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ATHENA/MOD1 CODE DEVELOPMENT
REQUIREMENTS DOCUMENT

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ATHENA/MOD1 CODE DEVELOPMENT REQUIREMENTS DOCUMENT

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ABSTRACT

This document states the requirements and capabilities of the ATHENA code for the Fusion Safety Program. The history of the development of ATHENA is given, along with requirements for the Fusion Safety Program, manuals, quality assessment, documentation, and support.

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REQUIREMENTS

GENERAL REQUIREMENTS

The inherent generality of the ATHENA modeling philosophy is primarily responsible for the successful applications of ATHENA to various plant designs. The code was designed around a basic hydrodynamic model instead of plant specific component models. This has the advantage that the code structure is not limited to specific systems or ,i.e. fusion power systems. If system specific models are necessary, then they can be included as auxiliary calculations to the basic hydrodynamic model.

The code solves separate independent flow paths. This particular feature allows for simulation of plant systems which contain several separate working fluids, a necessity for the fusion effort. This has necessitated use of a generalized equation of state representation so that any fluid with known properties can be easily installed into ATHENA. Currently, ATHENA has installed properties for water, helium, hydrogen, nitrogen, potassium, sodium, and lithium as two-phase systems, lithium-lead and NaK as a single phase liquids, and several single phase ideal gases.

The hydrodynamic model used in ATHENA is based on a one-dimensional, transient, two-fluid model for a two-phase fluid mixture which can contain a noncondensable component in the vapor phase and/or a nonvolatile component in the liquid phase. There are also options for several simpler hydrodynamic models. These include homogeneous flow, thermal equilibrium, and frictionless flow models. These options can be used independently or in combination. The two-fluid equations of motion, the basis of the ATHENA hydrodynamic model, are formulated in terms of area and time average parameters of flow. Phenomena which depend on transverse gradients, such as wall friction and heat transfer, are formulated in terms of bulk potentials using empirical transfer coefficient formulations.

The semi-implicit numerical solution scheme, which is used for time integration, is based on replacing the system of differential equations with a system of finite difference equations partially implicit in time. The implicit terms are formulated such that the resulting equations are linear in the dependent variables at new time. This results in a linear time advancement matrix solved by direct inversion using a sparse matrix technique. An additional feature of the scheme is that the implicitness (terms that are chosen to be at new time) is selected such that the field equations can be reduced to a single difference equation per fluid control volume in terms of the hydrodynamic pressure. Thus, only an $N \times N$ system of difference equations in terms of the system pressures need be solved simultaneously at each time step, where N is the total number of control volumes used to simulate a particular fluid circuit. The separate fluid circuits comprising the overall system are then solved in turn.

For problems where the flow is expected to change very slowly with time, it is possible to obtain adequate information from an approximate solution based on very large time steps. To facilitate this type of advancement, a fractional step time advancement scheme was developed. This scheme, called the nearly-implicit scheme, consists of advancing the expanded balance equations where the convective terms (those involving velocities) in the momentum equations are evaluated implicitly instead of explicitly. Since these terms are approximations and directly affect the advancement variables, a second stabilizing step must be taken. This step is a function of the implicit velocities and the intermediate values of the advancement variables which stabilizes the convective terms in the mass and energy equations. This type of scheme performs a time advancement with relatively little computational effort as compared to a fully implicit scheme which requires all of the advancement equations to be solved simultaneously. The net result is a time advancement scheme with implicit characteristics without the runtime and excessive memory penalties associated with implicit schemes.

Next, semi-empirical constitutive models based on measured data are included into ATHENA to account for interphase drag, wall friction, interphase heat and mass transfer, and heat transfer between the fluid and its

surroundings. These models are based on flow regime and local thermodynamic conditions.

Input to ATHENA consists of representing a closed piping system with a number of objects called components. These components are named after the physical hardware they represent, such as pipe, valve, pump, etc. This nomenclature is used for convenience to the user as well as to internally flag the use or nonuse of special process models where applicable and to initialize those component models which have separate transient calculations. In certain applications, the phenomena associated with a component includes effects that are beyond the scope of the basic hydrodynamic model. In order to simulate the phenomena, empirical models are used in conjunction with the basic scheme. These models include valves, turbines, jet mixers, pumps, separators, cross-flow junctions, and heat pipes.

Lastly, in addition to the special component models, a number of special process models have been incorporated to account for phenomena not effectively or efficiently simulated by the basic hydrodynamic model and/or by the special component models. These models consist of choked flow, horizontal stratification, entrainment, abrupt area change, vertical stratification, and magneto-hydrodynamics forces.

SPECIFIC REQUIREMENTS

The requirements for ATHENA as defined by the fusion community are as follows:

First, the fluids types required are: 1) Lithium, 2) Lithium-Lead, 3) Nitrogen, 4) Helium, and 5) Light Water. For these fluids, the constitutive models, i.e. convective heat transfer, interphase mass and heat transfer, wall drag, and interfacial drag, must be validated. The results of the validation process must be published.

Secondly, Magneto Hydro-Dynamic (MHD) effects must be calculated by the ATHENA code. This capability is to be considered an option for use with liquid metal systems.

Third, the ATHENA code must execute in a timely manner. This means that the code will use time step sizes commensurate with the transient being performed, within the limitations imposed by user time step controls, mass error time step controls, and Courant limit time step controls.

Forth, the code must be able to execute on 32-bit computers. This includes accelerated personnel computers with sufficient storage, workstations, and mainframes.

Lastly, the ATHENA code must be supported. The Fusion Safety Program is committed to maintain ATHENA on the NMFECC, to provide error corrections, and to provide on call assistance to all users in the fusion community. These same services will be provided to other users on a cost recovery basis.

Currently, the ATHENA capabilities extend past the needs of the fusion community. These capabilities are considered to be enhancements to ATHENA from the fusion prospective, thus support, development, and maintenance will come from other sources. The extensions to ATHENA are in the form of having other fluids are available for use in the code.

Table 1 is intended to show the current capabilities of ATHENA by indicating constitutive model applicability with each fluid type. All currently available fluid types are included. The constitutive models listed, from left to right, are: 1) wall drag, 2) interfacial drag, 3) interfacial mass and heat transfer, 4) convective wall heat transfer, and 5) MHD pressure drop. An "X" under the category where the ATHENA models are applicable. A blank space indicates the current model is either incorrect but usable or unsuitable for that fluid. Within the convective wall heat transfer model, there are three subcategories labeled pre-CHF, CHF, and post-CHF. The pre-CHF subcategory includes all correlations for the boiling regimes to the point

TABLE 1. TABLE OF ATHENA FLUIDS AND MODELS.

FLUID TYPE	CONSTITUTIVE MODELS					MHD	
	Wall Drag	Interphase Drag	Interphase Mass & Heat Transfer	Convective Heat Transfer pre-CHF	Convective Heat Transfer post-CHF	Pressure	Drop
Light Water	X	X	X	X	X		
Heavy Water		X	X	X	X		
Nitrogen		X	X	X	X		
Lithium						X	X
Potassium						X	X
Sodium						X	X
NaK						X	X
Helium	X	X	X	X	X		
Hydrogen	X	X	X	X	X		

where Critical Heat Flux (CHF) occurs. The post-CHF subcategory includes all correlations for the boiling regimes past the point where CHF occurs. The CHF subcategory is the CHF correlation.

MANUAL REQUIREMENTS

The ATHENA code is formed by installing generalized fluid property data, generalized heat transfer correlations, and fusion reactor specific models into RELAP5/MOD3.⁷ Consequently, all the model and correlation documentation for RELAP5/MOD3 forms a subset of the necessary documentation for ATHENA/MOD1. Therefore, the ATHENA/MOD1 documentation will consist of a set of supplements to the RELAP5/MOD3 manuals.

These supplements will provide the documentation of the unique ATHENA code capabilities and will be released with the transmittal of the code. The supplements will consist of specific and separate reports for each topic or subject. Thus, there will be a separate report that documents the generalized fluid property capability which will include model development, references, and procedures for including additional fluid properties. A second report will document additional models and correlations that were installed into ATHENA/MOD1 for the heat transfer model for nonaqueous fluids, as well as fusion specific models and correlations. Also, a report that gives the input requirements and guidelines for ATHENA specific model will be generated. Additional reporting for developmental assessment, code validation and verification, configuration control, and new modeling capabilities will be made available upon completion of these tasks.

SUPPORT REQUIREMENTS

Whenever a computer code is released, support functions are necessary from the releasing organization. This support usually consists of several tasks which are determined by the releasing organization. The Fusion Safety Program has determined that it will provide code maintenance, configuration control, user support, and user training as code support functions.

Code maintenance consists of maintaining transmittal files and record keeping of the user base and updating the code for error corrections. The configuration control task will provide a process for maintaining code corrections, improvements, documentation, and performance characteristics with corrections and improvements. User support consists of providing consultation on code errors, code problems, and system models of users applying the ATHENA code to fusion related tasks. This same support will be provide to other users under a cost recovery procedure, which also include code installation. Lastly, user training in the form of user workshops will be provided. This last task is also provided by a cost recovery procedure.

QUALITY TESTING AND DOCUMENTATION

INTRODUCTION

The purpose of this section is to describe the reasons, procedures, and activities for the assessment of the ATHENA code. Also given here is a matrix of test problems chosen to quantify and qualify the capabilities of the code.

PURPOSE

Currently, DOE Order 1330.1C mandates that "each software management program will include the use of one or more software management methodologies and the concepts of software quality assurance and software quality control." Furthermore, this order applies to "software proposed for use, under development, and being maintained and used, whether that software was being developed in-house, licensed from a commercial vendor, obtained from another organization, or otherwise obtained ...". This is the introductory remark from the SOFTWARE QUALITY ENGINEERING FOR SCIENTIFIC COMPUTING⁹ internal technical report produced by the SCIENTIFIC COMPUTING organization. This document provides guidelines for determining the necessary quality level (QP-2, level A, B, or C) for scientific software being used or developed at the INEL. The information contained in this report is used to define

The ATHENA code will be used for analysis of actual and conceptual fusion plant designs. From the definitions from the EG&G Quality Manual and the ASME NQS-1, QP-2 level B is desired. Part of the verification that the ATHENA code will meet this quality level is assessing the code performance as applied to several code calculations. To make the assessment meaningful, the code calculations are compared to analytical results or measured data. Additionally, the test cases used for comparison have to be in the calculational domain of the code.

Another important thing about achieving QP-2 level B is to have a Quality Assurance Plan in place, and to follow the requirements set down in

that document. The ATHENA code is an existing piece of software, which requires different guidelines than new software development. However, ATHENA is based on the RELAP5/MOD3 thermal hydraulic systems analysis code. Consequently, the RELAP5 SQAP can be used as a supplement for the ATHENA/MOD1 SQAP. Also, all assessment performed on RELAP5/MOD3 can be applied to the ATHENA code. Thus the ATHENA assessment is the RELAP5/MOD3 assessment with additional test cases required for those capabilities not contained in the RELAP5/MOD3 code.

Specifically, nonaqueous fluids, liquid metals, and MHD effects require testing that is independent from RELAP5. These capabilities do use the basic RELAP5 thermal hydraulic advancement scheme, heat conduction model, input/output capabilities, and generalized convective heat transfer package. Of these portions of the code, the models that require special consideration are the flow regime maps, interphase heat and mass transfer, interphase drag, wall drag, critical heat flux, and film/pool boiling. The assessment of these models require separate effects tests.

PROCEDURE

For assessment purposes, three types of problems are used. The first type consists phenomenological problems that have analytic solutions. This tests the fundamental advancement scheme. The next types of problems are separate effects experiments. These types of experiments are designed to isolate and measure unitary processes, such as critical heat flux or stratified two phase flow. The application of the code to these problems isolates the model tested. Lastly, integral experiments are used for assessment cases. These experiments include several different processes in one problem. This tests transitions between models and the capability to simulate several processes at any instant.

Several criteria are used to chose the problems in each category. Some of the more important criteria include the availability and quality of

measured data, the applicability of the measured data to the models in the code, and problems that present a significant challenge to code calculations.

The code calculations of the assessment cases are made. The calculated results are then compared to either analytic solutions or measured data, depending on the type of test problem. The results are then analyzed and reported. As the code is applied to the assessment cases, problems may be uncovered. These problems are reported as code deficiencies, and no attempt is made to correct them.

ASSESSMENT CASES

The assessment cases for ATHENA consist of a number of problems that are being used to assess RELAP5/MOD3 plus additional cases specific to ATHENA. This is necessary to assess the nonaqueous fluids and liquid metal capabilities in the code. The cases are divided into water cases, nonaqueous cases, and liquid metal/MHD cases. The water cases are further subdivided into phenomenological problems, separate effects tests, and integral tests. The nonaqueous cases are all separate effects tests due to lack of integral test data.

The following table, Table 2, shows the test matrix being used. The problem names or identifiers are given in the first column, fluid types in the second column, and notes (i. e. heat transfer, CHF, integral test, etc.) in the third column. All water problems are applicable to ATHENA.

Table 2. ATHENA assessment cases

<u>Problem Name</u>	<u>Fluid Type</u>	<u>Test Type and/or Requirements Addressed</u>
Water Faucet Problem	water	phenomenological, hydrodynamics
Edwards Pipe Problem	water	separate effects, hydrodynamics
ORNL Void Profile Test	water	interfacial heat transfer
Christensen Subcooled Boiling Test 15	water	separate effects, subcooled boiling
LOFT L2-5	water	large break integral test
Semiscale NC-x	water	integral test, natural circulation
MIT Pressurizer	water	separate effects, mass transfer
RIT Tube Test 261	water	separate effects
LOBI A1-04R	water	large break integral test
GOTA	water	separate effects
Flecht-Seaset	water	separate effects, boiling curve
<u>The next set of test cases are specifically for ATHENA.</u>		
Two Phase Pressure Drop	helium	separate effects, hydrodynamics
Flow Boiling	helium	CHF for helium
Vertical Tube Boiling	water/helium	two component mass and heat transfer, water and air/water and helium
Film Boiling in Horizontal Pipes Parts I and II	nitrogen	film boiling with several fluids
Dispersed Flow Film Boiling	nitrogen	film boiling
Convective Boiling	nitrogen	plate-fin heat exchangers
Heat Transfer and Hydrodynamics	nitrogen	nitrogen and helium CHF, film boiling and pressure drop
Two Phase MHD Flow	NaK/nitrogen	flow regimes, heat transfer, and MHD effects with nitrogen vapor over NaK.
ALEX	NaK	MHD effects

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