survey's description of the physical phenomena reported to be modeled by the codes. These codes include:

1. ABAQUS - This is a proprietary general-purpose structural and heat transfer analysis code developed and maintained by Hibbitt, Karlsson, and Sorenson, Inc., Providence, Rhode Island.
2. ADINAT - A finite-element program for Automatic Dynamic Nonlinear Analysis of Temperatures. ADINAT is part of the ADINA system together with the general purpose stress analysis program ADINA developed and maintained by ADINA R & D Inc., Watertown, Massachusetts. The most recent version is dated 1984.
3. ANSYS - ANSYS is a proprietary finite-element code first offered by Swanson Analysis Systems, Inc., Houston, Pennsylvania, in 1970. The most recent version, Rev. 4.2, was released in 1985.
4. EAL - The Engineering Analysis Language (EAL) is a high order command language for structural, fluid, and thermal finite element analysis. This system is marketed by Engineering Information Systems, Inc., San Jose, California.
5. HEATING6 - This code represents an extensive revision of the HEATING5 code, both of which are public domain codes maintained and developed for the DOE and NRC by personnel at Martin Marietta Energy Systems, Inc., Oak Ridge, Tennessee.
6. MITAS II - The Martin Marietta Interactive Thermal Analysis System, Version 2.0 (MITAS II) is a lumped parameter finite-difference code owned and maintained by Martin Marietta Corp., Aerospace Division, Denver, Colorado.
7. THTD - The Transient Heat Transfer Program, Version D (THTD) is a proprietary finite-difference code developed and maintained by the General Electric Company.
8. TRUMP - TRUMP is a public domain computer program, originally developed at Lawrence Radiation Laboratory (now Lawrence Livermore National Laboratory) in 1967, with its latest version released in 1974.

5.3.2 Budden Report

A major effort has been under way at SNL/TTC in conjunction with PNL to investigate structural and thermal computer codes that could be

used to analyze irradiated fuel shipping casks and to develop methods of benchmarking candidate codes. In October 1984 at the Second Industry/Government Joint Thermal and Structural Codes Information Exchange Meeting, held at the National Bureau of Standards in Washington, D.C., a paper was presented by M. J. Budden of PNL describing the results of a study which focused on thermal codes.⁷ This investigation was divided into five areas: (1) a literature survey of the thermal aspects of shipping cask design, (2) an inventory of available computer codes, (3) an evaluation of selected codes, (4) the development of a set of "model" problems to be used for code testing, and (5) the use of the "model" problems to test five codes selected for a detailed assessment.

The literature survey revealed that even though experimental testing has been used in the past, the use of analytical methods to demonstrate the adequacy of the cask design has been increasing with time. The major issue driving the cask thermal design was found to be the fire transient condition required by 10CFR71. The major thermal phenomena concluded to be important in modeling the fire transient were radiation, conduction, convection, phase change, and three-dimensional effects. A review of 31 publicly available, general-purpose heat transfer computer programs resulted in five being selected for further investigation. The selected codes were: (1) TRUMP (ref. 25), (2) HEATING5 (ref. 26), (3) TEMPEST (ref. 27), (4) CINDA-3G (ref. 28), and (5) COYOTE (ref. 29).

Six "model" problems were devised to exercise the selected codes in the areas identified by the relevant thermal phenomena. Because of time and funding constraints, the model problem set did not address three-dimensional effects, variable properties, or phase change. The model problems did, however, cover the three accepted methods of code comparison: "comparison with an exact analytical solution (verification), comparisons with experimental results (validation), and code-to-code comparison (benchmarking)".⁷ Three of the five selected codes (TRUMP, HEATING5, and TEMPEST) were exercised by PNL, but CINDA-3G and COYOTE were investigated by SNL/TTC. Based on a review of their

user's manuals, Budden stated that none of the five selected codes were without their weaknesses:

Of the three codes tested at PNL, only TRUMP had three-dimensional gray body radiation capability; TEMPEST and HEATING5 had only one-dimensional gap radiation capability. Only HEATING5 and TRUMP had phase change capability, and only TEMPEST had general convection capability.

The different problems experienced by PNL with TRUMP, HEATING5, and TEMPEST in solving the problem set were considered to be minor and correctable. For HEATING5, problems arose with small meshes, a loose convergence criterion, and cells too close to the centerline in cylindrical coordinates. For TRUMP, problems occurred when the temperature node was not placed at the centroid of the control volume. Also, an inaccurate restart feature was found with TRUMP. For TEMPEST, an inefficiency arose due to an explicit and too simplistic stability limit imposed on the time step. However, it was found that the mesh selection problems for TRUMP and HEATING5 and the explicit time step limiter problem in TEMPEST were easily correctable with changes in the input data rather than by a reprogramming effort. It was demonstrated that an accurate solution could be easily obtained with any of the three codes tested by PNL. Detailed assessments of the two codes tested by SNL/TTC were not provided in ref. 7.

5.3.3 Benchmarking

U.S. BENCHMARKS

A program has been established under the lead of SNL/TTC with the purpose of gathering and disseminating information on thermal and structural codes that are applicable to shipping cask design.³⁰ As a part of that program, a benchmarking effort has been initiated in which candidate thermal codes are used to solve a set of four model problems. These four problems are described in Fig. 2, as taken from ref. 31. The benchmarking method of code comparison was chosen over the validation and verification techniques due to the complex nature of the

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CYLINDER WITH INTERNAL
HEAT SOURCE.
MODEL PROBLEM 1

CASK WITH ANNULAR REGIONS.
MODEL PROBLEM 2

CASK WITH RADIATION SHIELD.
MODEL PROBLEM 3

CASK WITH ANNULAR REGIONS
AND RADIATION SHIELD.
MODEL PROBLEM 4

Fig. 2. U.S. Model Problems 1 through 4 (taken from ref. 31).

combined heat transfer mechanisms involved in rejecting heat from a shipping cask. It was their judgment that neither relevant closed-form solutions nor sufficiently reliable experimental data were available to allow a program based solely on validation or verification. It was intended that the model problem set be simple, exploring most of the relevant thermal phenomena, and be "cask-like" in nature. The problems involve simplified representations of typical cask geometries in two dimensions. The ability to model multiregion and multimaterial sections in axisymmetric (r - z), cylindrical (r - θ), and mixed cylindrical/cartesian coordinate systems is required. Steady-state and transient (simulating the fire transient) solutions are required with convection, external and internal radiation, and volumetric heat generation employed as boundary conditions. The fuel rod assembly was not addressed explicitly by the problem set, nor were the physical phenomena of phase change, internal convection, temperature dependent properties, or three-dimensional effects included.

Bryan et al.³¹ presents a comparison of benchmarking results for seven codes: HEATING6, TRUMP, HEATING5, TEMPEST, TAC-2D, COYOTE, and CINDA-3G. Model Problem 1 (Fig. 2) is a one-dimensional problem with a two-region cylindrical geometry, an internal heat generation source, and convective cooling to the ambient. This is the only model problem of the set of four for which an analytical solution is available. All of the tested codes produced results to within 0.5°C of the exact solution. Model Problem 2 is also a one-dimensional problem requiring both steady-state and transient solutions. The physical phenomena that must be modeled include internal heat generation, conduction, and radiation. The results indicate that all of the codes predicted the same transient behavior and calculated temperature profiles that were close to each other. Model Problems 3 and 4 both involve two-dimensional radiation problems simulating a cask geometry with an intervening radiation shield. The solutions generated by the tested codes fall into two groups depending on the code's ability to model radiant interchange between multiple surfaces. The codes with a simple radiation model (i.e., gap radiation) such as HEATING5, TEMPEST, and COYOTE, showed good agreement with each other. The codes that were capable of handling

radiation enclosure problems (enhanced radiation model), such as TAC-2D and HEATING6, also showed good agreement. TRUMP and CINDA-3G were used both with the enhanced and simple radiation models. Their predictions agreed with the results of the two groups. Recently, Sanchez¹⁶ also tested seven codes (i.e., TRUMP, HEATING5, TEMPEST, COYOTE, CINDA-3G, TAC-20, and Q-TRAN) for the four model problems related to shipping cask design. All codes evaluated yield reasonable solutions agreeable to each other.

INTERNATIONAL BENCHMARKS

An international effort is also proceeding, under the auspices of the Organization for Economic Cooperation and Development (OECD), to develop and implement a model problem set for the benchmarking of thermal codes used in the design of shipping casks.³² The Nuclear Energy Agency Committee on Reactor Physics (NEACRP) sponsored meetings in May and October of 1985; with sessions attended by international specialists for the purpose of defining such a problem set. The result was a series of seven benchmarking problems divided into two phases. The four problems in phase 1, designated US-1, US-2, UK-1, and UK-2, included two from the problem set developed by SNL/TTC (Model Problems 1 and 3). UK-1 addressed the very difficult computational task of modeling the internal radiant interchange within a fuel rod assembly, while UK-2 focused on the outside, finned surface of the cask during the fire transient. The three problems of phase 2, designated FR-1, US-3, and UK-4, were designed to test the candidate code's ability to model phase change, temperature-dependent properties and boundary conditions, and anisotropic thermal conductivity (simulating natural convection currents in a water-filled cavity). SNL/TTC has taken the lead in coordinating the effort to apply these problems in the benchmarking of thermal codes used in the United States. No comparison studies of the complete international benchmarking problem set were found in the literature. A comparison of results using three codes (HEATING6, COBRA, and RIGG) was published for problem UK-1 by a British investigator.³³ A

comparison of the results indicated agreement between RIGG, COBRA and HEATING6. The US-3 and four international problems are shown in Fig. 3.

5.4 REPOSITORY APPLICATIONS

A geologic repository is an underground system of tunnels resembling a large mining complex for the disposal of HLW. Salt domes, bedded salt, basalt, and tuff have been investigated by DOE for the first repository site. The Nuclear Waste Policy Act Amendments of 1987 require the site to be at Yucca Mountain, Nev. (tuff). Less dense, deeply buried salt forms a salt dome when the overlying pressure of sedimentary rock lessens, forcing the salt up toward the surface. Bedded salt consists of salt deposits interlayered with other sedimentary rock formations. These deposits were formed millions of years ago when ancient seas evaporated. Basalt is a fine-grained solidified lava, rich in iron and magnesium minerals. It is generally hard and dark in color. Tuff is a medium-grained rock formed of small, compacted fragments of volcanic glass, mineral grains, and rock particles. The thermal behavior of the repository within the geologic media is important in studying the effects on its natural moisture content, structural strength, heat capacity and conductivity, permeability, porosity, and solubility.

A typical repository can be modeled as a room and pillar construction having the room floor at a depth of 300 to 1200 m (1000 to 4000 ft) below the earth's surface. Eighteen-m (60-ft)-wide pillars separate very long rooms that are 7.6 m (25 ft) high and 6.1 m (20 ft) wide. The waste canisters provide the thermal loading and are buried in approximately 41-cm-diam (16-in.-diam) vertical holes in the room floor. A concrete plug may exist between the top of the waste canister and the floor level. The soil or rock has constant thermal properties from the earth surface to 305 m (1000 ft) above the repository room and from 305 m (1000 ft) to 3050 m (10000 ft) below the repository room. The initial isothermal temperature of the rock is dependent on the earth depth and the applicable geological zones.

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**BENCHMARK PROBLEM FR-1 GEOMETRY
(HALF SECTION OF CASK).**

BENCHMARK PROBLEM UK-1 GEOMETRY.

**BENCHMARK PROBLEM UK-2 GEOMETRY
WITH FINITE-DIFFERENCE MESH
SUPERIMPOSED.**

**BENCHMARK PROBLEM UK-4 GEOMETRY
WITH FINITE-DIFFERENCE MESH
SUPERIMPOSED.**

**BENCHMARK PROBLEM US-3 FIN
GEOMETRY.**

**BENCHMARK PROBLEM US-3 GEOMETRY
(HALF SECTION OF BASKET/CASK
ASSEMBLY).**

Fig. 3. International Model Problems (taken from ref. 32).

HEAT TRANSFER MECHANISMS

Conduction is assumed between contacted surfaces. Radiant heat transfer is considered important from the floor to the ceiling of the room, and convection is not a significant contributor. The emissivity and view factors of the structure need to be estimated. The thermal load from the buried waste canister can be treated as a time-varying heat flux load.

5.4.1 Code Comparisons

A code comparison study was carried out by Claiborne et al.⁸ of several heat transfer codes including HEATING5, TRUMP, ADINAT, and SINDA (a version that was very close to the earlier CINDA3G version). The focus of this study was a thermal analysis of a hypothetical nuclear waste repository buried deep in a geologic media (salt) 610 m (2000 ft) below the surface. Two- and three-dimensional transient models were developed using temperature dependent thermal properties, radiation and conduction heat transfer, and time dependent heat generation. ADINAT was found to agree within $\pm 5\%$ of the HEATING5 results for the full transient. TRUMP results agreed with HEATING5 to within $\pm 5\%$ in the early part of the transient, and then began an oscillatory behavior with up to 25% deviations at longer times. It was reported that this could have resulted from time steps that were too large or from some unknown system problems. Difficulties were encountered with SINDA in getting the temperature-dependent thermal conductivity feature to work with the IBM computer used for the study. Reasonable agreement with HEATING5 was obtained with SINDA when the problem assumed constant thermal conductivity.

In 1981 Matalucci et al.¹⁴ compared ANSALT, DAPROX, JAC, MARC, REM, SANCHO, SPECTROM, and STEALTH for a bedded salt repository. In 1984 Coffman et al.³⁴ evaluated ADINAT, ANSYS-THERMAL, HEATING6, SINDA, and STEALTH for use in waste package analysis, while Graham⁹ compared HEATING6 to TEMP, WECAN, and THAC-SIP-3D for a repository problem.

The Matalucci et al. study was primarily a structural code comparison but the Coffman results are limited to a portion of the repository (i.e., the waste package). Therefore, even though each study is a useful comparison of a few codes, no study allows a generalization of the codes that were compared. The Shuker study shows good agreement between HEATING6 and WECAN but is too limited for any general conclusion to be drawn.

5.5 CODE VERIFICATION

Computer code verification requires "assurance that a computer code correctly performs the operation specified in a numerical model".¹ This verification is usually accomplished by comparing code results with a hand calculation, an analytical solution or approximation, or a verified code designed to perform the same type of analysis (benchmarking). A verification procedure will require that a verification plan be prepared. The plan shall identify the computer code to be verified (name and code version number), outline the approach to be followed to verify the code, and define the documentation that will be required in the verification report to assure that the specified verification has been completed. In addition, the plan shall contain or refer to written description of the mathematical models and numerical methods used in the code, user instructions, and the development plan, if one exists.

Although most codes claim to be verified, the HEATING6 code has been verified in accordance with the rigorous procedure described above. The Verification Plan and the Verification Report for HEATING6 are given in refs. 35 and 36, respectively. HEATING6 has also been verified by Martin Marietta Energy Systems, Inc.,³⁷ and is used by NRC for benchmarking other thermal codes.

6. CODE ASSESSMENTS

6.1 THERMAL CODE SELECTION CRITERIA

Since actual benchmarking is beyond the scope of this report, the authors must rely on their experience and the various cited references for their code assessments. Twenty-one codes were analyzed by different code evaluators in their respective studies. These codes are tabulated in Table 7. Although each of these studies had different objectives, the criteria they used in selecting the codes for analysis and the conclusions they reached provide some insight into an overall assessment of thermal codes. Table 7 indicates that HEATING5,6 has been included in five out of the six studies, followed by SINDA (four studies), and TRUMP (three studies). THAC-SIP-3D, ADINAT, COYOTE, and TEMPEST have all been included in two studies. The Claiborne et al.⁸ study notes that the HEATING series has been used extensively in repository calculation, and that ADINAT and SPECTROM-41 are FE techniques which compare favorably with the FD techniques. Matalucci et al.¹⁴ evaluated the capabilities of different codes to solve thermal/structural interaction problems associated with a bedded salt repository, and therefore, the codes selected required displacement or strain capability. This capability is beyond the scope of this study, and therefore, few of the codes selected by Matalucci are useful to this assessment. Coffman et al.³⁴ included a summary of thermal analysis code capabilities, which is reproduced here as Table 8 and a selection criteria summarized in Table 9. The most flexible of the codes summarized is the ANSYS-THERMAL finite-element code and the SINDA finite-difference code. No numerical comparisons are presented in this study. Budden⁷ developed a code matrix and selected three codes for problem solution based on the capabilities of the code as stated in the user's manual. The three codes tested are HEATING5, TRUMP and TEMPEST.

As detailed in Sect. 1, the authors have selected criteria of thermal analysis code selection as follows:

- Used by a DOE/OCRWM contractor
- Suitability

Table 7. Thermal code comparisons

	Claiborne et al.	Matalucci et al.	Coffman et al.	Budden et al.	Sanchez et al.	Graham et al.
ADINAT	X ^a		X			X
ANSALT		X				
ANSYS-THERMAL			X			
COYOTE				X	X	
DAPROK		X				
HEATING5,6	X		X	X	X	X
JAC		X				
MARC		X				
Q-TRAN					X	
REM		X				
SANCHO		X				
SINDA/CINDA-3G	X		X	X	X	
SPECTROM-41	X					
STEALTH		X	X			
TAC-2D					X	
TEMP						X
TEMPEST				X	X	
THAC-SIP-3D	X					X
THTD				X		
TRUMP	X			X	X	
WECAN						X

^aX = code evaluated by study.

Table 8. Summary of thermal analysis code capabilities^a

Code	Dimension	Solution Procedure	Phenomena ^b					
			Conduction	Convection	Radiation	Mass Flow Transport	Non-linear	Change of Phase
ADINAT	3	Finite element	X	*	*		*	X
ANSYS-Thermal	3	Finite element	X	X	X	**	X	***
HEATING6	3	Finite difference	X	*	*		X	X
SINDA	3	Finite difference	X	X	X	X	X	X
STEALTH-Thermal	3	Finite difference	X	****	****	X	X	X

^aReprinted with permission from Coffmann et al. (ref. 34).

^bX = has capability;

* = convection and radiation heat transfer is allowed only at model boundary;

** = pipe flow element included;

*** = by table input of thermodynamic property relationships;

**** = solves for conductive heat flux; has convection and radiation boundary conditions.

Table 9. Thermal code selection criteria used^a

-
1. Codes currently being used by the DOE and NRC should be included.
 2. Other codes most likely to be of use to the NRC should be included.
 3. Each of these codes should satisfy at least one of the following criteria:
 - Be able to perform a function not included in the NRC codes.
 - Be superior to the NRC codes under some circumstances.
 - Be widely used and generally accepted.
 4. All the codes should be unclassified and documented well enough to permit preparation of a summary.
 5. If several versions of a code are available, the most recent should be used.
 6. The total number of codes selected should be consistent with the project budget.
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^aReprinted by permission from Coffman et al. (ref. 34).

- Verification and benchmarking
- Availability, ease of use, cost to use
- Math modeling technique
- Documentation and quality assurance
- Computer compatibility (type and language)

6.2 CODE ASSESSMENTS

6.2.1 Current DOE/OCRWM Code Use

In this assessment, DOE/OCRWM contractor code use is an important criterion in the recommendation and selection of thermal codes. The DOE/OCRWM contractors and subcontractors have been surveyed to determine principal code use by DOE/OCRWM. Concentrating on general-purpose codes from Tables 4 and 5 and using Table 7 to guide the selection process, fifteen codes used by DOE/OCRWM communities are selected to be evaluated further. The code names and user organizations are listed in Table 10. A matrix, shown as Table 11, is developed based on the capabilities stated in the user manuals.

6.2.2 Code Suitability and Modeling Capabilities

The computer codes that meet DOE/OCRWM needs must yield sufficiently accurate results for the physical system and phenomena they are to simulate. The codes must be capable of modeling the latest engineering concepts evolved in the design of shipping casks and repositories. The following discussion presents some previous evaluations on the suitability and capabilities of different codes.

CASK-LIKE PROBLEMS

Budden presents temperature histories and temperature distributions for six model problems for TRUMP, HEATING5, and TEMPEST. The following comparisons were among those noted:

- None of the three codes clearly outperformed the other two on all six model problems.

Table 10. OCRWM code use

Code	User
ADINAT	ORNL/Sandia
ANSYS	Sandia
COBRA-SFS/HYDRA-II	PNL/LLNL
COYOTE/NACHOS	Sandia
DOT	Fluor/Intera
HEATING5/HEATING6	ORNL/Battelle/ONWI
SINDA	Sandia
SPECTROM-41	RE/SPEC
STEALTH	ONWI
TEMP	ONWI
TEMPEST	PNL
THAC-SIP-3D	ORNL
TOPAZ/TACO	LLNL
TRUMP	LLNL

Table 11. Code capability matrix

CAPABILITY \ COMPUTER CODE NAME		ADINAT	ANSYS THERMAL	HYDRA	DOT	HEATING 6	NACHOS	COYOTE	SINDA	SPECTROM 41	STEALTH	TACO	TEMPEST	TOPAZ 3D	TRUMP
GOAL OF PROGRAM	GENERAL PURPOSE	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	COMMERCIAL	•	•						•	•	•				
	RESEARCH	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	PUBLIC			•	•	•	•	•	•			•	•	•	
	OTHER														
METHOD OF ANALYSIS	FINITE ELEMENT	•	•		•		•	•		•		•		•	
	FINITE DIFFERENCE			•		•			•		•		•		•
	BOUNDARY INTEGRAL														
	PERTURBATION TECH														
	HYBRID														
GEOMETRY	DIMENSIONALITY	1,2,3	1,2,3	1,2,3	1,2	1,2,3	1,2	1,2	1,2,3	1,2	1,2,3	1,2	1,2,3	1,2,3	1,2,3
	CARTESIAN	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	CYLINDRICAL	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	IRREGULAR CELL	•	•	•	•	•	•	•	•	•				•	
	VARIABLE GRID	•	•	•	•	•	•	•	•	•	•	•	•	•	•
SOLUTION ALGORITHMS	SIZE LIMITS			8000		10000			4100				6000		1000
	STEADY STATE	•	•	•	•	•	•	•	•	•		•	•	•	•
	TRANSIENT EXPLICIT	•		•	•	•	•	•	•		•	•	•		•
	TRANSIENT IMPLICIT	•	•	•		•		•	•			•	•	•	•
	SPECIAL STEADY STATE OPTION			•		•			•				•	•	
SOLUTION CAPABILITIES	AUTOMATIC TIME STEP		•	•		•					•		•		•
	CONDUCTION	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	CONVECTION		•	•		•	•		•	•			•		•
	RADIATION		•	•		•			•		•	•	•	•	•
	COMPUTED CONVECTION			•			•						•		
	VARIABLE PROPERTIES	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	PHASE CHANGE	•	•			•	•		•			•		•	•
	PHASE CHANGE + CONVECTION						•								
	MULTIPLE MATERIALS	•	•	•	•	•	•	•	•	•	•	•	•	•	•
BOUNDARY CONDITIONS	COMPANION STRUCTURAL CODE	•	•		•					•	•			•	
	TRANSIENT B C	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	TEMPERATURE	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	HEAT GENERATION	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	HEAT FLUX	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	CONVECTION	•	•	•	•	•	•	•	•	•		•	•	•	•
	RADIATION	•	•	•	•	•	•	•	•		•	•	•	•	•
MISCELLANEOUS	COMBINATIONS	•	•	•	•	•		•	•			•	•	•	•
	RESTART	•	•	•		•	•	•	•	•	•		•	•	•
	AGE	6		5	11,7	7	7	6	17	4	15		6	2	15
	DATA CARD INPUT	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	AVAILABLE ON OTHER MACINES	•	•			•		•	•	•	•		•	•	•
	INTERNAL GRAPHICS	•	•	•			•	•		•	•	•	•	•	
	VERIFICATION	•	•	•	•	•	•	•		•	•		•		•
	AVAILABILITY	•	•	•	•	•		•	•	•	•	•	•	•	•
	DOCUMENTATION	•	•	•	•	•		•	•	•	•	•	•	•	•

- All three codes could be made to obtain a very accurate answer to Model Problems 1, 2, and 4 (those model problems where an "exact" answer was known). For Model Problem 3, which was a natural convection problem, it was only appropriate to use TEMPEST, since HEATING5 and TRUMP did not possess the convection capability. For Model Problem 3, TEMPEST compared fairly well with the experimental data. For the other model problems all three codes were judged of approximately equal accuracy, although some changes in the default convergence criteria or time step were sometimes necessary.
- Conclusions about actual computer running speed should be made very cautiously because of the many variables involved. For Problem 1, TEMPEST was faster than TRUMP or HEATING5, by a factor of 2 or more. For some steady-state calculations, TEMPEST was roughly a factor of ten times faster than either TRUMP or HEATING5. However, the transient computing times for Model Problems 5 and 6 show that for these more realistic problems the TEMPEST timing advantage is reduced. Furthermore, in the one three-dimensional mesh that was tried on Model Problem 2, the TEMPEST times were much closer to the run times for HEATING5 and TRUMP. The TRUMP steady-state solution algorithm was less efficient compared with TEMPEST or HEATING5 on Model Problems 5 and 6. The reason for this difference is not clear, although the TRUMP steady-state convergence criteria may need to be relaxed for these problems.
- Conduction capabilities of all three codes are roughly equivalent, with TRUMP possibly having a slight edge because of its irregular geometry capability. However, caution should be used in selecting TRUMP nodes at positions other than the centroid of the control volume. Radiation capabilities are most general in TRUMP; HEATING5 and TEMPEST have a considerably more approximate radiation model. TEMPEST is the only one of the three codes that has convection capabilities.

Sanchez¹⁶ presents temperature histories and temperature distributions for the first four of the problems tested by Budden for SINDA, COYOTE, HEATING5, Q-TRAN, TAC-2D, TEMPEST, and TRUMP. He indicated good agreement among the various code solutions obtained with the same modeling technique. Sanchez notes that the most important feature of a code is its modeling capability. He points out the following limitations for each of the codes tested:

- A difficulty in using CINDA-3G/SINDA is that its generality results in long learning times.
- Limitations of COYOTE include its inability to handle convection and radiation generally.
- Limitations of HEATING5 include (1) it does not have general gray body radiation and (2) change-of-phase capabilities cannot be used with implicit techniques.
- A difficulty of using Q-TRAN is that it does not have options for cylindrically symmetric and spherically symmetric geometries.
- The principal limitations of TAC-2D are the necessity of fitting the problem to one of the three coordinate systems, the one-dimensional treatment of radiation, and no direct provision for phase change.
- Limitations of TEMPEST are twofold: (1) the code does not have irregular geometry capability and (2) it uses a simple one-dimensional "gap radiation" model where radiation occurs only between nearest neighbors.
- Limitations of TRUMP include (1) it cannot model convection generally and (2) its general mesh capability and lack of a computer-generated mesh map make it difficult to track down geometric modeling errors.

REPOSITORY-LIKE PROBLEMS

Claiborne et al.⁸ presents temperature histories of a two-dimensional repository problem for HEATING5, SPECTROM-41, TRUMP, and ADINAT with the following observations:

- The maximum temperatures predicted by each code occur at the same printout time.
- Typically, the largest separation, or error, is seen at the time the maximum temperature is seen; the exception is TRUMP, which begins an oscillatory behavior at that time.
- TRUMP predicts a higher temperature farther from the source and a lower temperature closer to the source than the other codes.

Claiborne et al. (ref. 8), presents temperature histories for the three-dimensional problem for HEATING5, SPECTROM-41, and ADINAT with the following observations:

- The peak temperature predicted by each code occurs at the same printout time.
- The curves tend to grow together with time.

Graham⁹ compared HEATING6, THAC-SIP-3D, and TEMP for a three-dimensional reference repository (noted as Problem 4) where the results are in good agreement.

The code TRUMP is dropped from further evaluation for the various limitations discussed above. TEMPEST is retained for its capability to handle computed convection. Because of the lack of general radiation and convection capabilities, and the limited application to two-dimensional models only, the code COYOTE is not considered any further. Similarly, DOT is two-dimensional and can not model internal convection, radiation and phase change, thus it is not evaluated further. STEALTH is a special rock mechanics program, designed primarily to analyze heat conduction for repository application. It is not considered very well suited for general applications. TACO is not evaluated because it is a two-dimensional code, and its solution capabilities are combined into the newly developed three-dimensional code TOPAZ3D. HEATING6 code is the enhanced version of HEATING5 with added gray body radiation capability. Therefore, HEATING5 will not be evaluated.

6.2.3 Verification and Benchmarking

All the codes from Table 11 have been verified to some extent. TOPAZ3D is the most recently developed code. Although it evolved from the code TACO and TOPAZ2D, the verification status has not been well established. However, the program is capable of modeling enclosure radiation and is coupled with a companion structure code, making it well suited for DOE/OCRWM application and justified for further verification effort. The program tape is loaded with sample problems to facilitate

this task. The HEATING6 code has recently been verified by ORNL. 31,32,37

6.2.4 Availability, Ease of Use, Cost to Use

In order for a DOE/OCRWM contractor to use a thermal analysis code for a particular application, the availability and cost to run the code must be considered. This includes license or membership fee to acquire the program, computer hardware required to run, and manpower investment needed to learn and effectively use the code.

The code COBRA-SFS was recently developed for DOE by Pacific Northwest Laboratory (PNL) to analyze spent fuel storage applications. COBRA is a thermal/hydraulic code that uses a hybrid method of lumped finite-volume nodalization and network model to solve for natural convection, radiation and heat conduction in physical models resembling typical fuel storage casks. Being very specialized in solving flow recirculation and radiation between fuel rods, the code COBRA can also be used for general purpose thermal analysis.

As a recent, specialized code that is still being developed, COBRA has a short history of validations and limited benchmarkings. The effective usage of this code requires comprehensive knowledge of the physical phenomena in the model in order to select appropriate parameters to be used as input. The code is limited to be run on mainframe computers CRAY and CDC. It is recommended that the code COBRA be considered in future assessments and evaluations as the code is further developed, verified and converted to be run on other mainframe computers. The code HYDRA-II is a FD thermal/hydraulic program developed by PNL for DOE. HYDRA-II has the similar convection and radiation capabilities as COBRA-SFS but is easier to use. The code HYDRA is available on more mainframe computers than COBRA-SFS. Therefore only HYDRA-II will be considered further.

NACHOS, developed by Sandia National Laboratories, is not yet authorized for release by DOE because of national security. SINDA/CINDA-3G is a powerful and versatile program but was judged difficult to use and requires a long learning time.

6.2.5 Math Modeling Technique

After the previous evaluation process, only seven thermal analysis codes remain to be evaluated. The codes are ADINAT, ANSYS-THERMAL, HEATING6, HYDRA-II, SPECTROM-41, TEMPEST and TOPAZ3D. All are general purpose codes. HYDRA-II and TEMPEST are thermal/fluid programs that have the only computed convection capabilities. The other codes are thermal/solid programs. The codes utilizing FEMs are each coupled with a structural analysis program. Table 11 lists the general capabilities of each code.

6.2.6 Documentation and Quality Assurance

The computer code for DOE/OCRWM use should be well documented according to NRC guidelines¹ in terms of the mathematical theory, numerical method, program flow chart, input/output utilities, sample problems and results, capabilities and incapacabilities, error interpretation, modeling optimization technique and, most importantly, the quality assurance record and current program updates and revisions.

Currently only the commercial program developers for ADINAT and ANSYS maintain traceable quality records and updates through the established user group organizations. HEATING6 and TEMPEST codes are documented in compliance with the NRC guidelines¹ but have no formal maintenance program. HYDRA-II and TEMPEST are excellent programs developed through DOE funding by Battelle Pacific Northwest Laboratory. The program support has been transferred to NESC, where the future code support, maintenance, and quality assurance may be limited.

6.2.7 Computer Compatibility (Type and Language)

All the programs listed for evaluation can be installed on all the major mainframe computers. The commercial programs ADINA and ANSYS are designed to be used on interactive work stations and PCs through a central mainframe computer. HEATING6 has a version being developed that

can be installed on the PC. TOPAZ has a two-dimensional version, TOPAZ2D, available on the IBM-PC.

6.3 CODE SELECTION

Based on the above discussion and the various studies cited in this report, three computer codes are considered the most applicable for OCRWM applications:

ADINAT - The companion heat transfer code of the general-purpose stress analysis code ADINA84, ADINAT is a FEM program, developed and maintained commercially by ADINA R & D, Inc. The ADINA program series can handle conduction, convection, radiation, fluids in porous media and phase change. It is very suitable for complicated geometry. The modeling grid is compatible with the companion stress analysis program ADINA and the fluid mechanics code ADINA-F, a great ease when nodal temperatures are required. The user manual is easy to understand and use. A very advanced graphics presentation program package is available for input checking and output interpretation. The program is widely used by the DOE/OCRWM community for benchmarking other thermal and stress analysis programs. A large pool of user knowledge can be drawn upon when help is needed. The program source codes are available on a large selection of computers. It is also installed on a network of timesharing services, such as Scientific Information Service of Control Data in Kansas City, Missouri, or Boeing Computer Service in Bellevue, Washington. The disadvantages are the following: (1) a licensing fee required for the user's own mainframe computer installation, (2) the ability to handle radiation and convection is limited to boundary elements, (3) the computer input is limited to fixed format (to an occasional user, this could be a frustrating experience), and (4) no thermal properties libraries can be used to expedite the thermal properties input process.

ANSYS - The code is commercially offered by Swanson Analysis Systems, Inc. It is a general-purpose, FE program for engineering analysis. ANSYS can solve a wide range of structural, electromagnetic, and heat transfer problems and is used to determine displacements, forces, stresses, strains, temperatures, and magnetic fields. Analysis types available in ANSYS are the following: static, eigenvalue buckling, mode frequency, nonlinear transient dynamics, linear transient dynamics, harmonic response, heat transfer, magnetics, and substructures. Structural and heat-transfer analyses utilize the same FE model that may be made in one, two, or three dimensions. One of the most powerful features of ANSYS is the ease with which a thermal model can be used in a structural analysis. The program is packaged with preprocessing and postprocessing capabilities that include automatic mesh generating, resulting plotting and color graphics. The program is available on all major mainframe computers and timesharing centers such as Scientific

Information Service of Control Data in Kansas City. The thermal analysis program has been previously verified by NRC in a licensing application for a shipping cask. ANSYS, Rev. 4.2, is the most current release. The program can model all the physical phenomena required in the waste applications with the exception of computed convection. The disadvantages are the cost to lease the program and the unavailability of the source code. The latter limits the application and input debugging capabilities of the thermal analyst, which may contribute to the lack of general verification and usage by the OCRWM communities.

HEATING6 - An upgraded code from the large general-purpose conduction computer code HEATING5, HEATING6 is capable of modeling convection, phase change, and spatial radiation in one, two, or three dimensions, during steady state and transients, and with all types of boundary conditions. HEATING6 is a FDM code, widely used by NRC and the DOE/OCRWM community not only for thermal analysis but also for benchmarking. It is very well verified. Actively maintained by Oak Ridge National Laboratory personnel through DOE and NRC funding, the program documentation is easy to understand and user oriented. A versatile post processor is available for graphic presentation of results. The thermal properties of common materials are stored in a computer library that can be extracted when the main program is running. The program is readily available from the code custodian at no cost to the user. A PC version is being developed. The disadvantages are the lack of provision to handle irregular geometries and limited internal modeling of convection and radiation. The radiation model is under improvement, but convection is calculated with an equivalent coefficient. The radiation and convection heat transfer are limited only to parallel or boundary surfaces. It is not designed to handle an irregular grid, but it is very easy to set up and use.

The following thermal analysis programs are considered applicable and can be used for special purpose and objectives.

HYDRA-II is a general-purpose, three-dimensional hydrothermal code that solves energy, momentum, and continuity conservation equations. This FD code can calculate temperatures within canisters containing spent fuel sub-assemblies. The code explicitly treats conduction, convection and thermal radiation in a fully coupled fashion. The code is intended primarily to provide steady-state solutions, but it has been used for transient problems. It can also compute the internal pressure distribution and gas velocities. Inertial forces are assumed small compared to viscous forces for the convection flow, and the surfaces of the fuel rods are assumed to emit and reflect radiation diffusely.

The code is available from National Energy Software Center. The cask model geometry needs to be axisymmetrical and regular shaped. No provisions have been made in the code to model phase change. No companion of structural analysis code is available. The analysis output provides only the printout form. No post-processing or graphic

capabilities are provided. It is a recently developed code, and verifications are not extensive. Because of funding restraints, further code support, maintenance, and developments are limited.

SPECTROM-41 - Originally developed under the name TRANCO specifically for the FE analysis of the thermal problems associated with the underground disposal of radioactive waste, SPECTROM-41 is a special-purpose thermal/rock mechanics code. The model is limited to two-dimensional geometry and predominant heat conduction phenomena. Convection is treated as a boundary condition. There is no radiation capability, and it can not treat phase change. Pre- and postprocessors are available to check input or to present output. There is a companion stress analysis code, SPECTROM-32. The documentation complying with NRC guideline¹ is being prepared and is soon to be released.

TEMPEST is a large, FD, general-purpose conduction/convection code developed at Pacific Northwest Laboratory. The advantage of TEMPEST is that it solves computed convection. The code is three-dimensional. It cannot compute phase change with or without convection. Its conduction and radiation capabilities are similar to HEATING5, thus it too has only a gap radiation model. Like HEATING5 it is very easy to set up and use, and the documentation and verification are excellent. It comes with a user's manual as well as a verification manual. Approximately 12 sample problems containing sample input and output are provided.

TOPAZ3D - An implicit FE program for three-dimensional heat transfer analysis, TOPAZ3D was developed and is used by Lawrence Livermore National Laboratory (LLNL). TOPAZ3D evolved from the code TACO3D and the two-dimensional heat transfer code TOPAZ2D. Besides conduction, enclosure radiation and phase change, it can handle chemical reaction kinetics. The boundary condition and internal heat generation can be represented by a user-defined function. Convection is treated as a boundary condition. Both natural and forced convection coefficients are calculated automatically by the program. Thermal stresses can be calculated using the solid mechanics code NIKE3D which reads the temperature state data calculated by TOPAZ3D. For complex models, a mesh-generation code and preprocessor INGRID is available from LLNL. The analysis results can be presented on an interactive post-processor program TAURUS for temperature contour, temperature-time history plots. The 2-D version TOPAZ2D can be run on an IBM-PC. TOPAZ series computer codes are actively maintained by the code developer. The codes are readily available at no cost from LLNL. Since the code is relatively new, extensive benchmarking or verification has not been performed. More verifications on this code will greatly enhance the value of this program.

7. CONCLUSIONS AND RECOMMENDATIONS

7.1 SUMMARY

A review of the open literature on the thermal analysis of shipping casks and repositories has been completed. The shipping cask analyses are carried out in support of structural studies that are used to demonstrate to the NRC that the proposed shipping cask design can satisfy the requirements of 10CFR71. The repository analyses are performed to demonstrate that the waste storage design can meet the general requirements of 10CFR72 and assist in the study of environmental impacts. An extensive program has been under way at SNL/TTC in conjunction with PNL to assess the capabilities of a wide range of publicly available thermal and structural computer codes. As a part of that effort, SNL/TTC has developed a set of "cask-like" model problems that are being used as benchmarks for code comparison studies. International efforts are also under way to encourage the use of benchmarking to evaluate the applicability of specific thermal codes to shipping cask analysis. Even though shipping cask evaluations may not address all the thermal issues that arise during the design of a nuclear waste management system, the design conditions for these containers do represent one of the more demanding thermal environments confronted by the analyst. The general guideline in the proposed regulation of 10CFR72 can be used to help design and analyze underground repositories. Several analyses have been performed to demonstrate the accuracy of thermal codes for use in a repository application [Claiborne et al.,⁸ Matalucci et al.,¹⁴ Graham⁹]. Sect. 5 summarizes these studies.

7.2 CODE RECOMMENDATIONS

No single code is sufficient for all applications. Every code has some deficiencies. We strongly recommend that the thermal analyst should first determine the primary physical phenomena to model and the principal heat transfer mechanism. If convection is the major phenomena, then fluid dynamics codes such as TEMPEST or HYDRA-II should

be used. If the radiation heat transfer is important compared with conductive heat transfer in the presence of air gaps between material, then a computer program specialized in computed gray body and spectral radiation should be utilized. The code matrix in Sect. 6, Table 11, may be used as a guide. The user manual should be consulted for the code capabilities.

Based on the assessment criteria identified in Sect. 1 and the assessment in Sect. 6, we recommend the following computer codes for primary DOE/OCRWM applications: ANSYS, HEATING6, ADINAT, and the following codes for further study and special purposes: HYDRA-II, SPECTROM-41, TEMPEST, and TOPAZ3D. The codes HEATING6, HYDRA-II, and TEMPEST are FDM programs; all the remaining computer codes are FEM programs. All codes selected are well supported by their code developer and readily available. ANSYS and ADINAT are commercial programs; a user or license fee is required to run the program. The advantage of commercial programs is the comprehensive user training and corporate technical support programs available. The remaining programs are developed and maintained through DOE funding. With the exception of TEMPEST and HYDRA-II, all the DOE-sponsored programs can be acquired at no cost from the code custodian listed in Sect. 3.

7.3 FUTURE RECOMMENDATIONS

The following recommendations are advanced as areas for additional work:

1. Benchmarking efforts, both U.S. and international, are proving to be a valuable source of code evaluation and comparison data. The waste package thermal analyst is urged to take advantage of this information when choosing analytical tools to be used in engineering evaluations. Benchmarking should be completed for more recently developed codes such as TOPAZ3D, FIDAP, COBRA-SFS and HYDRA-II. We suggest that a centralized and timely information service be established to facilitate future code assessments.
2. As of this writing, validation of general-purpose thermal codes with reliable data from full-scale shipping cask experiments has yet to be employed. We consider

validation to be a final and necessary step in the evaluation of both the codes and modeling methodology used in the analysis of shipping casks. It is recognized that such integrated testing is very costly and not economically feasible as a standard requirement for all new designs. However, within a class of designs, the experience gained in comparing code prediction with experimental data would not only prove invaluable in determining the accuracy of the codes themselves but also would be of great importance in gaining insight into the validity of the initial assumptions required by the analysis. The test program carried out at PNL on a Ridihalgh, Eggers, and Associates REA 2023 boiling-water reactor (BWR) spent fuel storage cask provides a good illustration of the kinds of experimental data that can be obtained.

3. The phase-change capabilities of most codes listed in the code matrix are limited to tracking the input of latent heat and the change in thermal properties as the material melts. An estimate of the movement of the phase-change front is also possible if one assumes no change in volume or mass distribution. Since the melting of a lead gamma shield would most likely entail the "slumping" of the material, and thus result in a change in its radiation shielding characteristics, the capability of the thermal analysis to account for such shape changes would be of value in thermal, shielding, and criticality studies.
4. The natural convection currents that can be established in a shipping cask, particularly in the neutron shield, represent a potentially significant mechanism for heat transfer. Many general-purpose heat transfer codes approximate the effect of a convection current by using a material that has a fictitious anisotropic thermal conductivity. The thermal conductivity in the direction of the dominant path of heat flow is assigned a value much higher than the value used for the perpendicular direction. It is unclear what level of accuracy is obtained by this approximation. The capability of calculating the characteristics of the flow field directly could be a significant asset in a shipping cask analysis. The recently developed codes, HYDRA-II and COBRA-SFS, are capable of modeling natural convection. We recommend that continued developments and validation/verification efforts be funded for these special capabilities.
5. Thermal calculations involving shipping casks have typically been limited to either one- or two-dimensional models; however, there are areas in which a complete analysis requires the correct modeling of

three-dimensional effects. For example, the effects of fins must usually be approximated in two-dimensional cask models. Temperature profiles within the fins themselves are generally not available from these calculations. If details regarding temperature gradients in regions with pipe fittings, bolts, valves, pressure gauges, drain plugs, lifting trunions, etc., are required, then a three-dimensional analysis may be indicated. An investigation into the applicability of three-dimensional modeling would be beneficial.

6. As stated earlier, no single currently available thermal code is best for dealing with all possible heat transfer problems. When faced with a specific application, the thermal analyst must review the capabilities of a range of codes and make a judgment regarding the optimum tool to satisfy his needs. To assist in such an effort, the development of an interactive (possibly PC-based) program that would provide the analyst with an easily accessible data base of information on heat transfer codes would be most beneficial. The interactive session would guide the user to a selection of candidate codes based on the user's response to questions about the specific application in hand. Such an applications-specific guideline for selecting thermal codes system would include information on code modeling capabilities, availability and cost, documentation, benchmarking status, etc.
7. There are 116 codes identified by this study and listed in Table 2 through 6. The current status of the codes are not all updated. The first step towards the implementation of the above-mentioned database would be to survey the codes further to complete the information about the code usage, availability, hardware compatibility, maintenance, and documentation.
8. With the spread of PC computing capabilities throughout the engineering design community, it is becoming increasingly important that reliable and verifiable thermal analysis software be made available for such a PC-based environment. We therefore recommend that an investigation be carried out to determine the feasibility of converting such codes as HEATING6 to operate on a PC. As a part of that investigation, it would also be important to determine the most appropriate role that a PC thermal code should play in an analysis of nuclear waste packages. Table 12 is provided as an initial survey of PC thermal codes.

Table 12. Thermal assessment codes available for personal computers

Code name	Contact address	Maximum number of nodes	Maximum degrees of freedom	Cost	Comments
ANSYS-PC/ THERMAL	Swanson Analysis Systems P.O. Box 65 Houston, PA 15342-0065	N/A	400	N/A	Finite element; 8 thermal element types
COSMOS/M	Structural Research and Analysis Corporation 1661 Lincoln Blvd Suite 100 Santa Monica, CA 90404	5,000	20,000 (No limit w/substruc- turing)	\$2,500 Complete (Modules sold indi- vidually)	Finite element; 11 thermal element types, \$8,000 complete with pre and post processors, demo disk, CAD interface, ANSYS, and NASTRAN translators.
GIFTS	CASA/GIFTS, Inc. Maryland Trade Center II 7474 Greenway Center Dr. Greenbelt, MO 20770	N/A	N/A	N/A	Finite element; thermal element types; Demo disks; CAD interface, ABAQUS, ADINA, and NASTRAN translators.
I/TAS	R. F. Warriner Associates 3838 Carson St., Suite 300 Torrance, CA 90503	350	-	\$450	Finite difference
IMAGES-3D	Celestial Software Inc. 125 University Ave. Berkeley, CA 94710	400	2,400	\$1,995 Complete	Finite element - thermal elements available 1988.
LIBRA	Intercept Software 3425 S. Bascom Ave. Campbell, CA 95008	4,000	N/A	\$700	Finite element; 14 thermal element types, \$1,600 complete with structural, dynamics, and post processor; Demo disks

Table 12. (Continued)

Code name	Contact address	Maximum number of nodes	Maximum degrees of freedom	Cost	Comments
MSC/CAL	MacNeal-Schwendler Corp. 815 Colorado Blvd. Los Angeles, CA 90041	1,000	N/A	\$1,495	Finite element; thermal element types; CAD interface, pre- and post-processors
NISAI-PC/ DISPLAYII- PC	Engineering Mechanics Research Corporation P.O. Box 696 Troy, MI 48099	200	10,000	\$1,500	Finite element; 6 thermal element types; \$7,000 complete with pre- and post-processors, CAD interface; Demo disk
SAP86/mTAB	Number Cruncher Microsystems, Inc. 1455 Hayes St. San Francisco, CA 94117	2,000	12,000	\$1,495 Complete	Finite element; No thermal element types at present, \$1,395 complete, CAD interface, SAPIV compatability
SAPIV/PC	Applied Science & Dev. Suite 141, 169 SE Cary Pkwy Cary, NC 27511	700	6	\$295	Finite element; No thermal element
SCADA/TW	American Computers and Engineers 11726 San Vicente Blvd. Los Angeles, CA 9004	N/A	N/A	\$3,000	Finite element; thermal element types; pre- and post-processor available
SUPERSAP	ALGOR Interactive Systems, Inc. Essex House Suite 15 Pittsburgh, PA 15206	Automatic minimizer; No limitations	10,000	\$795	Finite element; thermal elements \$1,495 complete, pre- and post- processors available, CAD interface; Demo disk

Table 12. (Continued)

Code name	Contact address	Maximum number of nodes	Maximum degrees of freedom	Cost	Comments
TAK-1	K&K Associates P.O. Box 2882 Lyons, CO 80540	150* *Varies	-	\$239	Finite difference; thermal Analysis Kit (TAK)
TEMPEST	TRUCOMP 18571 Las Flores Fountain Valley, CA 92708	16	N/A	\$595	Finite element
INTEMP	TRUCOMP (see above)	9	N/A	\$495	Finite element
TOPAZ2D	Methods Development Group P.O. Box 808, L-122 Livermore, CA 94550			N/C	Finite element
TRUMP	Herman L. Crawford 614 Garden Road Columbus, OH 43214	480	-	\$995	Finite difference analysis

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