CONTAIN Independent Peer Review

B. E. Boyack

M. L. Corradini*

R. S. Denning**

M. Khatib-Rahbar***

S. K. Loyalka[†]

P. N. Smith^{††}

*University of Wisconsin, Nuclear Engineering Department, 1500 Johnson Drive, Madison, WI 53706

**Battelle Memorial Institute, 505 King Avenue, Columbus, OH 43201

***Energy Research Incorporated, P. O. Box 2034, Rockville, MD 20847

[†]University of Missouri Columbia, E1425C Engineering, Columbia, MO 65211

^{††}AEA Technology, Winfrith Technology Center, Dorchester, Dorset DT2 8DH, UNITED KINGDOM

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ACRONYMS

Acronym	Definition
ALWR	Advanced light water reactor
BSR	Bulk spontaneous recombination
BWR	Boiling water reactor
DBA	Design-basis accident
DCH	Direct containment heating
DFB	Diffusion flame burning
ESF	Engineered safety feature
FCI	Fuel-coolant interaction
FITS	Fully instrumented test series
GDE	General dynamic equation
GFT	Gravitational fall time
HPME	High-pressure melt ejection
LWR	Light water reactor
MCCI	Molten core-concrete interaction
NAD	Non-airborne debris
NRC	US Nuclear Regulatory Commission
NTS	Nevada Test Site
ODE	Ordinary differential equation
ORNL	Oak Ridge National Laboratory
PCCS	Passive containment cooling system
PNL	Pacific Northwest Laboratories
PRA	Probabilistic risk assessment
PWR	Pressurized water reactor
QA	Quality assurance
RPV	Reactor pressure vessel
SBWR	Simplified boiling water reactor
SNL	Sandia National Laboratories, Albuquerque, NM
TFI	Time to first impact
TOF/KU	Time of flight/Kutateladze criterion
TRENDS	Transport R etention of Nuclides in D ominant S equences
VGES	Variable Geometry Experimental System

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CONTAIN INDEPENDENT PEER REVIEW

by

B. E. Boyack, M. L. Corradini, R. S. Denning, M. Khatib-Rahbar,
S. K. Loyalka, and P. N. Smith

ABSTRACT

The CONTAIN code was developed by Sandia National Laboratories under the sponsorship of the US Nuclear Regulatory Commission (NRC) to provide integrated analyses of containment phenomena. It is used to predict nuclear reactor containment loads, radiological source terms, and associated physical phenomena for a range of accident conditions encompassing both design-basis and severe accidents. The code's targeted applications include support for containment-related experimental programs, light water and advanced light water reactor plant analysis, and analytical support for resolution of specific technical issues such as direct containment heating. The NRC decided that a broad technical review of the code should be performed by technical experts to determine its overall technical adequacy. For this purpose, a six-member CONTAIN Peer Review Committee was organized and a peer review was conducted. While the review was in progress, the NRC issued a draft "Revised Severe Accident Code Strategy" that incorporated revised design objectives and targeted applications for the CONTAIN code. The Committee continued its efforts to develop findings relative to the original NRC statement of design objectives and targeted applications. However, the revised CONTAIN design objectives and targeted applications were considered by the Committee in assigning priorities to the Committee's recommendations. CONTAIN is approaching fulfillment of its original design objectives and targeted applications. This is a significant accomplishment. The essential phenomenological models are present in the code. The capability exists for performing sensitivity studies for the few important phenomenological models not currently in the code. The fundamental building block models are successfully functioning in an integrated manner. The Committee determined some improvements are warranted and provided recommendations in five code-related areas: (1) documentation, (2) user guidance, (3) modeling capability, (4) code assessment, and (5) technical assessment. The small number of high-priority modeling recommendations is a significant measure of the degree to which CONTAIN is approaching fulfillment of its original design objectives and targeted applications.

EXECUTIVE SUMMARY

CONTAIN is designed to provide integrated analyses of containment phenomena. It is used to predict nuclear reactor containment loads, radiological source terms, and associated physical phenomena for a range of accident conditions encompassing both design-basis and severe accidents. Its targeted applications are experiment analysis and support for containment-related severe-accident and advanced light water reactor experimental programs, light water reactor and advanced light water reactor plant analysis, and analytical support for resolution of specific technical issues such as direct containment heating. CONTAIN is being developed at Sandia National Laboratories under the sponsorship of the United States Nuclear Regulatory Commission (NRC).

The NRC has instituted a program of peer reviews of its severe-accident codes. The peer reviews of the MELCOR and SCDAP5/RELAP5 codes are complete. A review process was developed and refined during the course of these two reviews and this process was applied to the CONTAIN Peer Review. A CONTAIN Peer Review Committee has been organized using recognized experts from the national laboratories, universities, the CONTAIN user community, and independent contractors. Specific design objectives and targeted applications for the code, along with associated success criteria have been provided by the NRC. The Committee primarily focused on Code Version 1.2.

The objective of this report is to document the findings of the CONTAIN Peer Review Committee that was formed to fulfill the charter described in the next section.

Committee Charter

The charter of the CONTAIN Peer Review Committee was to (1) provide an independent assessment of the CONTAIN code through a peer review, (2) determine the technical adequacy of CONTAIN for the analyses it is expected to perform, and (3) issue a final report describing the technical findings of the Committee.

Peer Review Process

The Committee developed and followed a multistep process for the CONTAIN Peer Review. The steps in the process are as follows:

1. Identify design objectives for the code.
2. Identify targeted applications for the code.
3. Identify the code version to be reviewed.
4. Identify and distribute the code document database to Committee members.
5. Select severe- and selected design-basis-accident scenarios.
6. Identify dominant phenomena for containment types and scenarios.
7. Develop a common Committee perspective regarding technical adequacy.
8. Define a "Standard of Technical Adequacy" to be used in developing findings.
9. Define a process for reviewing for technical adequacy.
10. Assess technical adequacy of individual phenomenological models and/or correlations within the code (bottom-up review).
11. Assess technical adequacy of the integral code against the design objectives and targeted applications (top-down review).
12. Document findings in a summary report.

Detailed descriptions of each step in the review process are provided in Sec. 1, Introduction.

Major Findings

Background

The review was conducted in an environment of ongoing code development. Therefore, the participation and support of the CONTAIN code development staff at Sandia National Laboratories was essential. Indeed, the code development staff provided excellent support to the Committee and exhibited professionalism in preparing and presenting the additional information that was essential to the review. Using both formal documentation and the extensive presentation materials, the Committee conducted a detailed review of the individual phenomenological models in the code to determine their technical adequacy (bottom-up review). In addition, a review of the total code was conducted (top-down review). The review was conducted using code design objectives, targeted applications, and success criteria provided by the NRC.

After the Committee had completed its bottom-up review and while it was approaching completion of the top-down review, the NRC issued a revised severe-accident code strategy for review and comment. Included in this strategy package were revised design objectives, targeted applications, and success criteria for the CONTAIN code. The Committee did not repeat its review using the revised CONTAIN design objectives, targeted applications, and success criteria. However, it did carefully consider this information when assigning priorities to its recommendations by assigning a low priority to correction of code deficiencies for features that will no longer be maintained, e.g., fission product models.

On the basis of the success criteria for design objectives and targeted applications, the Committee determined the overall technical adequacy of the code and provided recommendations for improvements.

General Committee Findings

The Committee conducted a thorough review of both the individual phenomenological models and integral performance of the CONTAIN code. The formal code documentation, both released and in draft form, was reviewed as were the extensive presentation materials prepared by the code development staff. The Committee has concluded that the following general findings summarize the outcome of the CONTAIN Peer Review effort.

1. CONTAIN is approaching fulfillment of its original design objectives and targeted applications. This is a significant accomplishment. The essential phenomenological models are present in the code. The capability exists for performing sensitivity studies for the few important phenomenological models not currently in the code. The fundamental building block models are successfully functioning in an integrated manner. Committee reservations regarding specific phenomenological models are identified in Sec. 6.
2. CONTAIN is also approaching fulfillment of its recently revised design objectives and targeted applications that were developed within the context of the revised severe-accident code strategy. The models to be carried into the future simulate a more limited set of physical phenomena.

3. CONTAIN can be applied to both selected design-basis accidents and severe accidents for both current reactors and advanced light water reactors. A large number of plant application calculations have been performed and these have demonstrated the applicability of the code to the satisfaction of the Committee. Significant development and assessment efforts are still in progress for advanced light water reactors.
4. The available documentation for the CONTAIN code represents a significant accomplishment. It is approaching completeness. The Committee received draft documentation that is not fully integrated and it is important that existing plans to integrate the documentation be completed. Those in the user community that responded to the CONTAIN user survey stated that the documentation was good. The Committee concurs but has concluded that additional documented user guidance is desirable. Further, the Committee has recommended that the documentation of selected models should be improved. Specific recommendations are provided in Sec. 6.
5. CONTAIN code development has benefited from an extensive assessment effort using data from a variety of experimental facilities. The Committee notes that the assessment effort for advanced light water reactors has just begun and, therefore, is only partially complete. For the assessments performed to date, however, code applicability has been demonstrated, development needs have been identified, and work is in progress to make needed improvements. Continued expansion of the Standardized Problem Set is encouraged.
6. CONTAIN can be run on a variety of computational platforms. Users experience few difficulties in performing calculations. The code is robust. Run times are practical.

Specific Committee Findings

The Committee has determined that recommendations in five code-related areas are appropriate:

- (1) documentation,
- (2) user guidance,
- (3) modeling capability,
- (4) code assessment, and
- (5) technical assessment

The Committee has included prioritized recommendations that it believes will have an important impact on either code usage or code adequacy. The Committee concluded that complete and adequate documentation is essential and, therefore, that all documentation deficiencies should receive a high priority for correction. The Committee also felt that improved user guidance is closely related to effective code usage and recommendations have been made in this area, as appropriate. An extensive effort was put forth in assessing the capabilities of basic CONTAIN phenomenological models. A detailed review of each model and a finding of its technical adequacy is presented in App. D. Committee findings regarding the adequacy of CONTAIN relative to its original design objectives are presented in Sec. 3 and findings relative to CONTAIN's original targeted applications are presented in Sec. 4.

As noted above, there are five areas in which recommendations have been made. The Committee has assessed the priority of each recommendation. The priority assigned to

each recommendation considered the importance of the processes and phenomena being modeled relative to their impact on containment source terms and pressure and temperature loadings. The state of scientific knowledge regarding the associated process or phenomena was also considered. The Committee's recommendations, assessed as either high, medium, or low priority, are presented in Tables 6-I to 6-III, respectively. Each table provides a brief description of the recommendation, characterizes the recommendation as belonging to one or more of the five recommendation areas identified above, and identifies the specific section(s) in this report wherein the recommendation is generated. Recommendations related to aerosol and fission product models are assigned a dual priority to reflect both the original and newly revised design objectives and targeted applications for CONTAIN.

Fourteen high-priority recommendations are listed in Table 6-I. Of these, four recommendations deal with documentation. The remaining high-priority recommendations are for user guidance (four), modeling capability (three), code assessment (one), and technical assessment (two). The small number of high-priority modeling recommendations is a significant measure of the degree to which CONTAIN is approaching fulfillment of its original design objectives and targeted applications.

1. INTRODUCTION

The CONTAIN code (Ref. 1-1) "...is an analysis tool for predicting the physical, chemical, and radiological conditions inside the containment and connecting buildings of a nuclear reactor in the event of an accident. CONTAIN has been developed at Sandia National Laboratories (SNL) under the sponsorship of the US Nuclear Regulatory Commission (NRC) for analyzing containment phenomena under severe- and design-basis-accident (DBA) conditions. It is designed to predict the thermal-hydraulic response inside containments and the release of radionuclides to the environment in the event of containment failure." The modeling capabilities of CONTAIN are also sufficiently flexible that they can be used for other nonreactor applications. Conservation equations for momentum, mass, and energy are solved for containment applications. The code employs a lumped-parameter control-volume approach that determines some of the fundamental characteristics of the code with respect to spatial resolution of phenomena and processes. In the present two-tier severe-accident analysis code structure used by the NRC, CONTAIN is a lower-tier, mechanistic, severe-accident code.

A number of organizations, both foreign and domestic, are using CONTAIN. Although the quality control, model development, and validation efforts are proceeding, there is a need to have a broad technical review of CONTAIN by recognized experts to determine or confirm the technical adequacy of the code for its intended applications. In addition, the peer review can be used by the NRC to assess the priority of the elements of its ongoing code development program.

A peer review committee has been organized using recognized experts from the national laboratories, universities, the CONTAIN user community, and independent contractors. Specific design objectives and targeted applications for the code, along with associated success criteria, have been provided by the NRC (Ref. 1-2). Using the NRC information, SNL-prepared documentation, presentations by the code development team and other technical sources, and a basic understanding of the underlying design-basis and severe-accident phenomena, the CONTAIN Peer Review Committee developed a consensus on the overall adequacy of the CONTAIN code.

The objective of this report is to document the findings of the CONTAIN Peer Review Committee.

1.1. Committee Charter

The charter of the CONTAIN Peer Review Committee was to (1) provide an independent assessment of the CONTAIN code through a peer review, (2) determine the technical adequacy of CONTAIN for the analyses it is expected to perform, and (3) issue a final report describing the technical findings of the Committee.

1.2. Committee Membership

The Committee membership was selected to conduct a broad peer review of the CONTAIN code using recognized technical experts from universities, the national laboratories, the community of CONTAIN code users, and other technical organizations. The Committee membership selection was based on the expertise required to evaluate the specific code models, as well as the overall code performance. Brief experience summaries of each Committee member are presented in App. A. The Committee members are as follows:

Dr. Brent E. Boyack (Committee Chair), Los Alamos National Laboratory
Dr. Michael L. Corradini, University of Wisconsin, Madison
Dr. Richard S. Denning, Battelle
Dr. Mohsen Khatib-Rahbar, Energy Research, Incorporated
Dr. Sudarshan K. Loyalka, University of Missouri, Columbia
Dr. Paul N. Smith, AEA Technology, Winfrith, United Kingdom

1.3. Peer Review Process

The Committee implemented a process for conducting the peer review of the CONTAIN code. A substantial effort was undertaken previously to develop a multistep process for the MELCOR Peer Review (Ref. 1-3). The peer review of the SCDAP/RELAP5 code also followed a similar process (Ref. 1-4). Because that process proved very workable for reviewing the MELCOR and SCDAP/RELAP5 codes for technical acceptability, a nearly identical procedure was adopted by the CONTAIN Peer Review Committee.

1.3.1. Identify Design Objectives

Both the design objectives and the associated success criteria for the CONTAIN code were provided by the NRC (Ref. 1-2). The numbering and formatting of (Ref. 1-2) have been preserved.

1. Modeling detail shall be capable of representing key and important phenomena of severe accident experiments, and anticipated plant accidents and transients.

General Success Criterion: The code can model all pressurized water reactor (PWR) and boiling water reactor (BWR) containment systems including advanced light water reactor (ALWR) designs (e.g., AP600 and SBWR), as well as operator actions and experimental facilities used for code assessment.

a. Expected modeling uncertainties should be comparable to uncertainties in integral severe-accident experiments.

Success Criterion: Uncertainties in important parameters calculated by the code should be less than or equal to measured values. For example, if the uncertainties in the measured temperatures and associated boundary conditions are $\pm 20\%$, then the success criteria for the code would be $\pm 20\%$ for calculated temperatures.

b. User-defined parameters, other than those needed to define experiments, plant unique features [or prepare uncertainty estimates as specified for Design Objective 2, below],¹ should be eliminated only where an experimental or other credible basis exists to define those parameters (e.g., user guidance documentation is required).

Success Criterion: The code will not contain any user-defined parameters other than those noted.

2. The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected DBAs. It

¹ Expanded definition adopted by Committee was documented in B. E. Boyack, "Minutes for April 20, 1993 Meeting at Sandia National Laboratories," Los Alamos National Laboratory Group N-12 letter N-12-93-210 to A. Notafrancesco, April 23, 1993.

should permit estimates of uncertainties of containment loads and fission product release predictions without requiring modifications to the code.

Success Criterion: The code predicts dominant phenomena based on assessment against integral facility data. The code also predicts values of important parameters associated with dominant phenomena within measured uncertainty when assessed against integral facility data.

3. The code should be applicable for containment transient studies under various accident sequences for PWRs, BWRs, and ALWRs.

Success Criterion: The code can predict containment loads resulting from risk-dominant accident sequences identified by probabilistic risk assessment (PRA) studies for PWRs, BWRs, and ALWRs, as well as DBAs for the AP600 and simplified boiling water reactor (SBWR) configurations. Physical models, as well as component models, exist sufficiently to accurately predict dominant phenomena. The code must model important phenomena in a much more detailed manner than the MELCOR code (with the exception of cases where MELCOR contains first- or higher-order models) (see footnote 1, previous page).

4. The code should be robust, portable, and fast running.

General Success Criterion 1: Although run time is machine dependent, the following general expectation can be used: running time should be reasonable so as to not handicap the user's ability to perform sensitivity/uncertainty analyses for the phenomena/conditions the code is design to model. Run time should be a small fraction of the time required to perform the entire analysis.

General Success Criterion 2: Based on user's guidelines and lessons-learned information in the code manual, code users shall be able to set up a plant model (e.g., input deck) to accurately represent a full-scale light water reactor (LWR) plant, and successfully perform plant calculations for various severe-accident scenarios and selected DBAs that are in the domain of targeted applications of the code

a. The code should not abort prematurely because of user input errors or numerical nonconvergence, but should exit with sufficient diagnostic messages for users.

Success Criterion A: Code performs as noted.

a. Numerical precision should be comparable with modeling precision. Spatial convergence should be comparable with modeling scale.

Success Criterion B: Code performs as noted.

b. The code should be transportable for mainframe and workstation computing machines.

Success Criterion C: The code is transportable.

5. The maintenance of the code should follow accepted quality assurance (QA) standards for configuration control, testing, and documentation.

General Success Criterion: Code QA procedures and associated documentation should be sufficient and consistently applied for all NRC applications.

- a. All code changes should be controlled and verified by redundant means.

Success Criterion A: Code changes should be made as noted.

- b. Testing standards and benchmarks should be defined for all versions released for production applications.

Success Criterion B: These should perform as noted.

- c. Documentation should define the theoretical basis, experimental database, limits of applicability, quantification of uncertainties, user guidance, and testing of assessment results of the code.

1.3.2. Identify Targeted Applications

The specific code-targeted applications were defined by the NRC (Ref. 1-2). The Committee adopted several clarifying statements (see item 1 below). The NRC also provided success criteria to be used by the CONTAIN Peer Review Committee in assessing the technical adequacy of CONTAIN in Ref. 1-2. The targeted applications for the CONTAIN code are:

1. Experimental analysis and support for containment-related severe-accident experimental programs such as HDR, LACE, NTS, and SURTSEY; and analyze relevant ALWR test programs, such as the Westinghouse large-scale Passive Containment Cooling System (PCCS) facility.

Success Criterion: Code has been or can be used to analyze these facilities and can provide reasonable predictions of associated dominant phenomena (compared with experimental data, the calculated results will be within the experimental uncertainty bands).

2. LWR plant analysis to predict the physical, chemical, and radiological conditions inside containment, and fission product releases as a result of predicted containment failure.

Success Criterion: Code has been or can be used to analyze LWRs and can provide reasonable predictions of associated dominant phenomena, or the ability to perform sensitivity studies. Code must have been shown to predict the dominant phenomena by assessment against sufficient experimental results.

3. Selected detailed analysis for specific technical issues—hydrogen combustion and migration, build-up of noncondensable gases, direct containment heating, and accident management evaluations.

Success Criterion: Code has been or can be used to provide detailed analysis of these specific technical issues predicting the associated dominant phenomena with reasonable agreement, or the ability to perform sensitivity studies. Code must have been shown to predict the dominant phenomena associated with these specific technical issues by assessment against sufficient experimental results.

4. MELCOR benchmarking and assessment.

Success Criterion: Code can be used to benchmark and assess the MELCOR code containment-related behavior at least for integral experiments.

5. ALWRs design-basis and severe-accident evaluation.

Success Criterion: Code can be used to evaluate ALWR severe accidents with reasonable prediction of the dominant phenomena and evaluate selected DBAs in accordance with its intended use in the NRC's regulatory process (see item 1 above).

1.3.3. Identify the Code Version to be Reviewed

The Committee primarily focused on CONTAIN Version 1.2. Development work on this version continued during the period the peer review was conducted. Some of the deficiencies identified during the peer review are being or will be corrected before public release of Version 1.2. In addition, the Committee considered and acknowledged the planned development program as part of its review effort.

1.3.4. Identify and Distribute Code Document Database to Committee Members

A CONTAIN Document Database was compiled and continually updated as new information was identified. Included in the Document Database are (1) Reports (Sandia National Laboratories, Albuquerque, NM), (2) Reports (Other), (3) Journal Articles (Sandia National Laboratories, Albuquerque, NM), (4) Journal Articles (Other), (5) Papers (Sandia National Laboratories, Albuquerque, NM), (6) Papers (Other), (7) Correspondence and Memoranda, (8) Presentation Materials (Sandia National Laboratories, Albuquerque, NM), (9) Presentation Materials (Other), and (10) Other. The complete database is found in App. B.

1.3.5. Select Severe-Accident and Selected DBA Scenarios

Both high- and low-pressure melt ejection (severe-accident) scenarios were considered and the phenomena expected to occur during such scenarios were identified. (App. C). The phenomena associated with selected design-basis scenarios are less complex and the Committee believes that these may be considered as a subset of the more complex severe-accident scenarios.

1.3.6. Identify Dominant Phenomena for Containment Types and Scenarios

Nine classes of LWR containment designs are identified in Sec. 3, Table 3-I. The key containment safety features that affect thermal-hydraulic and fission product behavior for ex-vessel accident conditions are listed in Sec. 3, Table 3-II. A summary of ex-vessel severe accident phenomena is provided in App. C. The Committee identified the following key processes: high-pressure melt ejection (HPME), nonenergetic fuel-coolant interaction (FCI), molten-core-concrete interaction (MCCI), combustion, ex-vessel transport, thermal-hydraulics of engineered safety features (ESF), containment failure modes, aerosol transport and retention, vapor fission product transport, and fission product characterization. Within each process, the Committee identified the severe-accident

phenomena and ranked each for importance relative to the impact upon the source term to the environment and containment loads.

1.3.7. Develop a Common Committee Perspective Regarding Technical Adequacy

The Committee members hold a variety of perspectives in deciding the technical acceptability of CONTAIN. To develop a common perspective on "how good is good enough," three important factors were considered related to severe-accident phenomena:

Knowledge of Physical Processes. The current level of scientific knowledge about severe-accident processes varies. The physics of some physical processes are well understood, while the physics of other physical processes are partially or poorly understood. Therefore, the Committee cannot expect CONTAIN to accurately model any phenomena that the scientific community has not yet fully understood. The CONTAIN code should therefore permit the consideration of uncertain physical processes by other means (e.g., sensitivity studies).

CONTAIN Physics. The objective of any modeling effort should be to mathematically represent the physical processes correctly, because incorrect mathematical representations cannot be expected to accurately predict reality. CONTAIN is a best-estimate, mechanistic code, and one of the success criteria for the first design objective (see Sec. 1.3.1) is that "...expected modeling uncertainties should be comparable to uncertainties in integral severe accident experiments." Therefore, sufficiently accurate mathematical representations of physical phenomena should be present in the model to accurately reproduce the physical behavior.

A model that captures the major features or trends of dominant phenomena and leads to the physically correct end state will be defined to be a "zeroeth-order" model. A first-order model improves the characterization of features or trends that affect event timing and magnitude and more accurately represent the passage to the end state. All models that are important to the prediction of dominant phenomena in severe-accident simulations must be of first order for the code to be considered best estimate and mechanistic.

Importance. Some models are more important than others in determining the course of a severe-accident simulation. Importance reflects the code's ability to predict (1) the source term from the containment to the environment, and (2) the loads on the containment structure. For those more important models, either the physics must be well understood and modeled or the sensitivity of results must be well quantified. However, for models of less importance (i.e., having less impact on the outcome of the simulation), the physics and modeling are less important, as are the sensitivity studies.

An importance value will therefore be determined for each model reviewed. The technical acceptability of the more important models will carry the most weight in determining overall technical acceptability of the code. Models that are inadequate, but are of less importance, should be flagged for future code improvement but should not impact the Committee's statement of overall code technical adequacy. Appendix C provides additional details regarding importance and ranking of severe-accident phenomena.

1.3.8. Define a "Standard of Technical Adequacy" to be Used in Developing Findings

A two-stage approach to defining a standard for technical acceptability was used by the Committee. Stage 1 is applicable to the detailed models in CONTAIN (the bottom-up view). Stage 2 is applicable to the total or integrated CONTAIN code (the top-down view).

Stage 1: The Committee's standards for technical adequacy of the individual CONTAIN models are that (1) the model pedigree is known, documented, and acceptable, (2) the model is used appropriately or stated in another manner, and the application of the model is acceptable, and (3) the prediction of, or fidelity to, the dominant phenomena modeled is acceptable.

Stage 2: The Committee's standards for technical adequacy of the total or integral code are that (1) the total code is applicable and (2) the prediction of integral phenomena is acceptable.

1.3.9. Define a Process for Reviewing for Technical Adequacy

Having defined the Standard of Technical Adequacy, the Committee performed the following two review actions.

A bottom-up review was conducted by examining the pedigree, applicability, and fidelity of the many individual models and closure relationships in CONTAIN. This was accomplished by reviewing the CONTAIN code documentation and other related literature from the CONTAIN Document Database (see App. B for citation). A classification scheme was proposed, assigning a category number to each model consistent with the methods used in the MELCOR Peer Review.

A top-down review was conducted on the applicability and fidelity of the total code by examining benchmarking efforts available. The top-down review was documented for the specific version of the code that was reviewed. In the absence of such information, code-to-code comparisons and expert opinions became stronger elements of the top-down stage of the review.

1.3.10. Assess Technical Adequacy of Individual Phenomenological Models Within the Code (Bottom-Up Review)

A bottom-up review was conducted by examining the pedigree, applicability, and fidelity of the individual models in CONTAIN. The code documentation database (App. C) provided most of the necessary model information. The Committee employed a set of classifications and definitions as depicted in Fig. 1-1 and defined in Table 1-I. Findings of Categories 1, 2, or 3 indicate that the code model is technically adequate. Findings of Categories 4, 5, and 6 indicate its technical inadequacy. A finding of Category 7 indicates the code model's technical inadequacy but low importance. (For comparison purposes, the crosshatched regions in Fig. 1-1 show technically acceptable categories for CONTAIN, and the shaded regions show technically acceptable regions for the MELCOR code.) MELCOR is a upper-tier or integrated code in the NRC's two-tier severe-accident code structure.

The Committee conducted reviews of the individual models and correlations and provided documentation of their results in the format shown in Table 1-II. The model review summaries (provided as subsections to Sec. 2) provide a qualitative overview of the technical adequacy of the code using the standard-of-model pedigree, model applicability, and model fidelity. The detailed reviews (provided as sections to App. D) give additional information to support the overall qualitative assessment.

1.3.11. Assess Technical Adequacy of the Integral Code Against the Design Objectives and Targeted Applications (Top-Down Review)

CONTAIN is designed to provide integrated analysis of containment phenomena. It is used to predict nuclear reactor containment loads, radiological source terms, and associated physical phenomena for a range of accident conditions encompassing both DBAs and severe accidents. Its targeted applications are experiment analysis and support for containment-related severe accident and ALWR experimental programs, LWR and ALWR plant analysis, and analytical support for resolution of specific technical issues such as direct containment heating (DCH).

<div> <div>Technically Acceptable for CONTAIN</div> <div>Technically Acceptable for MELCOR</div> </div>			
<div> <div>KNOWLEDGE OF PHYSICS</div> <div>→</div> </div>			
MODELING DETAIL	Understood	Questionable	Poor
First Order	1	2	3
Zeroeth Order (Parametric)	4* or 7	3	3
Control Function Features Allow Sens. Studies	5 or 7	4 or 7	3
Not Reasonable No "Features"	5 or 7	5 or 7	6

* Includes inadequate first-order model.

Fig. 1-1.
CONTAIN bottom-up review matrix of technical adequacy findings.

A top-down review was conducted by examining the applicability and fidelity of the total code. Previous benchmarking efforts were reviewed. In the absence of this information, plant calculations and expert opinion were employed.

The Committee has documented its findings in relation to the code objectives (Sec. 3) and targeted applications (Sec. 4). For each code objective and targeted application, the Committee defined areas to be examined to adjudge the technical acceptability of the integral code.

1.3.12. Document Findings in a Summary Report

This report documents the findings of the CONTAIN Peer Review Committee and the process used to develop those findings.

**Table 1-I
CONTAIN Bottom-Up Review
Classification of Findings**

Finding	Definition
Category 1	The severe-accident phenomena are generally understood, and the physics are correctly represented with a least a first-order model.
Category 2	The physics are partially, but not fully understood; thus, the knowledge of physics is questionable. Reasonable physics (in the context of expert judgement) are represented with at least a zeroeth-order model.
Category 3	A poor understanding of the severe-accident phenomena exists. A model is provided in the code, or features are available in the code to perform sensitivity studies over the currently understood ranges of phenomenological behavior.
Category 4	The physics are understood, but they are represented by an inadequate first-order model or a zeroeth-order model. The physics are questionable, but they are represented by control function features.
Category 5	The physics are understood, but they are represented by (1) control function features, (2) an unreasonable model, or (3) no modeling features exist at all. The physics are questionable, but they are represented by (1) an unreasonable model, or (2) no modeling features exist at all.
Category 6	The physics are poorly understood. The code provides no mechanism (features) to perform sensitivity studies over the currently understood ranges of phenomenological behavior.
Category 7	A finding of either Category 4, 5, or 6 would apply, but the phenomena being modeled are not of sufficient importance to markedly influence either the major features or trends of the severe accident. (Note: This category relates more to prioritizing the correction of defects than condoning their continuance.)

1.4. Presentation of Committee Findings

The Committee decided to present its findings in a format similar to that employed for the previously cited MELCOR and SCDAP/RELAP5 reviews. Summarized findings for the detailed review of code phenomenological models are given in Sec. 2. More detailed findings for these bottom-up reviews are given in App. D. The findings relative to the code objectives are presented in Sec. 3; findings relative to the targeted applications are presented in Sec. 4; other findings are presented in Sec. 5. Recommendations resulting from the Committee's review findings are presented in Sec. 6. CONTAIN peer review assignments for individual Committee members are presented in Table 1-III.

Table 1-II
Format for CONTAIN Bottom-Up Detailed Review Documentation

Section 2. Model Review Summary Format	
1.	Phenomenological Description
2.	Qualitative Perspective
3.	Technical Adequacy
Appendix D. Detailed Review Format	
1.	Model Description and Pedigree
2.	Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena
3.	Results of Model Sensitivity Studies
4.	Results of Benchmarking/Validation Studies
5.	Identified Deficiencies and Options for Model Improvements
6.	Importance of Model to Prediction of Dominant Phenomena
7.	Technical Adequacy of Model and Documentation

REFERENCES

- 1-1. "CONTAIN 1.2 Code Manual: A Computer Code for Severe Accident Analysis," Sandia National Laboratories report SAND94-2358, in preparation.
- 1-2. F. Eltawila, US Nuclear Regulatory Commission, Division of Systems Safety Research, unnumbered letter dated October 23, 1994, to B. E. Boyack, Los Alamos National Laboratory.
- 1-3. B. E. Boyack, V. K. Dhir, J. A. Gieseke, T. J. Haste, M. A. Kenton, M. Khatib-Rahbar, M. T. Leonard, and R. Viskanta, "MELCOR Peer Review," Los Alamos National Laboratory report LA-12240, March 1992.
- 1-4. M. L. Corradini, V. K. Dhir, T. J. Haste, T. J. Heames, R. P. Jenks, J. E. Kelly, M. Khatib-Rahbar, and R. Viskanta, "SCDAP/RELAP5 Independent Peer Review," Los Alamos National Laboratory report LA-12481, January 1993.

**Table 1-III
CONTAIN Peer Review Assignments**

Description	Reviewer A	Reviewer B
Phenomenological Models (Bottom-Up)		
Intercell Flow Models/Thermal-Hydraulics	MKR	PNS
Cell Heat and Mass Transfer		
Convective Heat Transfer	MLC	SKL
Radiative Heat Transfer	MLC	SKL
Conduction Heat Transfer	MLC	SKL
Mass Transfer	MLC	SKL
Core-Concrete Interactions	MKR	MLC
Water Pool Heat Transfer	MLC	MKR
Direct Containment Heating Models	PNS	MLC
Aerosol Behavior Models	SKL	PNS
Gas Combustion Models (H ₂ and CO)	PNS	MKR
Fission Product Behavior Models	SKL	RSD
Engineered Safety Features		
Fan-Cooler Model	RSD	PNS
Ice Condenser	RSD	MLC
Containment Sprays	SKL	PNS
BWR Specific Models		
Suppression Pool Flow Model	MKR	RSD
Vent Clearing Model	MKR	RSD
Suppression Pool Scrubbing Model	RSD	SKL
Material Properties	MLC	PNS

Committee Members' Initials:

Boyack	BEB
Corradini	MLC
Denning	RSD
Khatib-Rahbar	MKR
Loyalka	SKL
Smith	PNS

Table 1-III (continued)
CONTAIN Peer Review Assignments
(continued)

Description	Reviewer A	Reviewer B
Integral Code Performance (Top-Down)		
Design Objective 1	RSD	BEB
Design Objective 2	RSD	BEB
Design Objective 3	RSD	BEB
Design Objective 4	MKR	
Design Objective 5	MKR	
Targeted Application 1	RSD	BEB
Targeted Application 2	RSD	BEB
Targeted Application 3	RSD	BEB
Targeted Application 4	RSD	BEB
Targeted Application 5	RSD	BEB
Fission Products	SKL	RSD
Revised Severe-Accident Code Strategy	Committee	
CONTAIN User Survey	BEB	

Committee Members' Initials:

Boyack	BEB
Corradini	MLC
Denning	RSD
Khatib-Rahbar	MKR
Loyalka	SKL
Smith	PNS

2. BOTTOM-UP REVIEW OF CONTAIN PHENOMENOLOGICAL MODELS

The objective of the bottom-up review was to determine the technical adequacy of individual phenomenological models in the CONTAIN code. To report its findings, the Committee used category numbers that identified to what degree a given model was technically adequate (see Sec. 1.3.10). The category numbers are depicted and described in Fig. 1-1 and Table 1-I, respectively.

A model that is assigned a category number of 1, 2, or 3 is deemed to be technically acceptable; otherwise, the model is deemed inadequate (Categories 4, 5, or 6) or unimportant (Category 7).

Detailed reviews of each CONTAIN phenomenological model are presented in App. D. However, the Committee decided that a summary of the review findings was advisable. The objective of this section is to present the summary reviews of each phenomenological model.

Each summary is divided into three subsections: (1) a brief description of the phenomenological model; (2) a qualitative perspective that considers, for example, factors such as the level of modeling detail; and (3) a discussion of the technical adequacy of each model. Table 2-I summarizes the findings for technical adequacy for each of the code models reviewed. Table 2-I summarizes the information in Table C-II. The order of model presentation in Table 2-I differs from the order of model review in the following subsections. The subsection containing the summary review for each model is identified in brackets.

2.1. Material Properties

See App. D.1 for the detailed model review.

2.1.1. Phenomenological Model Description

The materials properties routines used in CONTAIN are described in Sec. 3 of the CONTAIN manual. A library of physical properties for 50 standard materials that can be used in the modeling of containment systems is part of the CONTAIN code. This library provides temperature-dependent specific enthalpy, specific heat, density, viscosity, and thermal conductivity for these 50 materials that may be found in nuclear reactor containments under severe-accident conditions. Table 3-1 lists the standard materials available in the CONTAIN code and the corresponding code name for each material in the library. Viscosity functions are not included for solids, and gas densities are determined from the ideal gas law. The user is referred to App. B (Reports - Sandia National Laboratories, Albuquerque, NM, Ref. VAL88b) for the complete listing of each correlation as coded into the CONTAIN model. Some of the properties for each material have not been revised or have not been supported since CONTAIN-1.1. These are clearly noted in the aforementioned table. The properties for water are divided into water liquid and vapor properties with this method. Also averaging of mixtures of properties are accomplished according to accepted procedures for thermophysical properties (by mass fraction) and transport properties (by mole fraction). One should note that the molar averaging done for viscosity and thermal conductivity of gases is a gross simplification of the actual practice. However, such simplification does not have a significant effect on the simulation results. In addition, the dimensionless properties are given according to generally accepted definitions.

Table 2-I
Summary of Bottom-Up Review Findings for CONTAIN Models

Severe Accident Phenomena [Section]	Importance to Containment		Model Adequacy
	Source Term	Loads	
I. Direct Containment Heating			
a. Melt Ejection from RPV [2.4.1]	Medium	High	Adequate
b. Melt Oxidation by Gas [2.4.2]	Medium	High	Adequate
c. Melt Sweepout [2.4.3]	Medium	High	Adequate
d. Drop Entrainment/Fragmentation [2.4.4]	Medium	High	Adequate
e. Melt-Water Interactions [2.4.5]	Low	High	Inadequate
f. Fission Product Release [2.4.6]	Medium	Low	Inadequate
g. Melt Trapping and Carryover [2.4.7]	Medium	High	Adequate
h. Melt-Debris-Gas Heat Transfer [2.4.7]	Medium	High	Adequate
II. Non-Energetic Fuel-Coolant Interaction			
a. Melt Fragmentation in Water [2.4.5]	Low	High	Inadequate
b. Melt Water Heat Transfer [2.4.5]	Low	High	Inadequate
c. Melt Oxidation [2.4.5]	Low	Medium	Inadequate
III. Molten Core-Concrete Interaction			
a. Energy Generation [2.3.1]	High	High	Adequate
b. Crust Formation/Freezing [2.3.2]	High	High	Adequate
c. Heat Transfer (Concrete/Bulk) [2.3.3-4]	Medium	High	Adequate
d. Hydraulics in Pool (Mixing/Swell) [2.3.5-7]	Low	High	Adequate
e. Chemical Reactions [2.3.8]	High	High	Adequate
f. MCCI Material Properties [2.3.9]	High	High	Adequate
g. Melt Debris Spreading [2.3.10]	Low	Medium	Inadequate
h. Fission Product Release [2.3.11]	High	Low	Inadequate
IV. Combustion			
a. Ignition Criteria [2.7.1]	Low	High	Adequate
b. Mode of Combustion [2.7.2]	Low	High	Adequate
c. Diffusion Flame [2.7.3]	Low	Medium	Adequate
d. Bulk Spontaneous Recombination [2.7.4]	Low	High	Adequate
e. Deflagration [2.7.5]	Low	High	Adequate
f. Combustion Completeness [2.7.6]	Low	High	Adequate
g. Propagation in Multi-Compartments [2.7.7]	Low	Medium	Inadequate
h. Effect on Fission Product Release [2.7.8]	Low	Low	Adequate
V. Ex-Vessel Transport			
a. Materials Properties [2.1]	Low	Medium	Adequate
b. Water Pool Phenomena [2.2.2]	Medium	Medium	Adequate
c. Structure Conduction [2.8.1]	Medium	High	Adequate
d. Structure Radiation [2.8.2]	High	Medium	Adequate
e. Mass Transfer [2.8.4]	High	High	Adequate
f. Free/Forced Convection [2.8.3]	High	Medium	Adequate
g. Thermodynamics [2.8.5]	Medium	High	Adequate
h. Intercell Flow [2.2.1]	High	High	Inadequate ¹
i. Stratification [2.2.1]	Low	High	Inadequate ¹

¹ Evaluation based on the original CONTAIN design objectives. However, based on the revised CONTAIN objectives associated with the revised severe-accident code strategy (App. E), this model is adequate.

Table 2-I (continued)
Summary of Bottom-Up Review Findings for CONTAIN Models

Severe Accident Phenomena [Section]	Importance to Containment		Model Adequacy
	Source Term	Loads	
VI. Engineered Safety Features Thermal-Hydraulics			
a. Ice Condenser [2.10.2]	Low	High	Adequate
b. Containment Sprays [2.10.3]	Low	High	Adequate
c. Suppression Pool Flow [2.9.1]	Low	High	Adequate
Suppression Pool Vent [2.9.2]	Low	High	Inadequate
d. Containment Fan Coolers [2.10.1]	Low	High	Adequate
e. PCCS for ALWR - PWR [2.10.4]	Low	High	Adequate
PCCS for ALWR - BWR [2.10.4]	Low	High	Adequate
VII. Containment Failure Modes			
a. Local Leakage Rate [2.2.1]	Medium	High	Inadequate ¹
b. Gross Failure [2.2.1]	High	High	Adequate
VIII. Aerosol Transport/Retention			
a. Size and Composition Distribution [2.5.1]	High	Low	Inadequate ²
b. Agglomeration [2.5.2]	High	Low	Inadequate ²
c. Deposition [2.5.3]	High	Low	Inadequate ²
d. Steam Condensation [2.5.4]	High	Low	Inadequate ²
e. Removal by ESF-Suppression Pool [2.5.5]	High	Low	Inadequate ²
Removal by ESF-Ice Condenser [2.5.5]	High	Low	Adequate
Removal by ESF-Containment Spray [2.5.5]	High	Low	Inadequate ²
f. Resuspension	Medium	Low	Not Evaluated ³
g. Surface Physical Reactions	Medium	Low	Not Evaluated ³
h. Surface Intraparticle Chemical Reactions	High	Low	Not Evaluated ³
i. Charge Effects	Medium	Low	Not Evaluated ³
IX. Vapor Fission Product Transport			
a. Noble Gas	High	Low	Not Evaluated ³
b. Organic Iodide Source	High	Low	Not Evaluated ³
c. Organic Iodide Retention	High	Low	Not Evaluated ³
d. Volatile Iodine	High	Low	Not Evaluated ³
e. Retention by ESFs	High	Low	Not Evaluated ³
X. Fission Product Characterization			
a. Transmutation [2.6]	Medium	Low	Adequate
b. Fission Product Grouping [2.6]	Medium	Low	Adequate
c. Decay Heat [2.6]	Medium	Low	Adequate

² Evaluation based on the original CONTAIN design objectives. The revised CONTAIN design objectives associated with the revised severe-accident code strategy (App. E) discontinue further CONTAIN model development related to these phenomena.

³ Evaluations were not performed because the model does not exist in the CONTAIN code and the revised CONTAIN design objectives associated with the revised severe-accident code strategy (App. E) dictate that there be no further CONTAIN model development effort related to the phenomenon.

2.1.2. Qualitative Perspective

The methods used for specifying material properties seem quite adequate. However, the CONTAIN manual notes that the standard material property library cannot be used to specify the properties for the debris species used in the DCH model within CONTAIN, nor is it used for the MCCI process in CORCON. The committee feels that this may result in possible inconsistencies between modules within CONTAIN, and must be corrected so that a consistent properties database is used within the DCH, MCCI, and other parts of CONTAIN or that the user be given precise advice to avoid unwanted inconsistencies. Other than this identified concern, the materials package is quite reasonable.

2.1.3. Technical Adequacy

The material properties used reflect the current state of knowledge of a first-order equation-of-state model. The physics is well understood based on materials properties references within the CONTAIN manual and the properties have been validated by direct reference to well-known property tables. Therefore, although possible inconsistencies are present by the lack of a common material properties database for DCH and MCCI as well as the rest of CONTAIN, it is judged to be technically adequate (Category 1). The priority for resolution of these inconsistencies is discussed in Sec. 6, Recommendations.

2.2. Atmosphere/Pool Thermodynamic and Intercell Flow Models

See App. D.2.1 for the detailed model review.

2.2.1. Intercell Flow Model

2.2.1.1. Phenomenological Model Description

The model used for computing flow between control volume compartments is described in Sec. 4.2 of the CONTAIN manual. The model allows for various flow path options that the analyst can choose from: a single flow path between control volumes, an engineering vent flow path between control volumes that allows for multiple flow paths, as well as variable area junctions. The flow model also has four different flow path models to calculate the mass flow between any control volume: inertial flow model, quasi-steady flow model, critical flow model, user-specified flow rate model. The normal choice for most calculations is the inertial flow model, although there are instances where the other choices are more advantageous. A containment failure model that allows for calculation of flow based on user-specified failure location and size is also included. For the most part, the manual does a good job in describing the various models and giving guidance to the analyst as to what is the best choice.

The complete one-dimensional momentum equation used for the inertial flow model is given in Table 4.1 of the CONTAIN manual. The definition of the body force term in the CONTAIN momentum equation can introduce errors in predicting natural circulation flows, and has been shown to be incapable of accurately predicting temperature and/or species stratification under simulated conditions. The recent modifications to the CONTAIN flow solver package in response to the concerns expressed by the peer review group are based upon several alternatives to the numerical approximations of $\int \rho dz$ term under conditions that variations in density are either large or discontinuous along the flow

path direction. The proposed approach is based on a "hybrid" of the average density and the donor density numerical approximations depending on the density difference between the cells, and the previous time-step flow direction, corrected for isothermal stratification effects.

2.2.1.2. Qualitative Perspective

The one-dimensional momentum equation used in the CONTAIN model is developed with the assumption that any two control volumes, which model compartments within the containment, are approximately connected by an opening (doorway or open area) which can be modeled by an orifice of some specific flow area with an associated momentum loss coefficient. In fact, the derivation of the equation (inertial flow model), as depicted in Table 4.1 of the CONTAIN manual, can be derived in a straightforward manner using this physical picture. One should note that such a characterization of the flow geometry leaves one with the interpretation that the inertial length of the junction is approximately equal to the center-to-center distance between the two control volumes and the buoyancy term in the momentum equation must be referenced to the control volume cell-centered elevations. With this interpretation, the one-dimensional momentum equation used in CONTAIN (or its quasi-steady simplification) seems quite consistent and reasonable. The committee found it difficult to come to this conclusion, because the manual describes the formulation in a different way and allows the analyst the flexibility to choose other options for the inertial length and the definition of the buoyancy term and the associated elevations. With the change to the Implicit Flow Solver logic, the committee feels a better explanation of the flow formulation would be in order.

The recent hybrid formulation of the buoyancy term is based on heuristic physical and numerical arguments that appear reasonable. However, additional application cases are needed to determine all potential pitfalls, and to confirm technical adequacy under conditions of most interest to containment analysis.

2.2.1.3. Technical Adequacy

The current state of knowledge for this flow model is well established in the open literature and the physics is understood. In addition, this type of momentum flow model has been validated in past analyses. Also, the recent modifications to the buoyancy head formulation were shown to improve the prediction of intercell and thermal stratification behavior; however, the CONTAIN simple control volume model cannot be used in predicting intracell distributions of flow, temperature, and concentration fields in large, open volumes. Furthermore, additional experimental validation of the revised buoyancy head formulation is needed to confirm its applicability under all conditions of interest.

Within the limitations of the control volume, lumped-parameter approximation, the intercell flow models are adequate under homogeneous and well-mixed conditions. On the other hand, these simple, zeroth-order, lumped-parameter models are inadequate under conditions of large thermal and species stratification. The recent numerical fixes introduced in CONTAIN show promise for resolution of intercell distributions; however, the present model is inadequate for prediction of intracell effects. The containment failure model is appropriate for large failure sizes, while it is inadequate for application to flow through cracks and tortuous pathways. Overall, a finding of Category 4 is assigned to the intercell flow, stratification, and containment failure models.

It should be noted that under the "Revised Severe Accident Code Strategy" (App. E), the detailed mechanistic specification and accompanying requirements for models to be first order no longer exist. Therefore, with the exception of the identified

deficiencies, the intercell flow model is acceptable within the revised severe-accident code strategy and practical constraints on a systems code. No action to render the intercell flow model first order is recommended.

2.2.2. Water Pool Model

See App. D.2.2 for the detailed model review.

2.2.2.1. Phenomenological Model Description

The water pool model is partially described in Sec. 4.3 of the CONTAIN manual. It is used as the appropriate model for a source or sink of water associated with the transport from ESF systems, as well as the destination for water film drainage off of structures within the containment or as overflow locations from other higher water pools. Besides providing the water inventory for the containment for open pools, it serves as the source of water vapor or steam provided by energy input from the core debris. This feature of water pools is described in detail in Sec. 4.3 and is termed the "implicit boiling model." This is actually part of the original CONTAIN lower cell model that is less frequently used. The mass of steam produced within a time step is equal to the energy deposited because of decay heat or other energy sources into the water pool divided by the enthalpy required to raise the water from its initial enthalpy to its saturated vapor enthalpy. Thus, the updated mass of the pool is set equal to the initial mass plus any water added (or subtracted) minus the water boiled away. The documentation seems to indicate that this CONTAIN water pool model assumes that any pool within the containment is assumed to become and remain saturated, although one would not have to maintain that restrictive of a condition. The SNL staff stated that the model does consider subcooled water pools as a lumped-parameter liquid pool.

2.2.2.2. Qualitative Perspective

The models used for the implicit boiling pool source was not clearly documented in the CONTAIN manual. The equations used to explain the vapor source term (Eqs. 4-21 and 4-24) were redundant and confusing to the reader. In addition there is a mention of an App. K, which was absent from the documentation and appears irrelevant. After a discussion with the SNL staff, it seemed clear to the committee that there were errors in the documentation, not in the code software, that needed corrections. The actual approach used for a saturated boiling pool was described by Dr. K. Murata and seemed correct. Thus, the manual should be corrected to reflect the correct physical relations. In addition, the SNL staff should consider that documentation for the subcooled pool model be included into the CONTAIN formulation. These changes are necessary for better understanding.

2.2.2.3. Technical Adequacy

The water pool model, as described by the SNL staff, reflects the current state of knowledge for a systems model and is judged to be of first order. The physics is well understood and validation of the model is possible with simple thought experiments as well as simple test problems. Although the documentation errors need to be corrected in the CONTAIN manual and the subcooled model completely documented, the model is judged to be technically adequate (Category 1).

2.3. Core-Concrete Interactions

CORCON-Mod3 models the thermal attack of core debris on concrete using a quasi-static approach that includes the core debris pool, the concrete cavity, and the water and/or atmosphere above the debris pool. The decay and chemical reaction energy generated within the debris pool is transferred to the concrete basemat and sidewalls, as well as the overlaying water pool and/or atmosphere.

See App. D.3 for the detailed model review.

2.3.1. Energy Generation

2.3.1.1. Phenomenological Model Description

The core debris/concrete interaction process is driven by decay and chemical reaction heat generated in the pool. The decay heat includes contributions from actinides, decay products, and irradiated structural material. The decay heat is approximated by contributions from 27 elements (excluding noble gases) which were found to account for nearly all of the energy production in the ORIGEN calculations. The initial core inventory of fission products is assumed to be proportional to core operating power, as specified through user input. The energy generation due to chemical reactions is also included.

2.3.1.2. Qualitative Perspective

The approximate representation of the decay heat is consistent with the present conceptual framework of CONTAIN and represents adequate level of details for containment analyses.

2.3.1.3. Technical Adequacy

Typically less than 10% uncertainty exist in the ORIGEN predictions. The present approach is based on a simple fit to a SNL-ORIGEN calculation. Even though the approach is not truly a first-order model, nevertheless, it is an adequate representation of first order behavior. The technical adequacy of this model is classified as Category 1.

2.3.2. Crust Formation and Freezing

2.3.2.1. Phenomenological Model Description

This model is based on CORCON-Mod2, where a quasi-steady one-dimensional analysis is performed. Crust is assumed to begin to form when the local interface temperature falls below the solidus temperature. Crust thickness is determined by matching the energy generation rate with the net heat loss rate. Using a one-dimensional conduction model, it treats liquid layers, solid layers, and liquid layers with solid crust.

2.3.2.2. Qualitative Perspective

The model does not account for crust history; therefore, during calculations the crust may appear and disappear in a single time step. In addition, the model for crust growth and its evolution is not correct, especially in the presence of water, so crust breakup upon interaction with water and crust instability are not considered.

2.3.2.3. Technical Adequacy

The severe accident physics are partially, but not fully understood; thus the knowledge of physics remains questionable. Reasonable physics are represented with at least a zeroeth order model. The technical adequacy of this model is classified as Category 2.

2.3.3. Bulk Pool Heat Transfer

2.3.3.1. Phenomenological Model Description

Pool is considered to be composed of several metal and oxide layers in a stratified configuration, with well defined interfaces. The CORCON-Mod3 model considers inter-layer heat transfer as well as heat transfer at pool boundaries. Empirical correlations reported in the literature are used for calculation of heat transfer by convection (with and without gas flow) from the top, bottom, and radial boundaries of the molten pool.

2.3.3.2. Qualitative Perspective

The heat transfer processes within the pool remain uncertain, and many models are available in the literature; however, none of these models have been found to be able to predict the experimental measurements adequately. This is a complicated problem, and it is not expected that a universally accepted model can be developed that will capture the physics observed in the experiments; therefore, it appears that adequate dials are built into the present CORCON models so that parametric studies can be performed over the expected range of uncertainties.

2.3.3.3. Technical Adequacy

The severe accident physics are not fully understood; however, reasonable physics are represented with a first-order model. The technical adequacy of this model is classified as Category 2.

2.3.4. Melt-Concrete Heat Transfer

2.3.4.1. Phenomenological Model Description

In CORCON-Mod2, for a horizontal surface, a pseudo film boiling model based on the concept of Taylor instability was used, and this model is still an option in CORCON-Mod3. Radiation heat transfer is also included in the model. In addition to the original stable gas film model of CORCON-Mod2, a new model based on intermittent contact of debris pool and concrete surface is included as an option in CORCON-Mod3.

2.3.4.2. Qualitative Perspective

The use of gas film flow path length in calculating heat and mass transfer is not supported by the laboratory data reported in the literature. The code does not allow a transition from the original stable film model to the new slag film model. Here again, it is not expected that a universally accepted model can be developed that will capture the physics observed in the experiments; therefore, it appears that adequate dials are built into the present CORCON models that parametric studies can be performed over the expected range of uncertainties.

2.3.4.3. Technical Adequacy

The severe accident physics are not fully understood; thus the knowledge of physics remains questionable. Reasonable physics are represented with a first-order model. The technical adequacy of this model is classified as Category 2.

2.3.5. Coolant Layer Heat Transfer

2.3.5.1. Phenomenological Model Description

Fits to standard correlations for nucleate boiling, film boiling, maximum heat flux and minimum heat flux are used. Radiation contribution in film boiling is also included. The effect of gas injection on film boiling is based on the correlation proposed by Greene.

2.3.5.2. Qualitative Perspective

The use of nucleate boiling and critical heat flux correlations applicable to water boiling on a solid, flat surface, to heat transfer from a molten pool/solid debris to an overlying coolant layer remains in question. The effect of gas injection on film boiling is based on the correlation proposed by Greene. This correlation is based on small temperature difference of about 100 K, and its applicability to reactor calculations is not established. Superposition of combined effects of gas injection and liquid subcooling is not based on experimental evidence. The correlation for effect of gas barbotage on minimum film boiling temperature is not justified.

2.3.5.3. Technical Adequacy

The severe accident physics are not fully understood; however, reasonable physics are represented with at least a zeroeth-order model. The technical adequacy of this model is classified as Category 2.

2.3.6. Bubble Phenomena

2.3.6.1. Phenomenological Model Description

Bubble behavior affects heat transfer and interlayer mixing within the molten debris pool. The terminal velocity of the bubbles is calculated for different bubble shapes (i.e., spherical, ellipsoidal, and spherical cap bubbles) using the correlations/models available from the literature.

2.3.6.2. Qualitative Perspective

Changes resulting from variations in chemistry, pressure, temperature and composition are accounted for; however, coalescence or breakup of bubbles has not been considered. Chosen bubble size is not substantiated with experiments. Froth formation at the pool free surface and at the layer interfaces has not been considered.

2.3.6.3. Technical Adequacy

Overall the model is adequate but there may be substantial error in calculated void fractions, which in turn will affect the convective heat transfer coefficient. The physics are

not fully understood; however, reasonable physics are represented with a first-order model. The technical adequacy of this model is classified as Category 2.

2.3.7. Interlayer Mixing

2.3.7.1. Phenomenological Model Description

Models are included to address the effects of mixing between molten layers within the debris pool. If this option is activated, mixing can occur instantaneously (within one time step). The code can currently model two types of mixture layers: a layer of light oxide with suspended metal drops or a layer of metals with suspended heavy oxide drops. In addition, single layers can also be formed (stratified) due to the de-entrainment mechanism.

2.3.7.2. Qualitative Perspective

This is one of the most important modeling aspects in terms of CORCON-Mod3 predictions of core-concrete interactions. The models for the entrainment of liquid droplets by the rising gas bubbles and the de-entrainment mechanism are based on a single particle model that may prove to be simplistic. The experimental basis of this model is very weak (solely based on one set of experiments). The effects of gas flow rate, interface conditions (i.e., waviness), and particle interactions and coalescence are not included in these models.

2.3.7.3. Technical Adequacy

The physics remain questionable; however, reasonable physics are represented with a first-order model. The technical adequacy of this model is classified as Category 2.

2.3.8. Chemical Reactions

2.3.8.1. Phenomenological Model Description

CORCON-Mod3 can treat two types of chemical reactions: (1) between evolved gases from the concrete (water vapor and carbon dioxide), other chemical reactions within the pool, and the metallic phase leading to oxidation and release of hydrogen and carbon monoxide in the process, and (2) between condensed phases (metals and oxides).

Chemical equilibrium is attained by minimizing the Gibbs free energy for the species (56 chemical elements and 15 elements are included) between the reactants and products at each time step. The species list has been expanded to include uranium, aluminum, silicon, and calcium. Additional condensed phase reactions probably should be included. The effects of non-ideal solution chemistry only treated for vaporization release models as part of the VANESA models are not yet working. In addition, the effects of condensed phase chemical reactions can be introduced by setting an option flag. The effect of coking reaction and production of C_2H_2 can also be suppressed through a user-option flag; in this case large amounts of methane (CH_4) and ethane (C_2H_6) are produced.

2.3.8.2. Qualitative Perspective

It is not clear from the documentation why the CORCON and VANESA chemistry models are not integrated together into one package. The addition of the condensed phase chemistry models is a positive development. However, with condensed phase chemistry option activated, the equilibrium model leads to reaction of most of the zirconium content of the melt within the first time step, provided zirconium initially is present in large quantities

in the pool (greater than a few percent). This leads to an early escalation of chemical reaction heat and the melt temperature. The effect of non-ideal solution chemistry is not yet operational. Furthermore, the chemistry package needs additional condensed phase chemical reactions for SiC, U_3O_8 , and other species. Lack of additional chemical reactions may be the reason for prediction of coking reaction in CORCON.

2.3.8.3. Technical Adequacy

The physics are not fully understood; however, reasonable physics are represented with a zeroeth-order model. The technical adequacy of this model is classified as Category 2.

2.3.9. Material Properties

2.3.9.1. Phenomenological Model Description

CORCON-Mod3 calculates thermophysical properties over a large range of temperatures. The modeling of thermophysical data remains largely unchanged from CORCON-Mod2.

The phase diagrams include data built in for the three concrete types, while other concrete types the code requires user values for the liquidus and the solidus temperatures. The phase diagrams include data built in for the three concrete types, while for other concrete types, the code requires user values for the liquidus and the solidus temperatures. The phase diagrams for metallic mixtures consist of simple fits for chromium, iron, and nickel liquidus and solidus temperatures. The presence of zirconium, silicon, etc., which could substantially reduce melting temperature of metal phase, is currently ignored. In CORCON-Mod3, a new option is included for the user to provide the solidus temperature of the metallic phase and the code in turn adds 10 K for the liquidus temperature. The phase diagrams for oxidic mixtures (pseudo-binary system) are based on an ideal solution for the solid phase.

2.3.9.2. Qualitative Perspective

A much faster reduction in solidus temperature is expected with concrete addition (at 10-20% concrete, mixture solidus temperature falls to that of concrete). The user can select a parametric value of solidus temperature to represent eutectic interactions. A better representation of recent experimental observations is desirable. The phase diagrams between the in-vessel and ex-vessel severe-accident codes may not necessarily be consistent.

2.3.9.3. Technical Adequacy

The data base for material properties is still expanding. The CORCON material properties are, for the most part, adequate. The properties should be updated to reflect the recent experimental database. The CORCON approach is at least zeroeth order. The technical adequacy of this model is classified as Category 2.

2.3.10. Melt Spreading

2.3.10.1. Phenomenological Model Description

The radius of the debris pool can be specified as a function of time by the user.

2.3.10.2. Qualitative Perspective

The simple model for melt radius variations with time incorporated in the code is believed to be appropriate for comparison with experimental data where the melt spreading can be measured. However, in the event of an actual accident scenario, the progression of the melt radius with time is not known, and the present model is too limited to be of much use. It is desirable to implement a simple model for prediction of the melt spreading rate. Simple melt spreading models have been developed and are available in the open literature.

2.3.10.3. Technical Adequacy

The physics are partially but not fully understood; thus the knowledge of physics remains questionable. However, even though a parametric model is included in the code, nevertheless, the model is inadequate for severe-accident simulations. The technical adequacy of this model is classified as Category 4.

2.3.11. Fission Product Release

2.3.11.1. Phenomenological Model Description

The fission products are released from the melt concrete pool. CORCON-Mod3 models these releases based upon the chemical reactions (Sec. 2.3.8) which provide for the fission-product vapor injection and subsequent VANESA conversion of these vapors into aerosol particles in the rising bubbles. The transport of these condensed species via the bubble is affected by the thermal-hydraulics of the pool.

2.3.11.2. Qualitative Perspective

Calculation of vaporization of the fission products into the bubbles and their subsequent conversion to particles poses very difficult problems. The size/composition distribution of particles is, therefore, eventually estimated from integral experimental data rather than mechanistically.

2.3.11.3. Technical Adequacy

CORCON-Mod3 is an advance over previous models, but the overall model is a mixture of mechanistic models and empiricism. The technical adequacy of the overall model is Category 4.

2.4. Direct Containment Heating

See App. D.4.1 for the detailed model review.

2.4.1. Melt Ejection from Reactor Pressure Vessel

2.4.1.1. Phenomenological Package Description

The initial ejection of single-phase melt from the vessel is modeled using Bernoulli's equation to predict the discharge of core debris via the breach; a user input orifice coefficient allows some user control over the discharge. The Gluck correlation is used to determine the point at which gas blowthrough will occur. After blowthrough has occurred the two-phase discharge of debris and gas from the vessel is treated as a separated flow, with a correlation developed by Pilch and Griffith to predict the flow quality. During

this phase the debris discharge is treated as in the single-phase discharge and the gas is treated as an ideal gas undergoing choked flow. During the discharge of the debris, ablation of the vessel resulting from the thermal attack of the debris on the vessel is modeled; heat transfer is estimated using a modified flat plate heat transfer coefficient and all of the heat transferred to the vessel is assumed to be used in melting the steel vessel.

The RPV models are only available when the cavity entrainment models are used; otherwise the user must specify the debris ejection rate explicitly.

2.4.1.2. Qualitative Perspective

The models for most of the major processes are physically reasonable and agree with the available experimental data. No explicit allowance is made in the modeling for the presence of solids in the debris or for off-center discharges that could lead to incomplete discharge from the vessel. However, the breach area and discharge coefficients can be adjusted to scope the effect of solid debris on the discharge rate and the discharged fraction can be varied by varying the amount of debris input to the calculation. In view of the stochastic nature of the geometry of any solid debris present in the lower head and the uncertainty in the position of the breach in the lower head, the parametric treatment adopted in the code is appropriate. The neglect of thermal conduction in the vessel when estimating the hole ablation rate is justified in view of the high predicted ablation rates and the agreement between prediction and experiment.

2.4.1.3. Technical Adequacy

The phenomena for which the physics is understood have appropriate first-order models in the code. Where uncertainty exists in the behavior of the system, or the understanding of a process is questionable, there is adequate flexibility in the modeling to allow the magnitudes of the effects to be investigated. The documentation is adequate. The technical adequacy of this model is classified as Category 2.

2.4.2. Melt Oxidation by Gas

See App. D.4.2 for the detailed model review.

2.4.2.1. Phenomenological Package Description

The oxidation of zirconium, aluminum, chromium, and iron by oxygen and steam are all modeled. The metals are assumed to react in the above order, first with oxygen then with steam; all the reactions are assumed to go to completion except the iron/steam reaction, which is limited by the calculated equilibrium of the system. The heat of reaction is added to the debris in each case. The hydrogen produced by the reactions with steam can either be added to the atmosphere or can be immediately reacted with any available oxygen in the atmosphere.

The rate of oxidation is limited by mass transfer of oxidant to spherical debris particles through the gas and by diffusion in the stagnant drops. The oxidation of metals is allowed to occur in both the airborne debris and non-airborne debris (NAD). In the latter case the user must define a length scale for the mass transfer processes.

2.4.2.2. Qualitative Perspective

The modeling includes the major chemical reactions and physical processes, with the possible exception of heat transfer between the NAD and the structures, which it

contacts (which may lead to the over-prediction of debris oxidation and hydrogen production). The NAD model is parametric, though the length scale can be chosen to give good agreement with the measured hydrogen production in all of the relevant SURTSEY experiments.

The mass transfer modeling contains some approximations, but nevertheless is adequate for the intended purpose.

2.4.2.3. Technical Adequacy

The physics are mainly understood and first-order models of the relevant phenomena are in place. The possible exception is the modeling of non-airborne debris, for which the detailed behavior is unknown and therefore is treated parametrically, so care should be taken in interpreting the results if it is predicted to make a significant contribution to the oxidation of the debris. The technical adequacy of the airborne debris model is classified as Category 1. The technical adequacy of the NAD portion of the model is classified as Category 2. The documentation should include advice to the user on how to estimate the required particle size for NAD for reactor plant calculations.

2.4.3. Melt Sweepout

The breakup of melt to form droplets is discussed in Sec. 2.4.4 and trapping on structures is covered in Sec. 2.4.8. See App. D.4.3 for the detailed model review.

2.4.3.1. Phenomenological Package Description

The melt can be represented by a number of types each with its own mean particle size, initial composition, mass and temperature. Each type can in turn be resolved into a number of generations, which allows the chemical and thermal evolution of extended sources of debris to be followed.

The fragmentation of the melt to produce the particles is discussed in Sec. 2.4.4 and the trapping of particles on structures is considered in Sec. 2.4.8. The particles that are not trapped by structures flow with the gas are subject to a user-defined slip ratio, which can be different for each debris field type and for each containment cell. The debris transport is achieved by integrating it into the implicit flow solver. Choking of the flow is accounted for when appropriate.

2.4.3.2. Qualitative Perspective

The multi-field capability provides ample representation of the airborne debris. The use of parametric slip ratios to represent particle transport by the gas is justified in view of the lack of understanding of the detailed fluid flow patterns and processes in the complex geometry of the reactor containment.

The recommended slip factors were obtained by fitting to the SURTSEY experiments; sensitivity calculations at reactor scale are required to determine if the possibility of smaller slip ratios required in the cavity is of any significance.

It remains to be determined if all of the particles can be levitated out of the cavity by the flows produced by the lowest pressures of interest.

The choked flow model significantly overpredicts the mass flux in the limit of no slip between debris and gas.

2.4.3.3. Technical Adequacy

In general the phenomena are understood in outline, though not in detail, and appropriate parametric models are in place. Some confirmatory work is suggested in Sec. 2.4.3.2, which would improve confidence in the modeling. The technical adequacy of this model is classified as Category 2.

The manual for this area of the code is confusing in places; this is due in part at least to the fact that it currently consists of several documents. However, the appropriate sections have been expanded in the revised documentation (to be issued) and the explanations are now clear and concise.

2.4.4. Drop Entrainment/Fragmentation

See App. D.4.4 for the detailed model review.

2.4.4.1. Phenomenological Package Description

Correlations are provided for the debris entrainment rate and entrained fraction, based on small-scale, isothermal experiments. The user must supply a multiplier for each of the correlations and must input the surface area for entrainment. The size of the entrained debris particles is determined from a critical Weber number which can be input by the user, but defaults to a sensible value.

There is much user flexibility for performing sensitivity studies: the user can set the entrainment rate, entrained fraction, time for entrainment, and the particle size.

2.4.4.2. Qualitative Perspective

The experiments on which the entrainment correlations are based are small-scale and isothermal and may not adequately represent the reactor accident phenomena. The experimental data do not support the use of a critical Weber number criterion for determining the sizes of the particles in the cavity. However, preliminary comparison with the SURTSEY-IET- 9 experiment is encouraging, and the flexibility afforded the user allows many sensitivities to be determined. Several of the available correlations, including the Whalley-Hewitt and Levy correlations, should be tuned to the available experimental data and this applied to plant calculations to confirm scaling.

This model is pivotal to the prediction of containment loads as it affects the mass of debris available for energy transfer to the atmosphere, the size of particles for heat transfer and chemical reaction, and the coherence of the debris and steam discharges.

2.4.4.3. Technical Adequacy

The physical processes in the cavity are poorly understood. Therefore, despite the identified deficiencies in the modeling, it represents the current state of the art. In addition, the flexibility in the modeling allows the user to determine the sensitivity to the questionable aspects of the modeling. An alternative and more mechanistic approach to modeling debris entrainment is incorporated in the CORDE code. To significantly improve on the modeling would probably require considerable effort and success could not be guaranteed. The technical adequacy of this model is classified as Category 3. The documentation should be adequate when the various pieces have been consolidated into a single document.

2.4.5. Melt-Water Interactions

See App. D.4.5 for the detailed model review.

2.4.5.1. Phenomenological Package Description

There are no models in the code designed specifically to deal with melt-water interactions in the cavity. Water can be introduced into the cavity atmosphere using the source table option. This allows some aspects of heat transfer and oxidation of the melt by the water to be studied parametrically, though the user must input the amount of water with which the melt is to interact.

2.4.5.2. Qualitative Perspective

Energetic FCIs are poorly understood and are not modeled in the code.

Not all of the water in the cavity may interact with the debris. The user must decide how much of the water participates in the interaction and input the required to the cavity atmosphere using the source table option. Much of the water may be expelled from the cavity by the steam pressure resulting from the boiling of the water that takes part in the interaction. There are no features in the code to model water slug expulsion from the cavity and associated effects such as the exacerbation of the pressurization of the cavity due to the tamping effect of the water.

Heat transfer and oxidation of the debris can be studied parametrically, though the details of the melt to water heat and mass transfer processes are not represented.

Fission product release from the melt during the interaction with water is not modeled, but it is probably a minor effect.

2.4.5.3. Technical Adequacy

Energetic FCIs are poorly understood and are not modeled.

Less energetic interactions are better understood but there are no features in the code to predict processes such as water slug ejection from the cavity. Heat transfer and oxidation of the debris can be represented parametrically but without capturing the essential features of the physical processes.

Fission product release during melt-water interactions is poorly understood, not modeled and probably not important.

The technical adequacy of the model is classified as Category 4. There is no documentation on how to use the currently available code features to represent melt-water interactions.

2.4.6. Fission Product Release

See App. D.4.6 for the detailed model review.

2.4.6.1. Phenomenological Package Description

There are no models in the code specifically designed to estimate fission product release during high-pressure melt ejection. The phenomenon can be represented parametrically by the user specifying source tables of fission products and aerosols to the cavity.

2.4.6.2. Qualitative Perspective

A considerable amount of data is available on fission product release during high-pressure melt ejection from the SNL SPIT, HIPS, and SURTSEY experiments. However, the releases can be sensitive to conditions such as the oxygen potential in the cavity and the amount of dissolved gas in the melt. Extrapolation from the available experimental data to the reactor plant is therefore not straightforward. There is no code to estimate the release from HPME as VANESSA does for MCCI despite the same inventory of fission products being available for release; indeed if DCH were to result in containment failure, any released fission products would have little opportunity for deposition before being swept out by the gas, compared to the materials released during MCCI.

2.4.6.3. Technical Adequacy

The understanding of the processes by which fission products are released from the melt during high pressure melt ejection is questionable. The releases can only be represented in the code by user input of the released species via the fission product and aerosol source tables. The technical adequacy of this model is classified as Category 4. There is no documentation to advise the user how to use the source tables to represent fission product release during a DCH scenario.

2.4.7. Melt Trapping and Carryover

See App. D.4.8 for the detailed model review.

2.4.7.1. Phenomenological Package Description

The rate of trapping of debris on structures within a given volume can be specified by the user, or it can be calculated using one of the three available models.

In the simplest model the trapping rate is determined from the gravitational fall time to the floor.

The second option is to assume that the debris is transported on a turbulent gas jet to impact on a structure and then fall under gravity onto the floor.

The most sophisticated option is to assume that the debris is transported to its first impact as in the previous option. The code then determines if the debris will adhere to the structure or will be re-entrained into the gas flow, based upon a critical Kutateladze number criterion. Re-entrained debris is transported to a second impact by the convective flow past the structure and trapping/re-entrainment is again determined by the code. Debris that is not trapped at the second impact is deposited by gravitational fall or by the local gas flow, at the users discretion.

2.4.7.2. Qualitative Perspective

The gravitational fall option is appropriate to cells that are well mixed or in which the debris is lofted to the top without impact or sticking. This option is also useful for providing an approximate upper bound on the interaction of the debris with the atmosphere in a cell.

The models for debris transport to structures capture the basic processes and provide sufficient flexibility for the intelligent user to construct a suitable model for his/her needs.

The trapping model is adequate for steel structures, especially with the user control over the critical Kutateladze number. Outgassing from concrete is not modeled but its effect may be bounded by setting the critical Kutateladze number to zero.

2.4.7.3. Technical Adequacy

The basic physics of trapping and carryover are understood in outline, though the details for all possible geometries are not known. First-order models are in place for the important phenomena, which capture the essence of the processes. Ample flexibility is provided in the modeling for the user to adapt the models to suit his/her needs. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

2.4.8. Melt Debris-Gas Heat Transfer

See App. D.4.9 for the detailed model review.

2.4.8.1. Phenomenological Package Description

The debris-gas convective heat transfer is calculated using the Ranz and Marshall correlation for forced convection over a sphere.

A simple grey body law is used to estimate debris to atmosphere thermal radiation, with a user-defined multiplier which defaults to 1.

The atmosphere to structure thermal radiation model is that used for non-DCH calculations and has provision for the user to override the calculated emissivity of the atmosphere.

A grey body law is also used for the debris to structure thermal radiation model. Again there is a user-defined multiplier, which is recommended be kept close to the default value of 0 in view of the likely high opacity of the airborne debris. The surface area for this term is the minimum of the total surface area of all debris particles and the total surface area of all structures in the cell.

2.4.8.2. Qualitative Perspective

The convective heat transfer model is the appropriate model recommended by Bird, Stewart, and Lightfoot for spherical particles. The choice of flow velocity is not crucial due to the square-root dependence of the Nusselt number on this parameter.

The gas to structure thermal radiation model makes no allowance for the presence of airborne debris (including DCH aerosols). However, the user can override the atmosphere emissivity in order to estimate the likely importance of this effect.

The thermal radiation models are essentially parametric as the user must estimate the effective emissivity of the atmosphere in the presence of airborne debris particles. This could more easily be done within the code, where the time-dependent airborne concentration, size distribution, and composition of the debris particles is readily available.

2.4.8.3. Technical Adequacy

The heat transfer processes involved in DCH are reasonably well understood, with the exception of the effect of airborne debris on the atmosphere emissivity.

First-order models are in place for the important phenomena, with the exception of the parametric treatment of the effect of airborne debris on the atmosphere emissivity via the user-defined thermal radiation multipliers.

The technical adequacy of this model is classified as Category 1. The documentation is adequate.

2.5. Aerosol Behavior

See App. D.5.1 for the detailed model review.

2.5.1. Size and Composition Distribution

2.5.1.1. Phenomenological Model Description

The aerosol size and composition distribution is calculated by solving a set of simultaneous ordinary differential equations, derived from the spatially homogenized multicomponent aerosol dynamic equation by a group (section or size-bin) discretization. The equation includes aerosol source, agglomeration, deposition and steam condensation/evaporation terms. Brownian diffusion, gravitational settling, turbulence, thermophoresis, Stefan flow/diffusiophoresis, and solute effects are included. The set of equations is solved by standard ordinary differential equation (ODE) solvers such as Runge-Kutta methods. For condensation, a Lagrangian approach (the moving grid) is also used. The computations are rapid, as the nonlinear agglomeration integrals are pre-calculated and stored for later use.

2.5.1.2. Qualitative Perspective

The equation is an improvement over those used in most other nuclear aerosol codes, and it constitutes a practical approach to a very difficult problem. CONTAIN has had good success in predicting results of a number of large integral tests, and this provides confidence in use of the approach for the type of problems being addressed.

2.5.1.3. Technical Adequacy

The equation has proved practical, but a number of limitations are evident. These relate to non-physical assumptions such as same density for all aerosol species, spherical and neutral particles, neglect of chemical reactions at the particle surfaces as well as interior to them, and aerosol resuspension. Use of improved equations, however, would entail

major expenditures and code revisions. The technical adequacy of this model is classified as Category 4.

2.5.2. Agglomeration

2.5.2.1. Phenomenological Model Description

Agglomeration models for Brownian, gravitational, and turbulent motion are used. These derive from the works of Fuchs and Sutugin, and Fuchs, Saffman, and Turner (see App. D.5.2 for details). The Brownian model applies to all particle sizes and the gravitational model uses a collisional efficiency that depends only on particle size ratio. The models are simple in nature, and are conveniently integrated. Still, these integrations involve considerable computational expense, and the preference is to carry these computations only once at the start of the calculations (that is, the effects of changing environmental conditions on which the models depend are either not accounted for or are accounted in a piecewise fashion).

2.5.2.2. Qualitative Perspective

Agglomeration is a mass conserving but number reducing process that shifts particle distribution towards larger sizes (that is, the mean particle size increases). The larger particles diffuse (to the surfaces) more slowly, but they settle (on the floors) more rapidly; they also offer comparatively smaller surface area for condensation/reactions. For any dense aerosol (number concentration $>10^7$ /cm³), accurate modeling of agglomeration is essential to good predictive abilities.

2.5.2.3. Technical Adequacy

The CONTAIN models are reasonable. Improvements can and should be made via use of the available gravitational agglomeration models. Use of same density for all species introduces non-physical effects, the nature of which is difficult to ascertain in lieu of information from more detailed calculations. The use of shape factors is ad-hoc with a poor pedigree. The assumption of additivity among collisions induced by various processes introduces additional uncertainties. The technical adequacy of the Brownian agglomeration model is classified as Category 2 and that of the gravitational agglomeration model is classified as Category 4. The technical adequacy of the turbulent agglomeration model is difficult to ascertain.

2.5.3. Deposition

2.5.3.1. Phenomenological Model Description

Deposition models for Brownian, gravitational, thermophoretic, and Stefan flow/diffusiophoretic motion are used. The first two derive from the classical results in the field, while the latter are adopted from the research carried out during sixties. The models are meant to apply to all particle sizes. The models are simple in nature, and are conveniently used. Diffusion is effective for small particles, while settling is the dominant removal mechanism for large particle sizes. Stefan flow is important in condensing conditions, and thermophoresis is effective in presence of temperature gradients.

2.5.3.2. Qualitative Perspective

Deposition removes particles from suspension, and is the most important natural particle removal process. In a containment, aerosol is generally well mixed because of natural or forced convection, and for the homogenized aerosol equation, the deposition models are derived by solving particle continuity equation where one needs to consider convection-diffusion-body force terms all together.

2.5.3.3. Technical Adequacy

For a well mixed chamber all deposition models should be derived by solving particle continuity equation where one needs to consider convection-diffusion-body force terms all together. The CONTAIN models are a mixed bag, in that none of the models seem to be have fully constructed in this manner, and some of them require use of some ill-defined parameters. Nevertheless, the models for diffusion and settling appear reasonable, while the models for thermophoretic and Stefan flow/diffusiophoresis are conceptually quite flawed. The technical adequacy of the models for Brownian and gravitational deposition are classified as Category 2 and the models for thermophoretic and Stefan flow/diffusiophoresis deposition are classified as Category 4.

2.5.4. Steam Condensation/Evaporation

2.5.4.1. Phenomenological Model Description

For condensation/evaporation rate, CONTAIN essentially uses an expression due to Mason. This expression is based on simple mass and heat transfer with respect to a single spherical particle in a gas-vapor mixture in the continuum. The model accounts for the solute and Kelvin effects on the saturation density. Generally, the former enhances condensation, while the latter retards it.

2.5.4.2. Qualitative Perspective

Condensation is a number conserving but mass enhancement process that shifts particle distribution towards larger sizes (that is, the mean particle size increases). The larger particles diffuse (to the surfaces) more slowly, but they settle (on the floors) more rapidly; they also offer comparatively smaller surface area for condensation/reactions. For any aerosol in a vapor environment, good modeling of condensation is essential to good predictive abilities. Note that evaporation is not a number conserving process and requires very careful numerical treatment.

2.5.4.3. Technical Adequacy

The CONTAIN models is reasonable, but it is not clear if the Knudsen, shape, and gas-surface interaction (accommodation) effects have been incorporated in the model. Improvements can and should be made via use of the results available in the literature to make the model applicable to all sizes. The technical adequacy of this model is classified as Category 4. The model should be modified to allow more aerosol size classes to be used and the implementation of the Kelvin effect should be made consistent with the assumption of a single composition in each size class.

2.5.5. Removal by Engineered Safety Features

2.5.5.1. Phenomenological Model Description

CONTAIN has models for aerosol removal by fan coolers, containment sprays, ice condensers, and suppression pools. The ice-condenser model corresponds to deposition by Stefan flow/diffusiophoresis, the spray models to interception, impaction, diffusion, thermophoresis, and Stefan flow/diffusiophoresis, the ice-condenser models, to deposition on structures. The suppression pool modeling is borrowed from the SPARC and VANESA codes.

2.5.5.2. Qualitative Perspective

ESFs are important in removing aerosol particles from the suspension. The removal is often both direct (capture by spray droplets) as well as indirect (e.g., due to fogging). In removing aerosols through the use of ESFs, the goal always is to cause the aerosols to come near or in contact with spray droplet surfaces or structural surfaces.

2.5.5.3. Technical Adequacy

The CONTAIN models address the effects that are modeled either as agglomeration (with droplets) or deposition on surfaces. Adequacy of such models was discussed previously in Secs. 2.5.2 and 2.5.3. It should be noted, however, that the ESFs are generally quite effective, and the modeling limitations are less of a concern than that for the natural mechanisms.

The technical adequacy of suppression pool aerosol removal model is classified as Category 4.

The technical adequacy of the ice-condenser aerosol removal model is classified as Category 2.

The technical adequacy of containment spray aerosol removal model is classified as Category 4.

The technical adequacy of the PCCS aerosol removal model is classified as Category 2.

2.6. Fission Product Behavior

See App. D.10.6 for the detailed model review.

2.6.1. Phenomenological Model Description

The analysis of fission product behavior in CONTAIN includes the treatment of decay chains, decay heating, host exchanges, transport, generation during core-concrete interactions, and removal by ESFs. Fission products are associated with various hosts (repositories). A host can be gas, aerosol, heat structures, or a lower cell layer or pool. To the extent that the host is an aerosol, transport and removal mechanisms are discussed in Sec. 2.5. The treatment of fission product vapor or gas species is quite limited, however. Noble gases are treated appropriately (using gas as the host). In general, however, iodine vapor or gas species (e.g., I_2 or methyl iodide) are not treated mechanistically or in detail (although there is a simple model for spray removal).

2.6.2. Qualitative Perspective

The generalized treatment of fission product behavior involving hosts and the modeling of decay heat is quite flexible and satisfies the needs for ex-vessel analysis of fission product behavior. To address deficiencies in the treatment of iodine species, it had earlier been intended to incorporate some models from the TRENDS code into CONTAIN. Because this would not be consistent with the NRC's revised severe-accident code strategy (App. E), these improvements are no longer planned. The TRENDS models are discussed in Sec. 5.2 of this report.

2.6.3. Technical Adequacy

CONTAIN does not have an adequate capability of modeling fission product vapor (or gas) transport other than the transport of noble gases.

2.7. Combustion

See App. D.7.1 for the detailed model review.

2.7.1. Ignition Criteria

2.7.1.1. Phenomenological Package Description

For ignition to occur within a cell, the effective hydrogen mole fraction must exceed 7%; the effective hydrogen mole fraction is equal to the actual hydrogen mole fraction plus 0.541 times the carbon monoxide mole fraction.

In addition, the oxygen mole fraction must exceed 5% in the cell before combustion can commence.

The final condition to be met is that the diluent mole fraction should not exceed 55%. The diluent is taken to be the steam and carbon dioxide in the atmosphere together with 79% of any nitrogen in excess of that required to form air out of the available oxygen in the cell.

All of the above can be overwritten by the user on input.

2.7.1.2. Qualitative Perspective

The ignition criteria are approximate fits to experimental data. They are a reasonable representation of the conditions under which ignition can occur in the presence of igniters for the limited range of conditions of the experiments (e.g., initial pressure = 1 bar, initial temperature between 20 and 100°C). However, ignition is not guaranteed under these conditions and the user is advised to vary the criteria in order to determine their importance to a particular scenario.

In the absence of igniters, the possible ignition sources will be less well characterized. In plant studies, the initial conditions may well lie outside those used for the experiments (especially the temperature and pressure) and the atmosphere may contain more inhomogeneities. In addition the geometry is likely to be more complex.

Because of the variety and complexity of the containments that may be studied as well as the somewhat stochastic nature of ignition (if the ignition sources are not well characterized), it is appropriate that the user be left to vary the criteria parametrically to assess the various possibilities. Such sensitivity studies are extremely important as, in many cases, the default criteria give the lowest hydrogen concentration for which a burn may occur; a more energetic burn could occur if the combustible gas were allowed to concentrate further.

Some advice is given to guide the user in the choice of parameter ranges for sensitivity studies but it does not go far enough, especially in view of the non-conservative nature of the default values.

2.7.1.3. Technical Adequacy

For well characterized igniters, in well-mixed, relatively featureless volumes the ignition criteria are reasonably well understood for low initial temperatures and pressures.

For poorly characterized ignition sources, in more complex geometries or with initial conditions outside of those studied in the experiments ignition takes on a more stochastic nature. This is appropriately treated in the code by allowing the user the freedom to perform sensitivity studies on the criteria.

Some advice is given to guide the user in the choice of parameter ranges for sensitivity studies but it does not go far enough, especially in view of the non-conservative nature of the default values.

The technical adequacy of this model is classified as Category 2.

2.7.2. Mode of Combustion

See App. D.7.2 for the detailed model review.

2.7.2.1. Phenomenological Package Description

The code determines which form of combustion will take place, depending on the conditions in a given cell and the parameter values chosen by the user for the different combustion options.

The combustion modes available in the code are: deflagration, diffusion flame burning (DFB), and bulk spontaneous recombination (BSR). The conditions under which a deflagration is modeled by the code are discussed in subsection 2.7.1, above.

Bulk spontaneous recombination is intended for use if the temperature in a cell reaches the auto ignition temperature, e.g., during DCH or in a source room during hot hydrogen injection. BSR is modeled if either the gas temperature in the cell exceeds a critical value or the debris temperature and mass concentration (during DCH) exceed critical values

The diffusion flame model is included to allow the continuous burning of incoming fuel. This option is activated in the following circumstances. First, an ignition source must be present, i.e., either igniters are present or the BSR criteria are met. Second, the temperature of the incoming gas must exceed a user-specified threshold. Third, there must be sufficient oxygen in the receiving cell. Also the diluent mole fraction must be below a critical value. The mass flow of the incoming gas must be above a threshold value.

Finally, the diluent to combustible mole fraction in the incoming gas must be below a critical value.

2.7.2.2. Qualitative Perspective

The important burning modes are represented by first- or zeroth-order models, with the exception of detonations. Due to the multi-dimensional nature of detonations, it would not be appropriate to attempt to represent them in a lumped-parameter code such as CONTAIN. In light of the incomplete knowledge of when a burning mode is likely to occur under all conditions of relevance to PWR severe accidents, the parametric nature of some of the choices is appropriate.

2.7.2.3. Technical Adequacy

The choice of burn mode is uncertain and this is reflected in the parametric way in which the choice is made in the code. The user is pointed to relevant literature for guidance in setting the parameters. If simple methods exist for estimating some of the parameters it would make more sense to implement them in the code where the necessary variables are readily available for the computations. The technical adequacy of this model is classified as Category 3.

2.7.3. Diffusion Flame

See App. D.7.3 for the detailed model review.

2.7.3.1. Phenomenological Package Description

The diffusion flame model allows continuous burning of incoming combustible gases to be modeled parametrically, by the user specifying the fraction of the incoming fuel to be burned.

In addition to burning the incoming combustible gases, the code allows for the combustion of hydrogen and carbon monoxide that are entrained into the DFB jet from the surrounding atmosphere. This is not a mechanistic model; rather, it is assumed that sufficient oxygen is entrained to burn the user-specified fraction of the incoming combustible gas plus the hydrogen and carbon monoxide that must also be entrained in order to supply the required oxygen. The entrained gases are not allowed to exceed their inventories in the cell in which combustion is taking place.

The inflows from all other cells are treated separately when checking if DFB should take place and some inflows may burn while others do not. On the other hand, user input source tables to a given cell are combined into a single source before the BFD criteria are applied, so that a high steam input rate into a cell may preclude the diffusion flame burning of a combustible gas source to that cell.

2.7.3.2. Qualitative Perspective

Given the uncertainty in the details of diffusion flame burning in the complex geometry of a reactor containment and in the presence of hot core debris, it is reasonable that the magnitude of the effect be estimated using the parametric model provided in the code.

2.7.3.3. Technical Adequacy

Though the basic physics of diffusion flames is understood, the detailed behavior in the complex geometry of a reactor containment and in the presence of hot core debris is uncertain. A parametric model provided in the code enables the user to bound the magnitude of the effect that diffusion flame burning would have on containment pressurization. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

2.7.4. Bulk Spontaneous Recombination

See App. D.7.4 for the detailed model review.

2.7.4.1. Phenomenological Package Description

Two models are available to the user: the hydrogen recombination model and the bulk spontaneous recombination model. The former is a control function model, the latter a parametric model.

The hydrogen recombination feature allows hydrogen produced during DCH to be recombined with oxygen in the time step in which it is produced, providing there is enough oxygen in the cell. This feature can be turned on or off by the user.

The bulk spontaneous recombination model allows all of the hydrogen in a cell to burn at a user-defined rate, providing a set of user-specified criteria are met. The user is informed that the SENKIN code can be used to provide an estimate of the recombination rate.

2.7.4.2. Qualitative Perspective

The hydrogen recombination model is similar to the diffusion flame model when applied to a DCH situation, except that it does not burn combustible gas entrained into the plume with the oxygen required to burn the DCH hydrogen, nor does it have the parametric freedom to choose the fraction of hydrogen which is burned.

During DCH the hot debris particles lofted into the atmosphere provide a possible ignition source for pre-existing hydrogen in the containment. Due to the heating effect of the airborne debris, the hydrogen may ignite even if the atmosphere composition is such that it does not satisfy the ignition criteria at low temperature. The conditions under which the pre-existing hydrogen will burn (and the extent of any such burn) are uncertain. The parametric model provided allows the user to bound the magnitude of the effect.

The pessimism in the upper bound on the pressurization provided by the BSR model may be reduced by using the SENKIN code to estimate a finite rate of recombination.

2.7.4.3. Technical Adequacy

The understanding of hydrogen recombination during DCH is questionable. Parametric models provided in the code enable the user to bound the effect on containment pressurization. If the SENKIN code allows significant reductions to be made in the degree of pessimism in the predicted bounds, then fits to SENKIN calculations should be

considered for inclusion in CONTAIN. The technical adequacy of this model is classified as Category 2.

2.7.5. Deflagration

See App. D.7.5 for the detailed model review.

2.7.5.1. Phenomenological Package Description

The rate of combustion is determined by dividing the amount of combustible gas to be burned by the burn time. The burn time is determined by dividing the burn length by the flame speed. The burn length is a user-input parameter, which defaults to the cube root of the cell volume if not specified.

The flame speed is determined using correlations derived from experiments performed in a premixed hydrogen-steam-air atmosphere. The correlations give the flame speed as a function of the hydrogen and steam concentrations.

The correlations are generalized to include carbon monoxide in CONTAIN by replacing the hydrogen mole fraction by the combustible gas mole fraction. The correlations are further generalized to allow for diluents other than steam by replacing the steam mole fraction by the diluent mole fraction.

Two versions of the correlation are available: one for laminar flames and one that allows for the turbulence generated by the containment sprays.

The user may input a constant flame speed to be used in place the value calculated within the code.

2.7.5.2. Qualitative Perspective

The correlations are reasonable fits to the experimental data, though there is considerable scatter in the data.

The correlations apply to the relatively simple geometry of the vessels used for the experiments. Reactor containments have more complex geometries and there is no allowance in the correlations for effects such as flame acceleration around objects. Due to the large variety in containment geometries, it is not practical to allow for geometrical effects in the code. The provision of sufficient flexibility for the user to perform sensitivity studies is therefore reasonable. However, some advice to the user on how to choose the parameter ranges for sensitivity studies is needed.

The correlations account for only two levels of turbulence: no turbulence or turbulence caused by operation of the containment sprays. Other sources of turbulence exist in the containment during severe accidents, notably jets and/or plumes of hot gas (possibly carrying entrained debris). Such sources must be investigated by using the input option to override the calculated burn rate in order to perform sensitivity studies. Advice to the user on how to estimate parameter ranges for sensitivity studies is needed.

The burn parameters are not updated to allow for the input of combustible gas to the cell during the burn. The obvious case where this may be of concern is during DCH when combustion is likely to occur and the hydrogen source rate is likely to be high; however, in this case the BSR and DFB models can be used which do not suffer from the above drawback.

2.7.5.3. Technical Adequacy

The deflagration models provide a reasonable starting point for the analysis of low-speed combustion in the containment. However, the effects of turbulence and obstacles on the flame speed are difficult to quantify for complex geometries and are not allowed for in the code (with the exception of spray induced turbulence). There is adequate flexibility in the code to allow sensitivity studies to be performed to assess the effects by varying the flame speed, but the user is provided with no advice on the choice of parameter ranges for such studies. The technical adequacy of this model is classified as Category 2.

2.7.6. Combustion Completeness

See App. D.7.6 for the detailed model review.

2.7.6.1. Phenomenological Package Description

In the absence of any diluent the combustion, completeness rises linearly from 0 at a combustible gas concentration of 4.2057% to complete combustion at 7.4845% in a quiescent atmosphere and from 0 at a combustible gas concentration of 3.6535% to complete combustion at 7.1454% for an atmosphere with sprays on.

For both quiescent and turbulent atmospheres, the combustion completeness is reduced in the presence of a diluent by a factor of $\exp(a)$, where a is given by

$$a = X_d(-4.1966 + 3.3985 X_d),$$

where X_d is the mole fraction of diluent.

The above correlations are derived from the experimental data from the Nevada Test side (NTS), Variable Geometry Experimental System (VGES), Whiteshell, ACUREX, and Fully Instrumented Test Series (FITS) test series.

2.7.6.2. Qualitative Perspective

The correlations capture the major trends in the data but there remains much scatter in the data.

The experiments all had hydrogen concentrations less than 20% so the accuracy of the correlations cannot be guaranteed for concentrations significantly above this. The experiments used to generate the correlations all had well-mixed atmospheres and recent experiments have shown that combustion completeness can be greater in stratified atmospheres than in homogeneous ones. Hence sensitivity studies are required.

The experiments all had hydrogen as the combustible gas and steam as the diluent. The rationale behind the method of generalization to include carbon monoxide as a combustible gas and carbon dioxide and excess nitrogen as diluents is not clear.

2.7.6.3. Technical Adequacy

There is considerable scatter in the experimental data, indicating a degree of uncertainty in the current understanding of combustion completeness. The process is represented by correlations that capture the major trends in the data but necessitate the use of parametric sensitivity studies to take into account the uncertainty in the data. The model is therefore zeroth order and its adequacy is assessed to be Category 2. The documentation adequately describes the model but fails to provide advice to the user on reasonable parameter ranges to use for sensitivity studies.

2.7.7. Propagation in Multi-Compartments

See App. D.7.7 for the detailed model review.

2.7.7.1. Phenomenological Package Description

For the burn to propagate into another cell the mole fraction of diluent (as defined in subsection D.7.1) must be less than a critical value, which can be user defined but defaults to 55% if not specified. Similarly, the oxygen mole fraction in the cell must exceed a user-specified value, which defaults to 5%.

In addition the combustible mole fraction must exceed a critical value. The critical values can be user-specified or can be left to default to 4.1% for upward propagation, 6% for horizontal propagation, and 9% for downward propagation. The mole fraction of combustible gas is defined to be the mole fraction of hydrogen plus a fraction of the mole fraction of carbon monoxide, where the fraction is 0.328 for upward propagation, 0.435 for horizontal, and 0.600 for downward.

The relative heights of the cells are specified by the user and may be different to the heights specified for the flow solver.

If the conditions for propagation are met in a cell adjacent to the burn cell then the burn will propagate to the adjacent cell after a time delay, which is a user-specified fraction of the burn time in the burn cell. The delay fraction defaults to 0.5 if not specified.

2.7.7.2. Qualitative Perspective

The correlations capture the major trends in the experimental data, but there is considerable scatter in the data. The user must therefore perform sensitivity studies to properly interpret the results of any calculations.

If combustion occurs in one or more cells, then the pressurization of that cell or cells will result in gas flowing into adjacent cells which are not burning. Such flows are likely to be energetic and will generate a certain amount of turbulence in the downstream cells. The effect of this turbulence on the burn rate in the downstream cells is not modeled in the code. This process was found to double the pressure rise in experiments in the Battelle model containment.

In addition the gas flowing from burning to non-burning cells carries with it a mixture of burnt and unburnt gases in the code model. The introduction of unburnt gases will reduce the concentration of fuel in the downstream cells, which may effect the occurrence, rate, and completeness of burns in those cells.

2.7.7.3. Technical Adequacy

The basic physics is understood, though the generation of turbulence in complex geometries and its effect on burn rate are not known in detail. The model does not represent two of the most important processes in propagation (segregation of burnt and unburnt gases by the flame front and vent flowpath induced turbulence). The technical adequacy of this model is classified as Category 5. The documentation is adequate.

2.7.8. Effect of Combustion on Fission Product Release

See App. D.7.8 for the detailed model review.

2.7.8.1. Ignition Criteria

The targeted host and release mechanism in the code could be used to represent some aspects of the effect of combustion on fission products. This feature allows fission products to be hosted on aerosols, on structure surfaces, in the gas, and in water pools. The fission products can be released from their hosts at user-specified rates and accepted by other user-specified hosts. The release rates can have an Arrhenius temperature dependence with the constants specified by the user. The constants could be set to release the iodine from aerosols and structure surfaces at high temperatures and host them on the gas, thus representing the conversion of iodine to more volatile forms during combustion.

The alternative is to use the source tables to provide a control function representation of the phenomena.

2.7.8.2. Qualitative Perspective

Experiments indicate that the amount of iodine converted to the vapor phase depends upon a number of factors, such as the amount of steam in the atmosphere, the concentration of airborne cesium iodide, and perhaps the amount of water condensed on the cesium iodide. None of these factors is currently allowed for in the targeted host and release mechanism.

2.7.8.3. Technical Adequacy

Though the targeted host and release mechanism could be used to qualitatively represent the conversion of cesium iodide to more volatile forms, there is no mechanistic model to estimate the extent of the conversion for the relevant range of atmospheric conditions. Though models for some aspects have been described, the processes are still poorly understood on the whole. As control functions are available to represent the processes that are not modeled, the technical adequacy of this model is classified as Category 3.

2.8. Heat and Mass Transfer

See App. D.8.1 for the detailed model review.

2.8.1. Structure Conduction

2.8.1.1. Phenomenological Model Description

Heat transfer through structures to some heat sink by conduction is one of the major resistances to energy loss from the containment. CONTAIN considers this mechanism of

heat loss in a one-dimensional fashion (Sec. 10.4 of the CONTAIN manual). Any structure within the containment or acting as a boundary to the containment can be subdivided into control volumes of one-dimensional slabs of material (steel, concrete, paint, or any other prescribed material) through which energy can pass from a higher surface temperature (or ambient temperature with a prescribed or calculated heat transfer coefficient) to a lower surface temperature (or ambient temperature with a prescribed heat transfer coefficient). In general this energy transfer process occurs under the constraint of constant mass. However, if the material being heated by fission product decay heat through atmospheric convection or radiative transfer, is concrete, then it can decompose, releasing gaseous decomposition products. The CONTAIN model includes an outgassing model for the release of water vapor and carbon dioxide gases from the heated concrete. Both evaporable and chemically bound water vapor are considered to be released due to excessive heating. The gas release model used within the CONTAIN formulation is not completely mechanistic in that it does not model explicitly the transport (i.e., diffusion) of these gases within the porous concrete internal structure. Rather, the temperatures within the heated concrete solid (i.e., temperatures of individual control volumes) are computed and once the temperature exceeds the appropriate values for evaporable water release, or chemically bound water vapor or carbon dioxide release, and the proper amount of energy is absorbed at the control volume interface, then outgassing occurs. It is as if the concrete at these particular temperatures has very large values of heat capacity. Thus the enthalpy of decomposition is preserved without the need to calculate the transport of these gases through the porous structure. The choice of considering if the concrete is able to be heated and then decomposed is done by user input.

2.8.1.2. Qualitative Perspective

The heat conduction model developed seems quite reasonable. The Committee saw no particular problems with the conduction heat transfer model. In fact it found it to be quite versatile and well documented. The concrete outgassing model included in the conduction heat transfer model needs to be referenced to specific data comparisons rather than just comparisons to other more sophisticated models, e.g., SLAM or USINT.

2.8.1.3. Technical Adequacy

The conduction heat transfer model represents the current state of knowledge and is judged to be of first order. The knowledge of the physics of the process is well known and validation of the conduction portion of the model has been benchmarked relative to more fundamental analyses. We feel the outgassing model could be more directly compared to data; e.g., the data generated at SNL by T. Y. Chu and J. F. Muir. The technical adequacy of this model is classified as Category 1.

2.8.2. Structure Radiation

See App. D.8.2 for the detailed model review.

2.8.2.1. Phenomenological Model Description

If the gas temperature in containment rises to high values because of gas combustion or energy transfer from the surface of an ex-vessel molten corium pool or debris, then radiation heat transfer would become a significant heat transfer mechanism. In CONTAIN, the analyst can choose from two radiative heat transfer models. The first model is the net enclosure model, and the second is the simple radiation model. The former model allows for simultaneous calculation of radiative heat transfer between the compartment (control volume) atmosphere (which can include aerosols or corium debris), all heat

structures, and the upper boundary of the compartment below, as gray surfaces or gases with known average properties.

The major limitation of such a model is that only the inner surfaces of the structures facing the compartment atmosphere can be included in such an analysis. The latter model considers the direct radiative heat transfer between the compartment atmosphere and the heat structures (inner and outer surfaces of the structure if both are within the compartment), and between the atmosphere and upper layer of the compartment below. This latter model is recommended for use with the direct containment heating model since it is consistent with the additional direct radiative transfer models for corium debris to atmosphere and debris to structure heat transfer. A separate model consistent with the simple radiation model allows for radiative energy transfer from a lower compartment to inner heat structure walls.

Both of these radiation models can account for the optical properties of the atmosphere based on the emissivity of water vapor, carbon monoxide, or dioxide—i.e., the Cess-Lian correlation when water vapor is the dominant participating gas species, or the Modak correlation when the other two gases are significant species in the atmosphere. The presence of aerosols can be accounted for by a simple parametric model or by considering the aerosol cloud emissivity due to the aerosol mass loading. The presence of corium fuel debris resulting from high-pressure melt ejection must also be considered separately. This consideration is not straightforward and the CONTAIN model includes a parameter KMX which allows the analyst to alter the atmosphere properties with the debris present. The CONTAIN manual does a reasonable job of explaining this uncertainty and warning the user of the possible effects.

2.8.2.2. Qualitative Perspective

The radiation model is clearly state of the art, and the Committee sees no specific weaknesses in the models used and feels that, once the analyst picks either model, the formulations are consistent. However, the one area of uncertainty is the interaction of the dispersed corium fuel debris and its radiative properties with the normal considerations for radiative energy transfer within the compartment and its structures. The corium fuel debris would come out as a cloud of hot particles and it seems that the interaction of these particles and the surrounding atmosphere is complex enough to make this mode of heat transfer highly uncertain; e.g., radiative self-shielding could reduce this form of energy transfer to a cloud surface phenomena. The CONTAIN manual should expand its discussion of the limitations of the simple radiation model used under these conditions with airborne fuel debris, and perhaps indicate the importance of this portion of the energy transfer process. What is given within CONTAIN for the analyst is completely consistent with the other models, but more user guidance or some parametric effects should be discussed.

2.8.2.3. Technical Adequacy

The radiation heat transfer model is considered to be consistent with and representative of the current state of knowledge. The Committee feels it is a first-order model with a well-understood knowledge of the underlying physics. The models used in CONTAIN are felt to be validated. The major recommendation for this section is that the manual description of the use of radiation parameters given the presence of corium fuel debris needs to be further refined to give the analyst more guidance and the uncertainties associated with its use. Although these changes need to be implemented, the technical adequacy of this model is classified as Category 1.

2.8.3. Convection Heat Transfer (Free and Forced)

See App. D.8.3 for the detailed model review.

2.8.3.1. Phenomenological Model Description

The transfer of energy from the gas atmosphere to the heat structures due to temperature differences is driven by convection. The CONTAIN logic distinguishes between free and forced convection by calculating the average control volume velocity (or it is input by the analyst as a parameter) and then computing the heat transfer coefficient by either free and forced correlations. The larger coefficient then is used in the computations. For the free convection correlation, CONTAIN uses the standard Nusselt correlation where there is no inherent system length scale required, and for forced convection, uses the standard Nusselt correlation for a flat plate. The average control volume velocity is estimated by an arithmetic average of the inlet and outlet velocities to the compartment control volume, where the inlet and outlet velocities are computed from the known mass flows and the density of the gas mixture. This can be superseded by user input of some specific constant velocity.

2.8.3.2. Qualitative Perspective

The convective heat transfer model used in CONTAIN is standard for control volume modeling of fluid systems. The Committee sees no inconsistencies or flaws in its use here, except that the Grashof number should be based on density difference and not only on the temperature difference. However, we would recommend that the SNL staff consider further guidelines for the analyst who is to use CONTAIN on how to approach the question of free versus forced convection treatment of the heat transfer (and mass transfer), with some considerations of the effect of entry or exit velocities to the velocity in the compartment control volume. This recommendation is open-ended because the Committee is not sure what is the proper approach and recognizes simply that current discussions seem too sparse.

2.8.3.3. Technical Adequacy

The convective heat transfer model is state of the art and accurately reflects the proper knowledge of physics within a first-order model that is consistent with the rest of the system model. Better guidelines need to be added to the manual to help the analyst in handling the use of a forced velocity and the associated characteristic length scale in the compartment control volume for convective coefficients. In addition, the Grashof number should be modified so that its definition is based upon a density difference. Given this improvement, the technical adequacy of this model is classified as Category 1.

2.8.4. Mass Transfer

See App. D.8.4 for the detailed model review.

2.8.4.1. Phenomenological Model Description

Mass transfer of water vapor to and from heat structure surfaces due to condensation and evaporation is driven by the concentration differences (exhibited by pressure differences) at these surfaces. For example, if a condensate film layer exists on the heat structure surface below the dew point temperature (local saturation at the total pressure), the partial pressure of the noncondensable gas (air or hydrogen) at this interface

in the boundary layer will be higher than the bulk mixture value. This condition occurs because the noncondensable gas is carried with the vapor toward the interface where it can accumulate. The increase in the partial pressure of the noncondensable gas produces a driving force for diffusion of the noncondensable gas away from the surface. This diffusion opposes the diffusive motion of the water vapor towards the surface. Although the total pressure of the system remains constant, the water vapor partial pressure is lower at this surface interface within the boundary layer than in the bulk mixture and condensation occurs. If the surface temperature of the heat structure is above the point of local saturation, then the partial pressure gradient is reversed and we have evaporation from the surface.

To model this condensation phenomenon, the CONTAIN mass transfer model uses the Reynold's analogy between momentum transfer and heat transfer and applies it to mass transfer processes. By this analogy, one only needs some empirical information for the local (or average) friction coefficient for momentum transfer on the structure surface and the effect of molecular (or turbulent) diffusivities of mass to momentum to estimate the mass transfer coefficient. Once this mass transfer coefficient is estimated, one can compute the mass flux of water vapor condensing on the surface of a structure and the energy carried along with it. To model the evaporation process, one need only determine that the surface temperature is above the local saturation value and that any excess heat applied to the water on the structure wall would result in evaporation of a proportional amount of this condensate film.

The second resistance to condensation is the condensate film itself, which is due to the conduction of heat across the film. Outside the containment, a film can develop by water being added directly to the outer steel shell of the containment as an evaporative cooling aid. In either case, CONTAIN has developed a film tracking model to determine the inventory of water on the heat structures available for evaporation or as a barrier for condensation. Two different models are available. First, the analyst can specify a critical film thickness. If the condensate or added water film is below this value, the film simply accumulates or evaporates without motion. If it is calculated to go above this limit, then excess condensate is instantaneously diverted to the associated water pools for each compartment. The alternative approach is to use a more mechanistic film tracking model which assumes that the film flows in a laminar or turbulent flow regime down the structure surface. The CONTAIN model would track the thickness on these structures to determine the associated conduction resistance, which is similar to a Nusselt condensate film analysis.

2.8.4.2. Qualitative Perspective

The models for mass transfer are considered to be adequate for the level of detail in the CONTAIN system model. There were two deficiencies identified in this review. First, the Grashof number should be redefined based on density difference in the gas mixture instead of temperature difference. Second, the film tracking model methodology is not easily understood in the CONTAIN manual write-up. We are aware that the use of a laminar or turbulent film correlation-based model is crude especially for high film flow rates, but we feel it is consistent with the level of detail of the rest of the model. Although these models for condensation and evaporation are known to be useful estimates, the Committee feels that comparison to benchmark data is still warranted especially when the flow is in a mixed convection or natural convection regime. Such a regime is hard to determine, thus we recommend that the SNL staff continue its comparison to data being made available by the NRC and by the vendors for advanced reactor containment design.

2.8.4.3. Technical Adequacy

The mass transfer model reflects the current state of knowledge for condensation and evaporation processes off of heat structures and is consistent with the other CONTAIN models. The physics of the process is considered to be understood and the model is of first order. Validation is possible if the SNL staff focuses on new available benchmark data, particularly in the mixed convection regime. The improvements needed seem to be in the correction of the definition of the Grashof number and in the exposition of the film tracking model. Although these changes need to be implemented, the technical adequacy of this model is classified as Category 1.

2.8.5. Thermodynamics

See App. D.8.5 for the detailed model review.

2.8.5.1. Phenomenological Model Description

The modeling philosophy used in CONTAIN is similar to many other reactor-containment system models in that the containment compartments are considered to be divided into control volumes within which mass and energy for the gas mixture are balanced. The gas mixture has one mixture temperature and pressure and composition within the control volume which determines its thermodynamic state. The auxiliary equations of state for each material are then averaged to form the mixture values for mass and energy. These relations have been discussed in Sec. 2.1 of this review. There are separate mass and energy balances for the fuel debris that may be ejected into the atmosphere due to a high-pressure melt ejection, as well as separate mass and energy balances used to keep track of water pools.

2.8.5.2. Qualitative Perspective

The model used for the thermodynamics of the containment compartments is state of the art and seems quite reasonable. The Committee does not see any deficiencies or needs for improvement given the basic modeling philosophy. We do caution the analyst not to use the CONTAIN model inappropriately. Because it is a control volume (lumped) formulation, one must be careful to not over interpret the results and to consider other analytical or computational models if more detailed flows or spatially refined temperatures or pressures are required for analysis. The manual does indicate this and the Committee feels the proper cautions have been identified.

2.8.5.3. Technical Adequacy

The CONTAIN thermodynamic model represents the current state of knowledge for control volume formulations of containment analyses. The physics at this level of sophistication is well understood and validated based on past information. The technical adequacy of this model is classified as Category 1.

2.9. Boiling Water Reactor

2.9.1. Suppression Pool Flow Model

See App. D. 9.1 for the detailed model review.

2.9.1.1. Phenomenological Model Description

Before the initiation of vent flow actuation, the pool energy transfer process is governed by the CONTAIN "implicit boiling model." Once the liquid level reaches the vent elevation, the vent is assumed to be open/clear, and the energy transfer from the vented stream to the pool water includes the effects of vapor condensation and thermal equilibration of noncondensibles, pool flashing, and bubble re-saturation to 99% relative humidity. The gas flow rate is calculated based on an orifice flow equation with a discharge coefficient of unity.

The mass and energy transfer at the pool/atmosphere interface uses standard models for simultaneous heat and mass transfer (see also the comments on the atmosphere/pool thermodynamic and intercell flow models).

2.9.1.2. Qualitative Perspective

The suppression pool thermodynamics and flow models are physically reasonable, and for the most part, represent the current state of knowledge. The model does not include the potential effects of thermal stratification in the suppression pool. This could be important for ALWRs with passive containments. In addition, essentially no experimental benchmarking of the CONTAIN suppression pool thermal-hydraulics models is currently available.

The model documentation needs improvements including clear statement of model assumptions, limitations, and step-by-step derivation of the model equations. The App. K referenced on page 4-36 of the CONTAIN manual is missing from the documentation and could not be reviewed.

2.9.1.3. Technical Adequacy

In general, the suppression pool flow and thermodynamics models appear to represent most of the dominant phenomenological processes for BWR application. The physics is generally well understood, except for direct contact condensation of steam through the suppression pool in the presence of noncondensable gases, where experimental data are scarce. The CONTAIN modeling rationale appears to be technically sound and it is represented with a first-order model. The technical adequacy of this model is classified as Category 1.

2.9.2. Vent Clearing Model

See App. D. 9.2 for the detailed model review.

2.9.2.1. Phenomenological Model Description

The suppression pool vent clearing model is based on the solution of the steady-state Bernoulli's equation. Water overflow as well as vent flow direction (drywell to wetwell and vice versa) are also included. The effect of multiple vents is simulated by assuming that the effective vent area increases linearly with pressure difference, beginning at the gas pressure difference sufficient to support the liquid level

2.9.2.2. Qualitative Perspective

This formulation neglects the inertial effects of liquid within the vent, and the multiple, horizontal vents (that exist in BWRs with MARK-III containments) are lumped into a single equivalent vent, which is mechanistically inadequate.

2.9.2.3. Technical Adequacy

In general, the vent clearing model appears to adequately represent the general trends of major processes under thermal-hydraulics conditions of interest to BWRs. The major modeling limitation is due to the single/lumped treatment of the vent clearing model, which is not first order for mechanistic prediction of vent clearing behavior in a multi-vent pressure suppression pool system. In addition, the vent clearing model neglects the inertia effects of the liquid; however, this is not judged to be a serious limitation.

The current model is zeroeth order; however, it is not fully adequate for simulation of horizontal, multi-vent systems. The technical adequacy of this model is classified as Category 4. Plans currently exist to remedy this deficiency.

2.9.3. Suppression Pool Scrubbing Model

See App. D. 9.3 for the detailed model review.

2.9.3.1. Phenomenological Model Description

The CONTAIN code has two model options for aerosol retention in suppression pools. The SCRUB model, which was developed for the VANESA code, is based on Fuchs' treatment of sedimentation, impaction, and diffusion in spherical bubbles. The user may specify the initial bubble diameter, which is defaulted to 1.0 cm. The scrubbing efficiency is sensitive to the input parameter VROVR, the ratio of the gas circulation velocity to bubble rise velocity. Bubble expansion is calculated as a bubble rises in a pool, although vapor evolution effects are neglected.

The SPARC model includes some but not all of the model features of the 1985 version of SPARC. This model extends Fuchs' model to consider elliptical bubbles. It accounts for bubble growth and the deposition limiting effects of vapor evolution during bubble rise. The CONTAIN version does not include some important features in the 1985 version of SPARC or that have been included in more recent versions of SPARC (see App. D.9.3 for details) such as vapor evolution in rising bubbles, aerosol growth by condensation, the effects of hygroscopicity on aerosol growth, expansion work of rising bubbles, hydrodynamic description of bubble swarms, and bubble breakup models.

Neither model includes the analysis of vapor iodine retention in suppression pools.

2.9.3.2. Qualitative Perspective

The decontamination factor predicted for a suppression pool is very sensitive to modeling capability. Some of the model improvements in newer versions of the SPARC code could have a substantial effect on the values obtained in the analysis.

2.9.3.3. Technical Adequacy

The SPARC model in CONTAIN is a first-order mechanistic treatment, but cannot accurately predict suppression pool decontamination. Substantial improvement can be made in the validity of code results by the incorporation of model improvements from the SPARC-90 code. The technical adequacy of this model is classified as Category 4.

2.10. Engineered Safety Features

2.10.1. Fan-Cooler Model

See App. D.10.1 for the detailed model review.

2.10.1.1. Phenomenological Model Description

The fan-cooler model has a thermal-hydraulic model and an aerosol removal model. The MARCH fan-cooler model is not recommended. The more mechanistic fan-cooler model includes a condensation mass heat transfer coefficient and a convective heat transfer coefficient. The Nusselt number, which is used to determine the heat and mass transfer coefficients for flow over horizontal tubes, is based on a correlation for tube banks without fins.

Aerosol deposition in the fan cooler is calculated based on the condensation rate. The only mechanism modeled is diffusiophoresis. Aerosols travel with the condensate to sump volumes.

2.10.1.2. Qualitative Perspective

The level of detail of the fan-cooler model is consistent with analysis needs. Fan-cooler performance is not likely to be the focus of a technical issue requiring the use of CONTAIN for resolution. Ability to model the effects of fan coolers approximately could be important in CONTAIN applications, however.

2.10.1.3. Technical Adequacy

The fan-cooler physics are understood and the model is first order. The fan-cooler model may be more applicable to some fan-cooler designs than others but is assessed to be adequate. The documentation of the model within the manual is sufficient. The technical adequacy of this model is classified as Category 1.

2.10.2. Ice-Condenser Model

See App. D.10.2 for the detailed model review.

2.10.2.1. Phenomenological Model Description

The ice-condenser model involves a thermal-hydraulic model and an aerosol removal model. The thermal-hydraulic model is quite simple. Heat transfer by convection is calculated from flowing gases to a column of ice. Both turbulent natural convection and forced convection are considered. As the ice melts, the length of the column decreases and

reduces the heat transfer area. The condensate, aerosols, and associated fission products flow to a receiver volume. The outlet temperature of this effluent is an input parameter to the code.

The heat balance for the ice and melted water account for heating of the ice to its melting point, melting at constant temperature, and heatup of the melted ice water as it exits the ice bed. Radiative heat transfer is included for DCH conditions.

The effective velocity used for the forced-convection heat transfer correlations is based on the calculated inlet velocity and the assumption that the flow undergoes an isentropic expansion. Most of the input parameters for the model involve design data but some require "discretion" on the part of the user.

The aerosol decontamination model treats settling, impaction/interception, Brownian diffusion, diffusiophoresis, and thermophoresis. The model is based on the ICEDF model developed by A. Postma, P. Owczarski, and others (see App. D.10.2 for details).

2.10.2.2. Qualitative Perspective

A detailed mechanistic treatment of ice-condenser thermal-hydraulics would be a major effort that does not appear to be warranted. Some effort is required by the analyst in modeling the ice condenser to assure that results are not sensitive to nodalization or modeling assumptions. Sensitivities could be scenario dependent.

2.10.2.3. Technical Adequacy

Because of the potential for complex thermal-hydraulic flow patterns, the ice-condenser physics are questionable. The model is zeroeth order. The ice-condenser model satisfies the adequacy requirements established for the CONTAIN code. The technical adequacy of this model is classified as Category 2.

2.10.3. Containment Sprays

See App. D.10.3 for the detailed model review.

2.10.3.1. Phenomenological Model Description

CONTAIN has models for spray drop settling velocity, heat transfer to the drop, aerosol removal, and fission product gas (or vapors, I_2 and CH_3I or any gas/vapor species) removal. The drops are assumed to be monodisperse. The removals of the vapors and the aerosols are modeled as first-order rate processes, albeit in slightly different degrees of detail.

2.10.3.2. Qualitative Perspective

Containment sprays are effective in removing (scavenging) fission product gases/vapors and aerosol particles from the containment atmosphere. The removal is often both direct (capture by spray drops) as well as indirect (e.g., due to fogging). Cooling of structures by impingement of spray drops has been found to be important and is not modeled.

2.10.3.3. Technical Adequacy

The CONTAIN models for fission product (vapor) removal are based on convection diffusion, but those for aerosols include interception, impaction, and other subtle effects. Also the rate equations for the two are developed in slightly different ways. The modeling can be improved, particularly with respect to the drops characterization (size distribution, spatial distribution, composition, shape) and physicochemical interaction, but it appears to capture the dominant effects. The model should be modified to allow a fraction of the spray drops to be added to the water films on specified structures. The technical adequacy of this model is classified as Category 1.

2.10.4. Passive Containment Cooling System

See App. D.10.4 for the detailed model review.

2.10.4.1. Phenomenological Model Description

The passive containment cooling systems (PCCS) for the SBWR and AP600 are completely different systems and are modeled quite differently. Both can be used for DBA as well as severe-accident analyses. The elements of the SBWR PCCS are:

1. steam supply line,
2. vertical shell-and-tube single-pass heat exchanger,
3. condensate flow line, and
4. noncondensible gas vent line.

The difficult modeling aspect of the SBWR PCCS is the treatment of the film of condensed steam. A mass and momentum balance is performed for laminar film flow. An energy balance is performed at the liquid-film interface employing a heat mass transfer analogy (Dittus-Boelter Equation). Shear forces and suction are excluded from the model.

The AP600 PCCS involves heat transfer through the steel containment shell to water draining down the external surface of the containment and to air flowing by natural convection in an annular region between the containment and the shield building. The difficult modeling aspects of the AP600 PCCS are the treatment of the external water film and the condensing heat transfer at the inner wall surface. The distribution of water on the external surface is treated parametrically, rather than mechanistically. Evaporation of the liquid film is based on mass transfer coefficients in the duct.

The modeling of the interior of the containment includes mass transfer coefficients, steam stratification, and submerged concrete heat sinks. CONTAIN is also capable of modeling dry or long-term performance of the PCCS. In this case, radiative and convective heat transfer are modeled in the duct.

2.10.4.2. Qualitative Perspective

Both the SBWR PCCS and AP600 PCCS are important features of containment performance. The representation of the PCCS relies on existing phenomenological models

in the code. Both systems are represented with reasonable mechanistic detail and appear to provide good agreement with available integral test data.

2.10.4.3. Technical Adequacy

The physics of the PWR phenomena are understood but the BWR physics are considered questionable. Both models are first order. Both models satisfy the adequacy requirements established for the CONTAIN code. Neither model has been documented in the draft manual provided to the Peer Review Committee. The technical adequacies of these models are classified as Category 1 for the PWR and Category 2 for the BWR.

3. TOP-DOWN REVIEW: FINDINGS RELATIVE TO CODE DESIGN OBJECTIVES

Specific code design objectives for CONTAIN were provided by the NRC (Ref. 31). Along with the design objectives, the NRC also provided success criteria that could be used by the Committee members to evaluate the code. In this section, the Committee findings for each of the code design objectives is presented. Before the completion of the peer review, however, the NRC issued a draft revised code strategy (see App. E) in which no further development of fission product and aerosol models would be made within the CONTAIN code. In the future, any further model improvements in these areas will be made in the MELCOR code. In this peer review, evaluations have been made against the original design objectives and targeted applications provided by the NRC (Ref. 3-1).

The overall thrust of the top-down review is to assess the applicability and fidelity of the integrated or total code. A code is found to be applicable if it both includes and successfully integrates the individual models necessary to simulate the important systems, components, processes, and phenomena in targeted experimental facilities and plants. The fidelity of a code can generally be assessed by comparing code-calculated results to applicable integral test data from scaled experimental facilities. Another important top-down consideration relates to coding adequacy (numerics, usability, and quality control). In evaluating the extent to which CONTAIN satisfies its design objectives, applicability, fidelity, and coding adequacy may each be important considerations depending on the nature of the objective.

3.1. Design Objective 1

3.1.1. Statement of Objective and Success Criteria

Modeling detail shall be capable of representing key and important phenomena of severe accident experiments, and anticipated plant accidents and transients.

General Success Criterion: Code can model all PWR and BWR containment systems including ALWR designs (e.g., AP600 and SBWR), operator actions, plus experimental facilities used for code assessment.

a. Expected modeling uncertainties should be comparable to uncertainties in integral severe-accident experiments.

Success Criterion: Uncertainties in important parameters calculated by the code should be less than or equal to measured values. For example, if the uncertainties in the measured temperatures and associated boundary conditions are +/- 20%, then the success criteria for the code would be +/- 20% for calculated temperatures.

b. User-defined parameters, other than those needed to define experiments, plant unique features (or uncertainty estimates as specified in Sec. 3.2.1)¹ should be eliminated but only where an experimental or other credible basis exists to define those parameters (e.g., user guidance documentation is required).

¹ Expanded definition adopted by Committee was documented in B. E. Boyack, "Minutes for April 20, 1993 Meeting at Sandia National Laboratory," Los Alamos National Laboratory Group N-12 letter N-12-93-210 to A. Nofrafrancesco dated April 23, 1993.

Success Criterion: Code will not contain any user defined parameters other than those noted.

3.1.2. Specific Findings Relative to General Success Criterion

Table 3-I identifies each of the major containment design variations associated with commercial light water reactor design types. As indicated, CONTAIN is capable of analyzing containment conditions for each type of containment design. Example calculations were presented to the committee of CONTAIN analyses of a subatmospheric PWR containment design, an ice condenser PWR containment design, a Mark I BWR containment design, the AP600, and the SBWR.

Table 3-I
Containment Types

Reactor Type	Containment Type	CONTAIN Capability
PWR	Large-Dry	Yes
PWR	Large-Dry with Secondary Containment	Yes
PWR	Subatmospheric	Yes
PWR	Ice-Condenser	Yes
PWR	AP600	Yes
BWR	Mark I (Light Bulb and Torus) with Secondary Containment	Yes
BWR	Mark II (Drywell over Wetwell) with Secondary Containment	Yes
BWR	Mark III (Drywell with Annular Pool)	Yes
BWR	SBWR	Yes

Depending on the systems that are operable in a DBA or severe-accident scenario to be analyzed, a number of important containment safety features can influence the outcome of the analysis, either by affecting thermal-hydraulic conditions within the containment or by affecting the transport or retention of radioactive materials. Table 3-II identifies containment safety features for the different types of containment, identifies whether a capability exists within CONTAIN to model the safety feature, and provides a cross reference to where the phenomenological model is evaluated in App. D. A check mark indicating that a capability exists does not necessarily mean that the modeling capability is consistent with the expectations for a mechanistic computer code.

Although an ability to model each important safety system is indicated by the table, the ability to model the phenomenological aspects of the behavior varies. Limitations of these models are identified in App. D. These limitations potentially affect the fidelity of the model. It is important to recognize that, although CONTAIN is considered a mechanistic computer code, it does not treat all containment processes in full mechanistic detail. In particular, a lumped-parameter treatment is provided of containment thermal-hydraulics, rather than a three-dimensional solution of the Navier-Stokes equations. This is a necessary approximation in CONTAIN for practical use of the computer code. This approximation is adequate for a broad range of problems to which CONTAIN is applicable. There are other problems, such as those involving transition to detonation of combustible gases in the containment atmosphere, for which CONTAIN is not applicable. In the case of the Passive Containment Cooling System for the AP600, there may be some multi-dimensional effects for which the lumped-parameter modeling within CONTAIN is

Table 3-II
Containment Safety Features

Reactor Type	Containment Safety Feature	Capability	Reference
PWR	Containment Spray (and Heat Exchanger) - Thermal-Hydraulic	Yes	D.10.3
PWR	Containment Spray -Fission Product	Yes	D.10.3, D.5.5.1
PWR	Fan Cooler - Thermal-Hydraulic	Yes	D.10.1
PWR	Fan Cooler - Fission Product	Yes	D.10.1
PWR	Ice Condenser - Thermal-Hydraulic	Yes	D.10.2
PWR	Ice Condenser - Fission Product	Yes	D.10.2
PWR	Igniters/Glow Plugs	Yes	D.7
PWR	Ice Condenser Air Return Fan	Yes	Control Function
AP600	Passive Containment Cooling System Including Water Film	Yes	D.10.4
BWR	Drywell Sprays - Thermal-Hydraulic	Yes	D.10.3
BWR	Drywell Sprays - Fission Product	Yes	D.10.3, D.5.5.1
BWR	Suppression Pool -Thermal-Hydraulic	Yes	D.9.1
BWR	Suppression Pool - Fission Product	Yes	D.9.3
BWR	Igniters/Glow Plugs	Yes	D.7
BWR	Suppression Pool Cooling	Yes	D.9.1
BWR	Standby Gas Treatment System	Yes	Control Function
SBWR	Drywell Flooding	Yes	Control Function
SBWR	PCCS	Yes	D.10.4
SBWR	Multiple Path Suppression Pool	Yes	Planned

marginal (although preliminary comparisons with experiments indicate reasonable quantitative agreement).

Dynamic aspects of suppression pool behavior (e.g., chugging, pressure loads, and pool swelling) are not modeled in CONTAIN. The addition of this type of modeling would not be consistent with the planned end uses of CONTAIN. Thermal stratification of pools is also not considered, which in some cases could affect the fidelity of the calculation of pressure rise in the containment. CONTAIN also does not model the uncover of vertical layers of horizontal vents as in the Mark III configuration.

Although CONTAIN has the capability of analyzing several flow paths through an ice bed at different azimuthal positions, the thermal-hydraulics observed in the experimental program at Pacific Northwest Laboratories were very complex. The modeling in CONTAIN can only be expected to be able to simulate the gross behavior of ice bed melting and aerosol decontamination.

There are a number of limitations in the treatment of elemental and organic iodine in the containment and the effects of safety systems on elemental iodine removal.

The final aspect of this General Success Criterion relates to the ability to model operator actions and experimental facilities. Operator actions are typically straightforward to model in accident analyses through their impacts on the operation of systems. CONTAIN has the ability to turn systems on and off during the course of an accident scenario. Ability to predict results obtained in experimental systems is more challenging.

Table 3-III provides a list of the types of severe-accident integral experiments that relate to containment processes. Although CONTAIN is not applicable to some of these experiments, it would be unreasonable to undertake the major structural changes in the code that would be required to address three-dimensional and dynamic containment processes. These changes would also make CONTAIN less valuable to the applications for which these processes are not significant. The final column in this table relates to the evaluation of the next success criterion regarding model accuracy.

The experimental programs exist to support the development and validation of computer codes. Most of the severe-accident experimental programs undertaken by the NRC, the industry, and foreign partners are integral experiments in which a number of phenomena interact. These types of experiments are oriented more toward model evaluation than model development, although often the results are used to tune models. If integral tests could be performed in a manner that provided an exact simulation of severe accident conditions in a reactor, the modeling of experiments would introduce no additional code requirements. However, since integral experiments often involve distortion, scaling effects, or non-prototypic boundary conditions, sometimes features have to be added to a code to enable its use in modeling an experiment. Based on the use of CONTAIN in modeling a variety of experiments, the Peer Review Committee concludes that, in general, CONTAIN has the flexibility to model a wide variety of experiments involving coupled containment phenomena. A number of comparison calculations to these experiments were presented to the Committee during its review.²

3.1.3. Specific Findings Relative to Success Criterion "a"

The success criterion for code accuracy requires interpretation. The precision with which measurements can be made in experimental programs may be much more accurate than can reasonably be expected for the accuracy of the computer code. There are often substantial uncertainties in defining the boundary conditions of experiments that implicitly affect the accuracy of the measured parameters. Thus, in evaluating the measurement accuracy associated with experimental programs, it is necessary to consider the reproducibility of experimental results and the potential effects of uncertainties in determining experimental boundary conditions.

The fourth column of Table 3-III identifies the key parameters measured in integral experiments and the fifth column evaluates whether the uncertainties in CONTAIN predictions are comparable to the experimental uncertainties. Table C-II in App. C summarizes the bottom-up evaluations of models for ex-vessel severe-accident phenomena. A review of the state of knowledge of these phenomena indicates that there are a number of areas in which the level of understanding is questionable. As a result, there are some zeroeth-order models and control functions in CONTAIN. CONTAIN cannot be expected to represent phenomena with high accuracy until the scientific knowledge of the phenomena is improved. Nevertheless, the uncertainty in CONTAIN analyses are assessed to be

² Appendix B lists the presentations to the Committee as well as papers and reports describing CONTAIN comparisons with NUPEC, LACE, HDR, IET, PCCS, PNL Ice-Condenser Experiments, Battelle-Frankfurt Hydrogen Deflagration Experiments, DC, and core-concrete experiments.

comparable to the experimental uncertainties for a number of the integral experiments assessed in Table 3-III.

For some types of experiments CONTAIN is not applicable and a discussion of uncertainty is inappropriate. In Table 3-III it is concluded that CONTAIN was not designed to examine problems involving pressure pulses or three dimensional flow problems, such as hydrogen detonation or suppression pool dynamics. Similarly, because of the control volume approach employed in CONTAIN, it cannot be expected to reliably predict intra-compartment stratification over a wide range of conditions.

CONTAIN was assessed to be unable to meet the success criterion for code accuracy for elemental or organic iodine transport, suppression pool aerosol removal, ice-condenser aerosol removal, suppression pool thermal-hydraulics, fuel debris pour, quench and containment spray aerosol removal, and hydrogen stratification and intra-compartment hydrogen stratification. A number of the areas in which CONTAIN models do not satisfy the criterion involve elemental iodine and aerosol behavior. Within the revised severe accident code strategy (see App. E), any future improvements in modeling capability in these areas would be performed within the MELCOR code development effort.

3.1.4. Specific Findings Relative to Success Criterion "b"

CONTAIN has relatively few user-defined parameters in comparison with severe-accident codes that predict in-vessel core meltdown behavior. User-defined parameters are undesirable when they take the place of phenomenological models. The capability to enter user-defined parameters is essential, however, for the performance of uncertainty analyses.

3.2. Design Objective 2

3.2.1. Statement of Objective and Success Criteria

The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected DBAs. It should permit estimates of the uncertainties of containment loads and fission product release predictions without requiring modifications to the code.

Success Criterion: Code predicts dominant phenomena based on assessment against integral facility data. Code also predicts values of important parameter associated with dominant phenomena within measured uncertainty when assessed against integral data.

3.2.2. Specific Findings Relative to Success Criterion

The NRC, EPRI, and international safety community have undertaken an extensive severe-accident integral experimental program to provide benchmarks for validation and improvement of severe-accident computer codes. As indicated in Table 3-III, the containment-related experiments involve the prediction of transient pressures and temperatures in containments for various loads, such as direct containment heating and deflagration of hydrogen. Integral containment experiments have also been performed to examine the coupled thermal-hydraulic/fission product transport and removal processes in severe accidents. Table 3-III identifies the principal parameters measured in these experiments and the associated calculated versus experimental uncertainties. This comparison is discussed in Sec. 3.1.3.

Table 3-III
Ability to Model Integral Containment Experiments

Type of Integral Experiment	Examples of Integral Tests	Applicable	Key Parameter	Comparable Uncertainty
Blowdown to Containment	HDR	Yes	Delta P,P	Yes
High-Pressure Melt Ejection	Surtsey, HIPS, IET, CTF	Yes	P, Fraction Sweepout, moles H ₂	Yes
Passive Containment Cooling	Westinghouse Tests	Yes	P, Non-condensable Fraction	Yes
Hydrogen Detonation and Transition to Detonation	FLAME	No		
Hydrogen Deflagration, Igniter Testing	NTS, FITS, VGES, Whiteshell	Yes	P, T, Combustion Completeness	Yes
Inter-compartment Hydrogen Stratification	HDR, NUPEC, Factory Mutual, ACUREX	Yes	%H, T	No - Yes for hybrid flow solver
Intra-compartment Hydrogen Stratification	HDR, HIT	Limited	%H, T	No
Aerosol Agglomeration and Removal	LACE, CSE, DEMONA, ABCOVE, ACE	Yes	Airborne Concentration	Yes
Elemental or Organic Iodine Transport	CSE	Limited	Airborne Concentration	No
Core-Concrete Interaction	BETA, SURC, ACE	Yes	Gas Generation, Erosion, T	Yes
Core-Concrete Fission Product Release	ACE, SURC	Yes	Release Fraction	Yes
Suppression Pool Dynamics	GE Tests	No		
Suppression Pool Aerosol Removal	EPRI	Yes	Decontamination Factor	No
Suppression Pool Thermal-Hydraulics	Battelle	Yes	Condensation Rate, Exiting Steam Quality	In Progress
Ice-Condenser Aerosol Removal	PNL ICEDF	Yes	Decontamination Factor	No
Fuel Debris Pour and Quench	FITS, FARO	Yes	Steam Production, Coolability	No
Stratified Water and Debris Cooling	MACE, SWISS	Yes	Steam Production, Cooling, Quenching	Yes (Except for Crust Breakup)
Containment Spray	CSE, NUPEC, CVTR, HIT	Yes	P, Aerosol Concentration	Yes (Aerosol Unclear)

The capabilities of CONTAIN to predict the dominant phenomena of DBAs in ALWRS are still under development. Some testing against experimental data has been reported but additional experiments are still to be performed. Although the Committee endorses the use of CONTAIN for ALWR design basis analyses, it is premature to assess the accuracy of the current version of CONTAIN for these analyses.

3.3. Design Objective 3

3.3.1. Statement of Objective and Success Criteria

The code should be applicable for containment transient studies under various accident sequences for PWRs, BWRs, and ALWRS.

Success Criterion: Code can predict containment loads resulting from risk-dominant accident sequences identified by PRA studies for PWRs, BWRs, and ALWRS, as well as DBAs for the AP600 and SBWR configurations. Physical models, as well as component models, exist sufficiently to accurately predict dominant phenomena. The code must model important phenomena in a much more detailed manner than the MELCOR code (with the exception of cases where MELCOR contains first- or higher-order models).³

3.3.2. Specific Findings Relative to Success Criteria

Tables 3-I and 3-II indicate that CONTAIN has the capability to model all of the containment designs and containment systems identified in the design objective. A number of examples of accident sequence analyses were provided to the Peer Review Committee.

Appendix D provides an evaluation of the various phenomenological models and safety system models in CONTAIN. Models that were assessed to be inadequate for the CONTAIN code are:

- HPME - Melt-Water Interactions
- HPME - Fission Product Release
- Non-energetic FCI - Melt Oxidation
- MCCI - Melt Debris Spreading
- Combustion - Propagation in Multi-Compartments
- Ex-vessel Transport - Stratification
- Ex-vessel Transport - Intercell Flow-Natural Circulation/Forced Circulation
- ESFs - Containment Spray Aerosol Removal
- ESFs - Suppression Pool Fission Product Removal
- ESFs - Suppression Pool Thermal-Hydraulics (Multivent)
- Aerosol Transport/Retention - Resuspension
- Aerosol Transport/Retention - Charge Effects
- Aerosol Transport/Retention - Surface Physical Reactions
- Aerosol Transport/Retention - Surface Chemical Reactions

The bases for these evaluations are summarized in Sec. 2.0. Appendix C (Table C-II) documents the Committee's ranking of the dominant processes and phenomena and an evaluation of the CONTAIN models relative to those processes and phenomena.

³ See footnote 1.

The final element of the success criterion imposes the requirement that CONTAIN must model important phenomena in a much more detailed manner than the MELCOR code, except where MELCOR has incorporated first-order models. The version of MELCOR that was peer reviewed in 1992 had no models for ex-vessel processes that were of a higher order than those currently in CONTAIN. The Committee is unaware of any subsequent MELCOR improvements that would change this conclusion. Considerable convergence has occurred in the development of the two codes, resulting in a number of very similar models. The preceding paragraph lists CONTAIN models that were assessed to be inadequate.

3.4. Design Objective 4

3.4.1. Statement of Objective and Success Criteria

The code should be robust, portable, and fast running.

General Success Criterion 1: While the run time is machine dependent, the following general expectations can be used. Running time should be reasonable so as to not handicap the user's ability to perform sensitivity/uncertainty analyses for the phenomena/conditions the code is designed to model. Run time should be a small fraction of the time required to perform the entire analysis.

General Success Criterion 2: Based on user's guidelines and lessons-learned information in the code manual, code users shall be able to set up a plant model (e.g., input deck) to accurately represent a full-scale LWR plant, and successfully perform plant calculations for various severe-accident scenarios and selected DBAs, which are in the domain of targeted applications of the code.

a. The code should not abort prematurely because of user input errors or numerical nonconvergence, but should exit with sufficient diagnostic messages for users.

Success Criterion: Code performs as noted.

b. Numerical precision should be comparable with modeling precision. Spatial convergence should be comparable with modeling scale.

Success Criterion: Code performs as noted.

c. The code should be transportable for mainframe and workstation computing machines.

Success Criterion: Code is transportable.

3.4.2. Specific Findings Relative to General Success Criterion 1

Typical run-time statistics for CONTAIN simulation of design-basis and severe accidents are listed in Table 3-IV. The code run time is seen to be reasonable (it varies from a fraction of the real time for simulation of PWR direct containment heating scenarios, to several times the real time for design basis and other severe accidents). It should be noted that for accidents simulations consuming larger CPU times, the simulation time is typically short. Therefore, the user's ability to perform sensitivity/uncertainty analyses is not expected to be hampered. The recent proposed modifications to the CONTAIN flow

Table 3-IV
Examples of CONTAIN Runtime Statistics on an
IBM/RISC-6000 (320H) Computer

Scenario	Maximum Time Steps (s)	Simulation Time (s)	CPU Time (s)	Simulation /CPU
BWR/Main Steam Line Break	0.1, 0.2, 0.1	10, 410, 416	89	4.7
BWR/Recirculation Line LOCA	0.01, 0.1, 0.2	1, 10, 60	198	0.30
PWR Direct Containment Heating/5 Cells	0.002, 0.005, 0.01, 0.025	5, 10, 40, 80	1534	0.05
PWR Direct Containment Heating/11 Cells	0.002, 0.005, 0.01, 0.025	5, 10, 40, 80	4625	0.02
Typical Severe-Accident Analysis	2.5, 5.0	110, 10,000	720	14

solver are expected to reduce the overall computational efficiency of the code. In CONTAIN, like other large system codes, a considerable fraction of analyst's time is devoted to problem setup and not to running the code.

3.4.3. Specific Findings Relatives to General Success Criterion 2

The code users have been able to use CONTAIN to set up various plant models and experiments, as attested to by the large number of users, nationally and internationally. CONTAIN has been used for simulation of both design-basis and severe accidents. As an example, a large number of DBA cases were set up and simulated recently in a relatively short time frame (Ref. 3-2). The same experience has also been reported for CONTAIN simulation of severe accidents by those in the CONTAIN user community who participated in a recent user's survey (see Sec. 5.3).

3.4.4. Specific Findings Relative to Success Criterion "a"

In general, the code has not been found to abort prematurely because of user input errors or numerical nonconvergence. Upon user errors, the code exits with adequate diagnostic messages for users.

3.4.5. Specific Findings Relative to Success Criterion "b"

The code numerical precision is compatible with the modeling precision. The workstation version of the code operates with double-precision arithmetic, whereas the CRAY version operates in single-precision arithmetic. The spatial convergence is also compatible with the coarse spatial nodalization/modeling scale of the CONTAIN control volume/lumped-parameter approach. However, in CONTAIN, the global computational time step is not accuracy driven, despite the fact that the local computational time steps are accuracy controlled in the intercell flow/atmosphere/pool thermodynamics and the aerosol physics modules. Therefore, even though the code has not been found to be numerically unstable, numerical accuracy of the code calculated results cannot be assessed.

3.4.6. Specific Findings Relative to Success Criterion "c"

Mainframe and workstation versions (IBM, SUN, and HP) of the code are available from SNL. The SNL presentations to the peer review committee showed that the code produces the same results on different computer platforms (i.e., CRAY, IBM, SUN, and HP computers).

3.5. Design Objective 5

3.5.1. Statement of Objective and Success Criteria

The maintenance of the code should follow accepted QA standards for configuration control, testing, and documentation.

General Success Criterion: The code QA procedures and associated documentation should be sufficient and consistently applied as required for NRC applications.

- a. All code changes should be controlled and verified by redundant means.

Success Criterion: Code changes should be made as noted.

- b. Testing standards and benchmarks should be defined for all versions released for production applications.

Success Criterion: These should perform as noted.

- c. Documentation should define the theoretical basis, experimental database, limits of applicability, quantification of uncertainties, user guidance, and testing or assessment results of the code.

Success Criterion: Documentation defines these as noted.

3.5.2. Specific Finding Relative to General Success Criterion

A QA procedure exists (Ref. 3-3) to control, test, and document changes to the code. This procedure is currently being updated by SNL (Ref. 3-4). The QA process is considerably smaller than a full-scope ANSI NQA-1; however, the QA process appears to be working based on the long history of outside code use. The QA process is also compatible with the limited code development activities anticipated for the code.

3.5.3. Specific Finding Relative to Success Criterion "a"

Configuration control is maintained at a level such that every code version is uniquely identified. All of the code changes appear to be controlled and verified by the code developers.

3.5.4. Specific Finding Relative to Success Criterion "b"

Testing standards and benchmarks exist for all code versions released for production applications. The code undergoes three different types of testing prior to release for production calculations consisting of (1) developmental testing by the developers, (2) code testing against 28 standard problems which are documented, and (3) beta testing by members of the CONTAIN project. It should be noted that independent code testing is no

longer performed before code release. The standard problem suite should be expanded to include more benchmark problems, e.g., for condensation, the water pool model, and the outgassing model.

3.5.5. Specific Finding Relative to Success Criterion "c"

The approach to code documentation is for the most part satisfactory. The bases for some of the models are well documented (i.e., CORCON/Mod3 and the direct containment heating); while some of the other models lack the same level of documentation (i.e., the intercell flow models, the heat transfer models). The developmental assessment report (Ref. 3-5) is useful but not sufficient and up to date. A number of recently performed assessment activities were reported to the Committee via presentations. These are listed in App. B. A summary road map for all the assessment reports should be provided in the user's manual. In addition, the user guidelines and the lessons-learned aspects should be expanded and improved. Efforts are already underway at SNL to address these recommendations.

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4. TOP-DOWN REVIEW FINDINGS RELATIVE TO CODE-TARGETED APPLICATIONS

The specific code-targeted applications were defined by the NRC (Ref. 4-1). Along with each targeted application, the NRC provided success criteria that allowed the Committee members to evaluate the adequacy of the CONTAIN code to satisfy the application.

4.1. Targeted Application 1

4.1.1 Statement of Application and Success Criteria

The application is to experimentally analyze and support containment-related severe-accident experimental programs such as HDR, LACE, NTS, and SURTSEY; and analyze relevant ALWR test programs, such as the Westinghouse large-scale PCCS facility.

Success Criterion: Code has been or can be used to analyze these facilities and can provide reasonable predictions of associated dominant phenomena (compared with experimental data, the calculated results will be within the experimental uncertainty bands).

4.1.2. Specific Findings Relative to Success Criteria

This success criterion is redundant to the success criteria described in Sec. 3.1.1. In general, the CONTAIN code has the capability to analyze the dominant phenomena in the targeted facilities. Appendix B identifies the presentations that were made to the Committee by the CONTAIN staff. A number of comparison calculations to these experiments were presented to the Committee during its review. (Appendix B has the presentations to the Committee and papers involving CONTAIN comparisons with NUPEC, LACE, HDR, IET, PCCS, PNL Ice-Condenser Experiments, Battelle-Frankfurt Hydrogen Deflagration Experiments, DCH, and core-concrete experiments.) Those models found to be inconsistent with the requirements of a mechanistic code like CONTAIN are listed in Sec. 3.3.1.

4.2. Targeted Application 2

4.2.1. Statement of Application and Success Criteria

LWR plant analysis is to predict the physical, chemical, and radiological conditions inside containment, and fission product releases as a result of predicted containment failure.

Success Criterion: Code has been or can be used to analyze LWRs and can provide reasonable predictions of associated dominant phenomena, or the ability to perform sensitivity studies. Code must have been shown to predict the dominant phenomena by assessment against sufficient experimental results.

4.2.2. Specific Findings Relative to Success Criteria

A number of examples of comparisons with experiment and sample plant calculations using CONTAIN were presented to the Peer Review Committee. The ability of CONTAIN to represent dominant phenomena in the analysis of LWR transients was evaluated in Sec. 3. The state of validation of CONTAIN models has been evaluated in App. D. Table 3-III and Table C-II of App. C identify the dominant phenomena modeled by CONTAIN and provide evaluations of the accuracy of the models in predicting the

results of experiments. The state of validation of CONTAIN models has been evaluated and documented in App. D and summarized in Table C-II.

4.3. Targeted Application 3

4.3.1. Statement of Application and Success Criteria

The application is selected detailed analysis for specific technical issues, such as hydrogen combustion and migration, build-up of noncondensable gases, direct containment heating, and accident management evaluations.

Success Criterion: Code has been or can be used to provide detailed analysis of these specific technical issues predicting the associated dominant phenomena with reasonable agreement, or the ability to perform sensitivity studies. Code must have been shown to predict the dominant phenomena associated with these specific technical issues by assessment against sufficient experimental results.

4.3.2. Specific Findings Relative to Success Criteria

CONTAIN has been the benchmark code for the NRC in the evaluation of containment-related technical issues, as demonstrated by sensitivity analyses performed in support of NUREG-1150 (Ref. 4-2). CONTAIN is particularly valuable for containment issues involving coupled thermal-hydraulic and fission product transport phenomena. The status of CONTAIN model validation is summarized in Table C-II of App. C. CONTAIN has been used in pre-test and post-test predictions of a variety of integral experiments involving aerosol transport, containment thermal-hydraulics, high-pressure melt ejection, hydrogen combustion, and inter-compartment hydrogen stratification with excellent results. Extensive comparisons and sensitivity studies were presented to the Peer Review Team between CONTAIN and DCH experimental data.

4.4. Targeted Application 4

4.4.1. Statement of Application and Success Criterion

This application is for MELCOR benchmarking and assessment.

Success Criterion: Code can be used to benchmark and assess the MELCOR code containment related behavior at least for integral experiments.

4.4.2. Specific Findings Relative to Success Criterion

The assessment of the Peer Review Committee is that, in general, CONTAIN has the capability to be used as a benchmark for MELCOR code assessment. The limitations of CONTAIN phenomenological models are described in App. D. In some cases, CONTAIN has been used as a test bed for models that have subsequently been incorporated into MELCOR. It is clear that the two-tier structure originally intended for CONTAIN and MELCOR has not been maintained. However, the revised severe-accident code strategy (App. E) has markedly redefined the two-tier strategy and issues related to overlapping models in the two codes no longer appear to be issues.

4.5. Targeted Application 5

4.5.1. Statement of Application and Success Criterion

This application is for ALWRs design-basis and severe-accident evaluation.

Success Criterion: Code can be used to evaluate ALWR severe accidents with reasonable prediction of the dominant phenomena and evaluate selected DBAs in accordance with relevant NRC Standard Review Plans.

4.5.2. Specific Findings Relative to Success Criterion

Evidence for the ability of CONTAIN to model LWR DBA regulatory conditions was provided to the Committee. With regard to severe accident phenomena, this success criterion is largely redundant to success criteria in Sec. 3.1.1. The extent to which CONTAIN has been used to investigate severe accidents in ALWRs is quite limited, however. Work is in progress. The Committee has concluded that CONTAIN is an appropriate vehicle for performing both design-basis and severe-accident analyses for ALWRs. Some additional effort will be required to develop a CONTAIN model that can be used for regulatory applications and such efforts are currently underway.

REFERENCES

- 4-1. F. Eltawila, US Nuclear Regulatory Commission, Division of Systems Safety Research, unnumbered letter dated October 23, 1994, to B. E. Boyack, Los Alamos National Laboratory.
- 4-2. "Severe Accident Risks: An Assessment of Five U.S. Nuclear Power Plants," US Nuclear Regulatory Commission report NUREG-1150, Volumes 1-2, June 1989.

5. OTHER FINDINGS

During the course of the CONTAIN Peer Review, the NRC requested that the Committee review a revised severe-accident code strategy issued to code developers and code users for review and comment (Ref. 5-1). The new code strategy included an updated set of design objectives and targeted applications for the CONTAIN code. The Committee was asked to consider the impact of the revised design objectives and targeted applications on the Committee findings developed using the original CONTAIN design objectives and targeted applications (Ref. 5-2). Insights derived from the Committee's review of the revised severe-accident code strategy are provided in Sec. 5.1.

Before development of the revised severe-accident code strategy, design objective 2 for the CONTAIN code stated, "The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected design basis accidents. It should permit estimates of the uncertainties of containment loads and fission product release [to the environment] without requiring modifications to the code." During the course of the Committee's review, the NRC was considering whether to incorporate mechanistic models of fission products in CONTAIN. One candidate was the elements of the TRENDS code under development at Oak Ridge National Laboratory (ORNL). The Committee was asked to consider the adequacy of TRENDS and the review results are presented in Sec. 5.2. After completing the review, the revised severe-accident code strategy was issued (Sec. 5.1 and App. E) and fission product modeling was removed as a design objective for the CONTAIN code.

The Committee sought to obtain views and insights from the CONTAIN user community. A survey was prepared (App. F) and distributed to more than 30 users. Responses were received from nine users. Several key insights from the user community are summarized in Sec. 5.3.

5.1. Revised Severe-Accident Code Strategy

The revised severe-accident code strategy information package presented to the Committee for review is provided in App. E. The cover letter states the NRC's desire to eliminate duplication of code capability between the various codes it sponsors. Of most interest to the present review is the duplication of code capabilities between MELCOR and CONTAIN. One potential area of duplication was in existing plans to improve the fission product modeling capabilities in both CONTAIN (e.g., the addition of the TRENDS model reviewed in Sec. 5.2 of this report) and in MELCOR. The NRC revisited the original bases for the plans and determined that these had changed significantly as MELCOR performance has been enhanced. In addition, MELCOR calculates both the generation and release of radionuclides, as well as transport and deposition both within the reactor cooling system and the containment. In effect, MELCOR is a standalone code while CONTAIN must be supplied fission product releases from the reactor cooling system as input. Finally, the NRC concluded that because "larger uncertainties in fission product tracking are tolerable in comparison to the accuracy required for thermal hydraulic analyses," there was no need to use CONTAIN as a test bed for more detailed mechanistic fission product models that could later be simplified and incorporated into MELCOR.

The NRC provided a revised statement of objectives for CONTAIN. The revised CONTAIN objective statement is: "The CONTAIN code is intended as a thermal-hydraulic computer code for the integrated analysis of containment phenomena. It should have the capability of predicting pressure and temperature conditions inside a variety of containment types. The code should be useful for analyzing design basis accidents as well as postulated severe accident scenarios." As implied by the revised statement of objectives for

CONTAIN, the major difference between the original CONTAIN design objectives and targeted objectives (Ref. 5-2 and Secs. 1.3.1 and 1.3.2) and the revised objectives (App. E) is that the future focus of CONTAIN will be integrated thermal-hydraulic analyses of containment phenomena for a spectrum of accidents including severe accidents and selected DBAs. Given this focus, there will be no future development of the capability for fission product release predictions. The revised CONTAIN design objectives, targeted applications, and success criteria follow.

Design Objectives

1. The CONTAIN code is intended as a thermal-hydraulic computer code for the integrated analysis of containment phenomena. It should have the capability of predicting pressure and temperature conditions inside a variety of containment types.
2. The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected DBAs. It should permit estimates of the uncertainties of containment loads predictions without requiring modifications to the code.
3. Models incorporated in CONTAIN should be able to address key containment accident phenomena in adequate detail from the risk assessment perspective.
4. CONTAIN should permit relatively straightforward extrapolation of the results of simulation of small-scale separate effects and integral experiments to full-scale plant cases.
5. CONTAIN should be portable, maintainable, and have a structure that facilitates incorporation of new or alternative phenomenological models.

Targeted Applications

1. Containment response analysis in LWR plants under severe-accident conditions and certain design-basis events to predict thermal-hydraulic conditions inside containment.
2. As a code developmental tool for evaluating selected containment issue resolutions, and to analyze phenomena so that simpler models can be justified for incorporation into the MELCOR code.

Success Criteria

1. CONTAIN predictions of phenomenological events should be in qualitative agreement with the current understanding of the physics of such events based either on the results of certain well-defined and controlled experiments or on analytical results derived from first principles.
2. Uncertainties in key parameters describing a phenomenon as calculated by CONTAIN should not exceed the uncertainties in experimentally measured or analytically derived values of these parameters.
3. CONTAIN phenomenological models should, where feasible, be mechanistic in nature and capture the dominant processes to the practical

extent possible. Otherwise, parametric models are acceptable and uncertainties in the phenomena can be adequately represented through parametric variations and sensitivity analysis.

4. The code should be transportable for mainframe and workstation computing machines. The maintenance of the code should follow accepted QA standards for configuration control, testing, and documentation.

The Committee review of the CONTAIN code using the original CONTAIN design objectives and targeted applications was well advanced when the revised severe-accident code strategy was developed. As requested, the individual Committee members reviewed and commented on the revised severe-accident code strategy (Ref. 5-3). The Committee recognized the significant changes inherent in the revised design objectives and targeted applications for CONTAIN and concluded that it should complete its review using the original design objectives and targeted applications. This approach was taken, in part, because the revised strategy had been submitted for review and comment and seemed, therefore, to still be subject to further revision. Subsequently, it became clear that the revised severe-accident strategy had, in fact, been adopted in all material respects and that the NRC was proceeding with code-related decisions consistent with the revised strategy. Consequently, the Committee took this reality into consideration when considering the assignment of its priorities for correction of modeling deficiencies. For example, deficiencies related to fission product that would have been ranked as important and needing correction relative to the original code objectives were assigned a low (essentially no priority) for correction relative to the revised code objectives. Thus, the outcome of the revised CONTAIN code objectives for the CONTAIN Peer Review are reflected in Sec. 6, Recommendations.

5.2 TRENDS Review

The same format has been applied to the TRENDS review as was applied to the various CONTAIN models and correlations reported in App. D.

5.2.1. Model Description and Pedigree

Overall, fission products are not treated mechanistically or in detail in CONTAIN. There has been, however, an NRC-sponsored research effort underway at the ORNL on a computer program **TRENDS** (Transport and **RE**tention of Nuclides in **D**ominant Sequences), wherein the focus has been on defining and solving the basic set of rate equations. This program also has provided an avenue for related activities on experimental measurements of equilibrium properties and reaction rates associated with iodine/iodide gaseous, surface, and aqueous chemistry. The program has published a series of reports, and the CONTAIN peer review group also had the benefit of hearing presentations on TRENDS (ORNL), or rather uncertainties associated with some of the equilibria and the rate processes in TRENDS, and on how it might be, partially or completely, integrated into CONTAIN. Since the revised NRC strategy indicates that CONTAIN will not include computations of fission product fate and transport beyond its present capacities, and since the entire topic is in formative stages, the discussion below is confined to the some salient aspects of the modeling.

TRENDS addresses time evolution of fission product distribution in a chamber (cell), where the products might either be airborne (in the gaseous phase or adsorbed/absorbed (l/s) on aerosol particles), or surface bound (in liquid or on dry surfaces). The particles are regarded as single species and monodisperse. It is recognized that the iodine/iodide chemistry is strongly dependent on water pH and radiation fields, and

that needed data on the equilibria and the rate processes are not quite available. Within these constraints, the model follows 21 iodine inventory locations within each cell. Each of these is associated with a particular index as shown in Table 5-I.

With N_i representing the inventory (mass) in the location, the rate processes are described by the type of equations:

$$\begin{aligned} -\dot{N}_1 &= \dot{N}_4 = \alpha_4 N_1 - \beta_4 N_4, \text{ I}_2(\text{g}) \text{ depositing onto paint} \\ -\dot{N}_1 &= \dot{N}_5 = \alpha_5 N_1 - \beta_5 N_5, \text{ I}_2(\text{g}) \text{ depositing onto steel} \\ -\dot{N}_1 &= \dot{N}_6 = \alpha_6 N_1 - \beta_6 N_6, \text{ I}_2(\text{g}) \text{ depositing onto concrete} \\ -\dot{N}_1 &= \dot{N}_8 = \alpha_8 N_1^{0.82} - \beta_8 N_8, \text{ I}_2(\text{g}) \leftrightarrow \text{CH}_3\text{I}(\text{g}) \end{aligned}$$

and the overall rate equations are described by the system of ODEs consisting of the equations of the type (20 or 21):

$$\dot{N}_1 = \dot{Q}_1 - \left\{ (\alpha_4 N_1 - \beta_4 N_4) + (\alpha_5 N_1 - \beta_5 N_5) + (\alpha_6 N_1 - \beta_6 N_6) + (\alpha_8 N_1^{0.82} - \beta_8 N_8) \right\}$$

with appropriate initial conditions.

5.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The system of equations is reasonable, provided the sources, the rate constants, and the equilibria are known. The assumption of single-specie, monodisperse aerosol (solid/liquid) is quite unrealistic in so far as aerosols represent a large surface area for interaction, and a detailed modeling would be necessary for good predictions.

5.2.3. Results of Model Sensitivity Studies

However, the $\text{I}_2/\text{CH}_3\text{I}$ evolutions are known to be very sensitive to water pH (boron oxides, cesium hydroxides or borates, carbon dioxide, nitric acid, core-concrete aerosols, hydrochloric acid from cable insulations, etc.; a pH below 7, or more around 4, favors $\text{I}_2/\text{CH}_3\text{I}$ evolution) and radiation doses. Similarly, gas/solid iodine chemistry is sensitive to the environment.

5.2.4. Results of Benchmarking/Validation Studies

Good data on the rate processes are sparse, and results of TRENDS validation against experiments are either limited in scope or are not available.

5.2.5. Identified Deficiencies and Options for Model Improvements

The models are simple. Greater detail in the modeling, and a range of new data is needed for the modeling to be successful.

Table 5-I
Inventory Represented by N_i

Index i	Form	Location
1	I_2	Gas
2		Aerosol (airborne)
3		Liquid
4		Painted surface
5		Steel surface
6		Concrete surface
7		Deposited aerosol
8	CH_3I	Gas
9		Liquid
10		Painted Surface
11	CSI (or I^-)	Gas
12		Aerosol (airborne)
13		Liquid
14		Condensed on fixed surface
15		Deposited aerosol
16	HI	Gas
17		Aerosol (airborne)
18		Steel surface
19		Deposited aerosol
20	Not used	
21	AgI	Liquid precipitate

5.2.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct models is crucial to source term calculations.

5.2.7. Technical Adequacy of Model and Documentation

The models used are simple (a simple system of ODEs) to implement. The adequacy needs to be tested, but many limitations are apparent. Any ODE solver could solve a system of 20 ODEs, and to that extent, adoption of TRENDS in another code is straightforward. But good mechanistic modeling of fission product fate and transport is a problem that would require substantially more efforts and resources for resolution.

The TRENDS documentation is fragmented.

5.3. CONTAIN User Survey Summary

The SCDAP/RELAP5 Peer Review Committee designed a survey that was issued by the NRC to obtain insights from the user community regarding the capabilities and functioning of that code relative to its design objectives and targeted applications. A similar survey was designed and issued by the NRC to the CONTAIN user community. The survey form is presented in App. F. Survey forms were sent to over 30 users and 9 users completed the survey and returned comments. A summary of the results of the survey is provided here.

The survey proved to be of limited value for several reasons. First, the number of responses was disappointingly small. The Committee anticipated that there would be more respondents. Second, about two-thirds of the respondents reported that their experience level with the code was small. Third, some of the respondents reported that their experience was with dated code versions. Within the context of these reservations, the following general comments apply.

1. The code documentation was deemed to be adequate for the needs of the user community. This comment may appear to be contrary to the Committee recommendations in Sec. 6 for improved code documentation. However, it is likely that the differing perspectives on documentation reflect the need for more detailed documentation of models and correlations by the Committee as it carried out the bottom-up review of CONTAIN models and correlations.

2. Most institutions were able to implement CONTAIN on their computing systems with little difficulty.

3. The code was found to be user friendly and several institutions commented that the user guidance provided was helpful.

REFERENCES

- 5-1. A. Notafrancesco, US Nuclear Regulatory Commission, Division of Systems Safety Research, unnumbered letter dated December 27, 1993, to B. E. Boyack, Los Alamos National Laboratory.
- 5-2. F. Eltawila, US Nuclear Regulatory Commission, Division of Systems Safety Research, unnumbered letter dated October 23, 1994, to B. E. Boyack, Los Alamos National Laboratory.

- 5-3. B. E. Boyack, "Committee Member Comments on Revised Severe Accident Code Strategy," Los Alamos National Laboratory Group TSA-12 letter TSA-12-94-56 dated February 14, 1994, to F. Eltawila, US Nuclear Regulatory Commission.

6. RECOMMENDATIONS

The CONTAIN Peer Review Committee has determined that recommendations in five code-related areas are appropriate:

- (1) documentation,
- (2) user guidance,
- (3) modeling capability,
- (4) code assessment, and
- (5) technical assessment.

The Committee has included prioritized recommendations that we believe will have an important impact on either code usage or code adequacy. The Committee concluded that complete and adequate documentation is essential and, therefore, that all documentation deficiencies should receive a high priority for correction. The Committee also felt that improved user guidance is closely related to effective code usage and recommendations have been made in this area, as appropriate. An extensive effort was put forth in assessing the capabilities of basic CONTAIN phenomenological models. The Committee worked to identify the dominant PWR and BWR severe-accident phenomena. This effort had its genesis in the work documented in App. C of the MELCOR Peer Review report (Ref. 6-1). The earlier work was extended and refined as reported in App. C of this document. The ranking was used by the committee to identify the most important phenomenological models that must be provided, based on their potential effect on source-term and containment loads. Once the existence of the important models in CONTAIN was confirmed, model adequacy was assessed as part of the bottom-up review effort (App. D). Models assessed as having deficiencies were identified. Deficient models needed to simulate the key phenomena identified in App. C were assigned a high priority for improvement. For those models where code assessment was found to be deficient, recommendations were made. Finally, additional technical assessments in advance of, or related to, code modifications were identified and assigned a priority consistent with the importance of the underlying model.

As noted above, there are five areas in which recommendations have been made. The Committee has assessed the priority of each recommendation. The Committee's recommendations, assessed as either high, medium, or low priority, are presented in Table 6-I. The table provides a brief description of the recommendation, characterizes the recommendation as belonging to one or more of the five recommendation areas identified above, identifies the specific section(s) in this report wherein the recommendation is generated, and documents the basis for the recommendation. Recommendations related to aerosol and fission product models are assigned a dual priority. The NRC has recently issued a draft revised severe-accident code development strategy (App. E). Under this strategy, no further aerosol or fission product model development efforts will be undertaken in CONTAIN. These capabilities will be centered in the NRC-sponsored MELCOR code. Therefore, the Committee took this information into consideration when assigning priorities to its recommendations. For completeness, however, the Committee assigned a second priority that reflects the Committee's importance ranking using the design objectives and targeted applications originally specified for the CONTAIN Peer Review (Ref. 6-2). This second ranking may provide some insight into the relative importance that could be assigned to MELCOR development activities related to containment modeling.

Fourteen high-priority recommendations are listed in Table 6-I. Of these, four recommendations deal with documentation. The remaining high-priority recommendations are for user guidance (four), modeling capability (three), code assessment (one), and

technical assessment (two). The eleven medium priority recommendations given in Table 6-I relate to technical assessment (seven), modeling capabilities (three), and user guidance (one). Fourteen recommendations were assigned a low priority in Table 6-I. Of these, eight recommendations are related to fission product and aerosol modeling. Six of these are ranked as high priority, one is ranked as medium priority, and one is ranked as low priority for correction under the original CONTAIN design objectives and targeted applications (Ref. 6-2). All eight recommendations are assigned a low priority under the revised CONTAIN design objectives presented in App. E.

REFERENCES

- 6-1. B. E. Boyack, V. K. Dhir, J. A. Gieseke, T. J. Haste, M. A. Kenton, M. Khatib-Rahbar, M. T. Leonard, and R. Viskanta, "MELCOR Peer Review," Los Alamos National Laboratory report LA-12240, March 1992.
- 6-2. F. Eltawila, US Nuclear Regulatory Commission, Division of Systems Safety Research, unnumbered letter dated October 23, 1994, to B. E. Boyack, Los Alamos National Laboratory (note: this letter identifies the CONTAIN design objectives and targeted applications to be considered for the CONTAIN peer review).
- 6-3. K. E. Washington, Sandia National Laboratories letter dated May 31, 1994, to B. E. Boyack, Los Alamos National Laboratory (note: this letter identifies currently planned ALWR development tasks).

Table 6-I

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.2.1.5	Technical Assessment	Provide additional confirmation of technical adequacy of the hybrid formulation (flow solver) under conditions of most interest to containment analysis. Should the adequacy of the formulation be confirmed, appropriate model documentation and user guidelines should be provided.	High	The impact on containment loads is high and the phenomenon is understood (Table C-II, Item V.h). The hybrid formulation has shown promise in reducing some of the non-physical behavior of the code.
D.2.1.5	Documentation	<p>The condensation/evaporation heat transfer model should be better described in the code manual to show that the effect of high mass transfer on condensation and evaporation is correctly described.</p> <p>The choice of the characteristic length scale for the pool/atmosphere interface should be justified.</p>	High	The Committee has elected to assign a high priority to all documentation issues because they are important to the understanding and application of the code.
D.2.2.5	Documentation	Improve descriptions of the implicit boiling pool source and subcooled boiling models.	High	The Committee has elected to assign a high priority to all documentation issues because they are important to the understanding and application of the code.
D.4.2.2	User Guidance	Provide guidance on the length scale that should be specified for NAD	High	The value used for experimental analysis is a fit to small-scale experimental data and is inappropriate for plant-scale calculations.

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.4.5.5	Modeling Capability	Provide a model for the interaction of water with cavity debris.	High	The impact on containment loads is high, knowledge of the phenomenon is questionable, no model is provided, leading to a finding of inadequacy (Table C-II, Item I.e).
D.4.5.7	User Guidance	Provide guidance on how to use currently available features in the code to represent melt-water interactions	High	SNL presentations to the Committee claimed that some aspects of melt-water interactions have been successfully modeled. No guidance is currently provided.
D.7.1.5	User Guidance	Provide enhanced user guidance regarding the input values for sensitivity studies on (1) ignition criteria for combustion, (2) effects of turbulence and obstacles on flame speed, and (3) combustion completeness	High	Inappropriate application of a model potentially has the same impact as applying an inadequate model. The impacts on containment loads are high (Table C-II, Items IV.a, e, and f).
D.7.5.5				
D.7.6.5				
D.8.2.5	Documentation	The description of the use of radiation parameters given the presence of corium fuel debris needs to be further refined to give the analyst more guidance and the uncertainties associated with its use.	High	The Committee has elected to assign a high priority to all documentation issues because they are important to the understanding and application of the code.
D.8.3.5	User Guidance	Prepare improved guidelines for the use of a forced velocity and the characteristic length scale in the compartment control volume for convective coefficients.	High	Inappropriate application of a model potentially has the same impact as applying an inadequate model. The impact on source term is high (Table C-II, Item V.f).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority ¹	Basis
D.8.4.5	Modeling Capability	The Grashof number should be based on the density difference and not the temperature difference. Note: plans currently exist to make this correction (see Ref. 6-3).	High	The impact on containment source term and loading is high, knowledge of the phenomenon is understood, a first-order model is provided but is incorrectly formulated (Table C-II, Item V.e).
D.9.1.5	Documentation	Improve the description of the pool energy transfer model to show the analytic steps in deriving the model equations.	High	The Committee has elected to assign a high priority to all documentation issues because they are important to the understanding and application of the code.
D.9.2.5	Modeling Capability	Provide a mechanistic model for predicting vent clearing behavior in multi-vent pressure suppression pools and vents to multiple pools. Note: plans currently exist to provide this capability (see Ref. 6-3).	High	The importance of this phenomena on containment loads is ranked as high, the physics are understood, and a limited modeling capability exists.
D.10.3.5	Technical Assessment	Identify and document the most appropriate method (either using existing code models or by implementing a new model) to allow a user-specified fraction of the spray water at a physically appropriate droplet temperature to be added to water films on user-specified structures. Note: SNL specified a spray impingement fraction and used CONTAIN's film tracking model in its "Open Calculation of the ISP-35."	High	The CSNI ISP35 exercise has shown that direct cooling of structures by impingement of spray drops is an important effect.

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.10.4.5	Code Assessment	Complete assessment of AP600 and SBWR PCCS models as data become available. Document guidelines for representing the PCCS in ALWR calculations as this information becomes available.	High	The impact on containment loads is high, knowledge of the phenomenon is questionable, a zeroeth order model is provided, and the model is judged to be adequate but is conditioned on completion of assessment activities (Table C-II, Item VI.e).
3.5.4	Technical Assessment	Expand the CONTAIN standard problem set to include a benchmark problems for (1) condensation, (2) the water pool model, and (3) the data of Chu and Muir for the outgassing model.	Medium	The current standard problem set does not contain such a problem and it is feasible to do so. Directly relates to CONTAIN Design Objective No. 5.
D.2.2.5				
D.8.1.5				
D.1.7	Technical Assessment	Compare consistency of different materials data bases used by CONTAIN, DCH module, and CORCON and eliminate inconsistencies, as appropriate.	Medium	Potential for inconsistency. SNL states that under current code usage, the potential for inconsistency does not arise.
D.3.5	Modeling Capability	Provide a mechanistic melt spreading model. Models have been proposed and are available in the literature.	Medium	The impact on containment loads is moderate, knowledge of the phenomenon is questionable, a control function is provided, and the model is judged to be inadequate (Table C-II, Item III.g).
D.4.3.5	Modeling Capability	Modify the choked flow model so that it is consistent with established homogeneous choked flow models in the limit slip = unity	Medium	The impact on containment loads is high, knowledge of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be adequate (Table C-II, Item I.c).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority ¹	Basis
D.4.3.5	Technical Assessment	Perform a sensitivity study to determine the importance of the cavity slip ratio at plant scale to confirm the adequacy of the recommended value determined from the SURTSEY experiments.	Medium	The impact on containment loads is high, understanding of the phenomenon is questionable, a zeroeth order model is provided, and the model is judged to be adequate (Table C-II, Item I.c).
D.4.4.5	Technical Assessment	Determine if unstable debris particles break up before leaving the cavity and if predicted gas flows in the cavity are capable of levitating particles of the predicted size out of the cavity.	Medium	Small-scale experimental evidence indicates that large debris particles may be carried out of the cavity before breaking up into stable drops. The potential for occurrence at plant scale, together with the consequences, should be assessed. There appears to be no check in the code to ensure that the predicted particle sizes levitated and carried out of the cavity are consistent with the predicted carryover.
D.4.7.5	Technical Assessment	Because dispersal models consist of correlations which are based on isothermal, simulant experiments which may not adequately represent the phenomena under reactor accident conditions, several of the correlations (including the Whalley-Hewitt and Levy correlations) should be tuned to the available experimental data and then applied to plant calculations to confirm scaling.	Medium	The impact on containment loads is high, knowledge of the phenomenon is poor, a zeroeth-order model is provided, and the model is judged to be adequate (Table C-II, Item I.d). The information developed can be used to provide user guidelines for modeling this important process.

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.7.2.5	Technical Assessment	Determine if simple models exist to estimate the criteria for diffusion flame burning.	Medium	The impact on containment loads is moderate, knowledge of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be adequate (Table C-II, Item IV.c). If an adequate model is found, a corresponding medium priority modeling capability task should be identified.
D.7.4.5	Technical Assessment	Determine if use of the SENKIN code permits a significant reduction in the pessimism of the bulk spontaneous recombination calculation.	Medium	The impact on containment loads is high, knowledge of the phenomenon is questionable, a zeroeth order model is provided, and the model is judged to be adequate (Table C-II, Item IV.d).
D.7.7.5	Modeling Capability	Provide a model for propagation in multicompartments. Two possibilities are (1) include a flame front tracking model and (2) incorporating simplified models of turbulence generation (e.g., for specific geometries).	Medium	The impact on containment loads is moderate, knowledge of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be inadequate (Table C-II, Item IV.f)
D.2.1.5	Modeling Capability	Numerical inefficiencies associated with the new flow solver should be minimized.	Low	The recommendation addresses economic factors rather than technical adequacy.

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.3.5	Modeling Capability	<p>Improve the crust formation/freezing model. The model for crust formation and freezing does not account for crust composition changes and thermal inertia. The model for crust growth and its evolution is not correct especially in the presence of water, crust breakup upon interaction with water, and crust instability are not considered.</p> <p>The present melt-concrete heat transfer model does not allow a transition from the original stable film model to the new slag film model. This transition can be implemented via a simple gas velocity criterion.</p> <p>The coolant layer heat transfer model is limited to heat transfer from the pool surface (assumed to be represented by a flat plate). The model does not treat the potential for crust breakup, water ingress, debris fragmentation, quench, debris dryout, and remelt.</p>	Low	<p>The impact on containment loads is high, understanding of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be adequate (Table C-II, Item I.a).</p> <p>Should the phenomenon become understood, incorporation of appropriate models should assume a higher priority.</p>
D.4.1.5	Technical Assessment	Perform sensitivity studies to determine the impact of time of gas blowthrough.	Low	The impact on containment loads is high, understanding of the phenomenon is questionable, a first-order model is provided, and the model is judged to be adequate (Table C-II, Item I.a).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.4.2.5	Modeling Capability	Model heat transfer between NAD and structures.	Low	The impact on containment loads is high, understanding of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be adequate (Table C-II, Item I.b).
D.4.6.5	Modeling Capability	Provide a model for fission product release during HPME events.	Low/Medium	The revised CONTAIN design objectives issued with the revised severe accident code strategy (App. E) do not support new modeling CONTAIN modeling initiatives. The second ranking reflects the original CONTAIN design objectives. The impact on source term is moderate, knowledge of physics is questionable, and a CF is provided resulting in a Category 4 finding.
D.4.9.5	Modeling Capability	Incorporate in CONTAIN the capability to calculate the thermal radiation model multipliers now required as user input	Low	The impact on containment loads is high, the physics are understood, a first-order model is provided, and the model is judged to be adequate (Table C-II, Item I.h).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority ¹	Basis
D.5.1.5 2.5.1.3	Technical Assessment	Assess the need to generalize the dynamic equation to include density, shape, charge and physical-chemical interactions	Low/High	The impact on containment source terms is high, understanding of the phenomenon is questionable, a first-order model is provided, but the model is judged to be inadequate in that density, shape, charge, and chemical effects are not included (Table C-II, Item VIII.a).
D.5.2.5 2.5.2.3	Modeling Capability	Improve the gravitational agglomeration model	Low/High	The impact on containment source terms is high, the physics are only partially understood, first order models are provided but the gravitational agglomeration model is judged to be inadequate for modeling multicomponent effects (Table C-II, Item VIII.b).
D.5.3.5 2.5.3.3	Modeling Capability	Improve thermophoretic and Stefan flow/diffusiophoresis deposition models	Low/High	The impact on containment source terms is high, the physics are only partially understood, first order models are provided but some of the models are judged to be inadequate, e.g., a clarification of the impact of hydrodynamics on all deposition processes is needed and better models for phoretic effects that correctly capture the physics are needed (Table C-II, Item VIII.c).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority ¹	Basis
D.5.4.5	Modeling Capability	Improve the condensation model on aerosols (Eq. 7 of App. D.5.4.5. is recommended as a candidate)	Low/High	The importance of this phenomena on source term is ranked as 4, the physics are mostly understood, and a first order model evaluated as Category 4 currently exists. The model, however, can be improved in simple ways.
D.5.4.5	Modeling Capability	Implementation of the Kelvin effect should be made consistent with the assumption of single composition with an aerosol size class and more size classes should be provided for a given range of aerosol sizes.	Low/High	With the current implementation, the solution does not converge in time step if the Kelvin and solute effect models are used together. The restriction on number of size classes prevents converged solutions in size classes from being obtained for some calculations involving condensation onto airborne aerosols.
D.7.8.5	Modeling Capability	Include a model to predict the conversion of cesium iodide to elemental iodine during a hydrogen burn.	Low/Low	The impact on containment source term is low, knowledge of the phenomenon is poor, a control function capability is provided, and this is judged to be adequate (Table C-II, Item IV.g)
D.9.1.5	Code Assessment	Assess the adequacy of the pool energy transfer model (e.g., thermal stratification, bubbling phenomena, etc.) against data.	Low	The impact on containment loads is high, the physics are understood, a first-order model is provided, and the model is judged to be adequate (Table C-II, Item VI.c).

Table 6-I (continued)

Prioritized Committee Recommendations

Section	Type	Description	Priority¹	Basis
D.9.3.5	Modeling Capability	Incorporate models for bubble swarm, bubble breakup, condensation growth, expansion work effect on bubble saturation, and effect of hygroscopicity in the suppression pool scrubbing model. Provide a vapor removal model to predict the fate of vapor in containment.	Low/High	The impact on containment source terms is high, understanding of the phenomenon is questionable, a zeroeth-order model is provided, and the model is judged to be inadequate (Table C-II, Item VIII.e).

¹Proposed development activities related to aerosols and fission product transport are assigned a X/Y priority. The X priority reflects the revised severe accident code development strategy (see App. E) and the associated revised CONTAIN design objectives. The Y priority reflects the design objectives and targeted applications originally specified for the CONTAIN Peer Review.

APPENDIX A

Members of the CONTAIN Peer Review Committee

B. E. Boyack

Brent E. Boyack is the Chairman of the CONTAIN Peer Review Committee. He is leader of the Terrestrial Reactor Technology Team within the Reactor Design and Analysis Group at Los Alamos National Laboratory. He has published extensively on light water reactor accident behavior, thermal-hydraulic code assessment, code uncertainty quantification, gas-cooled thermal and fast reactor fluid dynamics and heat transfer, and computer model development. He was Chairman of the MELCOR Peer Review Committee. He has participated in NRC review groups focusing on the quantification of uncertainty in the NRC-developed thermal-hydraulics code TRAC-PF1/MOD1, quantification of uncertainty in the NRC-developed thermal-hydraulic code RELAP5/MOD3, the Severe Accident Scaling Methodology development, and the Expert Panel review of a proposed AP600 Integral Test Facility. Before accepting employment with Los Alamos National Laboratory, he was a Senior Staff Member at General Atomic Company where he held technical and management positions working in the High Temperature Gas-Cooled Reactor and the Gas Cooled Fast Reactor programs. He was also employed by the Boeing Company where he applied numerical methods to the solution of engineering analysis problems. He obtained his B.S. and M.S. degrees in Mechanical Engineering from Brigham Young University. He obtained his Ph.D. degree in Mechanical Engineering from Arizona State University and is a registered Professional Engineer in California.

M. L. Corradini

Michael L. Corradini is a professor of nuclear engineering and engineering physics, College of Engineering, University of Wisconsin-Madison. During the last 13 years, he has been engaged in research related to nuclear and industrial safety, with specific emphasis on subjects involving multiphase flow and heat/mass transfer. His current research focuses on vapor-explosion phenomena, jet-spray breakup, and mixing dynamics, as well as heat/mass transfer and chemical reactions involved in molten-core-concrete interactions. He is a Fellow of the American Nuclear Society and was a recipient of the 1990 Young Members Engineering Achievement Award. He serves as a consultant for the NRC Advisory Committee on Reactor Safeguards, as well as for the Department of Energy (DOE) National Laboratories (Los Alamos National Laboratory, Oak Ridge National Laboratory, Idaho National Engineering Laboratory, and Brookhaven National Laboratory), and participates in research with the national and international sponsors. He was a member of the SCDAP/RELAP5 Peer Review Committee. Professor Corradini obtained his B.S. degree in mechanical engineering from Marquette University in 1975 and his M.S. and Ph.D. from the Massachusetts Institute of Technology in 1978. He was a member of the technical staff at Sandia National Laboratories for 3 years before joining the faculty of the University of Wisconsin-Madison in nuclear engineering.

R. S. Denning

Richard S. Denning is Senior Research Leader for Nuclear Facility Safety at Battelle Memorial Institute. Dr. Denning directed the analysis of severe-accident progression and source terms for the Reactor Safety Study (WASH-1400). He subsequently managed the source term reassessment program at Battelle in which the Source Term Code Package was developed. He is a Fellow of the American Nuclear Society. He provided technical assistance to the TMI Special Inquiry Group. He was a member of the NAS committee to

review the safety of DOE's reactors following the Chernobyl accident. He was a member of DOE's Advisory Committee on Nuclear Facility Safety and was Director of ES&H for the Heavy Water Reactor/New Production Reactor project. He received his Bachelor of Engineering Physics degree from Cornell University in 1963 and Ph.D. in Nuclear Engineering Sciences from the University of Florida in 1967.

M. Khatib-Rahbar

Mohsen Khatib-Rahbar is President of Energy Research, Inc., of Rockville, Maryland. His research focuses on nuclear reactor safety and probabilistic risk assessment. He has published extensively on severe accidents, source terms, methods for uncertainty analysis, consequence assessment, thermal-hydraulics, and numerical methods. He has also developed computer models for simulation of thermal-hydraulics and neutronics transients in LWRs and LMFBRs. He was a member of the MELCOR and SCDAP/RELAP5 Peer Review Committees. Before founding Energy Research, Inc., he was a staff scientist at Brookhaven National Laboratory, where he managed programs dealing with level 2/3 PRA reviews, verification and benchmarking of STCP and MELCOR, source term uncertainties (QUASAR), Zion/Draft NUREG-1150, and regulatory implications of new source terms. He was a visiting scientist at Gesellschaft fur Reactorsicherheit (GRS) in Germany (1982), and the NRC Office of Nuclear Regulatory Research (1988-89). He is currently a consultant to the US Department of Energy, the US Nuclear Regulatory Commission, the Swiss Federal Nuclear Safety Inspectorate, and several national laboratories and private organizations. He received his Bachelor of Chemical Engineering degree from the University of Minnesota in 1974 and his Ph.D. degree in Nuclear Science and Engineering from Cornell University in 1978.

S. K. Loyalka

Sudarshan Loyalka is Curators' Professor of Nuclear Engineering, Chemical Engineering and Mechanical and Aerospace Engineering, and Director of the Particulate Systems Research Center at the University of Missouri-Columbia (MU), Columbia, Missouri. His research interests are in aerosol mechanics, the kinetic theory of gases, transport theory, and neutron reactor physics and safety. He is a member of the editorial board of the journal *Progress in Nuclear Energy* and served earlier as chairman of the Working Group on Aerosol Physics for the American Association for Aerosol Research and on the editorial board of the journal *Aerosol Science and Technology*. He has authored approximately 150 research papers and the recently published research monographs, Aerosol Science: Theory and Practice (Pergamon, 1991) with M. M. R. Williams, and Indoor Air: Quality and Control (Prentice-Hall, 1993) with A. Hines, T. K. Ghosh, and R. C. Warder. He received his B.S. in Mechanical Engineering from the University of Rajasthan, India (1964), and M.S. and Ph.D. in Nuclear (Mechanical) Engineering from Stanford University in 1965 and 1967, respectively. He has been at MU since 1967 and he was a visiting scientist at the Max Planck Institut fur Stromungsforschung, Gottingen, Germany during 1969-71. He is a Fellow of the American Physical Society (since 1982) as well as the American Nuclear Society (since 1985), and is a registered Professional Engineer in Missouri.

P. N. Smith

Paul Smith is a principal scientist in the Reactor Safety Studies Department of Consultancy Services, AEA Technology, Winfrith, United Kingdom. He is currently Section Manager of the Gas-Cooled Reactor and Degraded Core Section and coordinates AEA Technologies programs of gas-cooled reactor severe-accident research. For the previous 9 years he was manager of the Containment Section, where for 8 of the 9 years he used the CONTAIN code. Before moving to AEA Technology, Dr. Smith worked for 2 years in the Physics Department of Exeter University, and before that worked 2 years for a scientific consulting company (SCICON). Dr. Smith obtained a degree in mathematics and maths, part III, at Cambridge University, before moving to Hull University where he obtained a Ph.D. in applied math. He is a member of the Aerosol Society.

APPENDIX B

CONTAIN Document Database

This database identifies documentation of the CONTAIN code and its applications. Citations are collected into the following 10 categories:

- Reports (Sandia National Laboratories, Albuquerque, NM)
- Reports (Other)
- Journal Articles (Sandia National Laboratories, Albuquerque, NM)
- Journal Articles (Other)
- Papers (Sandia National Laboratories, Albuquerque, NM)
- Papers (Other)
- Correspondence and Memoranda
- Presentation Materials (Sandia National Laboratories, Albuquerque, NM)
- Presentation Materials (Other)
- Other

These 10 categories, in the order given, identify CONTAIN-related information sources in order of decreasing formality. Those items introduced with entries of the form [XXXYY] are listed in a database maintained by Sandia National Laboratories, Albuquerque, NM.

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APPENDIX C

Summary of Ex-Vessel Severe-Accident Phenomena for CONTAIN

The CONTAIN Peer Review process is described in Sec. 1.3. This process included several elements that formed the essential basis for accomplishing the Committee's objectives of: (1) developing findings regarding the adequacy of the CONTAIN code, and (2) assigning priorities to the Committee's findings for correcting code deficiencies. To support the Committee's first objective, it was essential that the ex-vessel severe-accident physiochemical processes and phenomena be identified. In this manner, the completeness of the CONTAIN code could be assessed by the Committee. However, additional insights beyond completeness were needed in support of the second Committee objective. If all processes and phenomena were modeled in equal detail, enormous resources would be required to (1) develop the scientific database for understanding and modeling each process or phenomena, (2) develop and demonstrate the adequacy of each analytical model developed to represent each process or phenomena, and (3) integrate and demonstrate the adequacy of the integrated code. Fortunately, when measured against key figures of merit such as containment source terms and containment temperature and pressure loads, not all processes and phenomena are of equal importance. Thus, the Committee first identified and listed ex-vessel severe-accident processes and phenomena and then ranked the phenomena with respect to importance using the key figures of merit of containment source terms and loads. Both the identification and ranking of phenomena represent the collective judgment of the Committee members. However, the identification of ex-vessel severe-accident processes and phenomena built upon the earlier MELCOR Peer Review effort (Ref. C-1).

A decomposition of ex-vessel severe-accident physiochemical processes and phenomena is presented in Fig. C-1, and consists of nine individual diagrammatic representations of the dominant ex-vessel severe-accident phenomena. Scenarios characterizing both high- and low-pressure introduction of molten core and metallic elements into the containment were considered by the Committee. The initial diagram, Fig. C-1.a, summarizes the severe accident as a progression through a series of ex-vessel events that can challenge the containment. These events are arranged as time progresses, in the order that might occur in containment after the reactor pressure vessel (RPV) fails. Because the challenge to containment by such loadings may extend from seconds to tens of hours after vessel breach, this set of events involves a progressively larger degree of system interactions. Each major physical process (e.g., fuel dispersal interactions by high-pressure melt ejection at high RPV pressures, which leads to DCH and non-energetic FCI at low RPV pressures) is shown in subsequent diagrams (Figs. C-1.b through C-1.i) that are keyed to Fig. C-1.a. A brief description of each of these key processes and is provided in Table C-I.

As summary tabulation of bottom-up review results is tabulated in Table C-II. This table summarizes many of the key findings of the CONTAIN Peer Review effort bottom-up review effort. The bottom-up review process and its relationship to the top-down review effort is described in Secs. 1.3.9 through 1.3.11. The following information is included in the table: (1) a listing of ex-vessel severe-accident processes and phenomena, (2) the sections of this report in which the Committee's findings (detailed in Sec. 2 and App. D) are found, (3) the importance of the processes or phenomena to containment source terms or loads, (4) an assessment of the current state of scientific knowledge regarding the process or phenomena, (5) the order of the CONTAIN model for the process or phenomena, (6) the validation status of the CONTAIN model, and (7) the Committee's finding of the models technical adequacy. Further information regarding the Committee's

perspective on how the state of scientific knowledge affects review findings is found in Sec. 1.3.6. Further information regarding order of code models and how this information affects findings of adequacy is also found in Sec. 1.3.6.

The information summarized in Table C-II helped the Committee to develop recommendations for correction of CONTAIN deficiencies and assign priorities to these recommendations. In general the following logic was applied. A high priority was assigned to the correction of those model deficiencies for which (1) the process and/or phenomena being modeled were highly important in determining containment source terms or loads, (2) the scientific knowledge of the process or phenomena was sufficiently advanced to permit modeling with a model of appropriate order, and (3) the existing CONTAIN model was either missing or inadequate.

The following information is provided as a guide to the content of Table C-II. The individual ex-vessel phenomena are listed in their order of appearance in the first column. The table then lists in the second column (Reference Sections) the location of the summary description of each process or phenomenon and its summary assessment in the main report and detailed in App. D. The next column (column A) presents the committee's judgment as to how important the process or phenomenon is to the magnitude of the containment source term and loading. Columns B to E give the Committee's collective judgment on each process or phenomenon related to the scientific communities knowledge of the physics (column B), the order of the CONTAIN model representing the process or phenomenon (column C), the validation status of the CONTAIN model (column D), and the Committee's assessment of the model's technical adequacy (column E). Additional information regarding the entries in the table follows.

Importance in setting the levels of the containment source terms and loads	5	- Most important
	3	- Moderately important
	1	- Unimportant
Knowledge of Physics	U	- Understood
	Q	- Questionable
	P	- Poorly Understood
Order of Model	1	- First Order
	O	- Zeroeth Order (Parametric)
	CF	- Control Function
	NM	- No model
Validation Status	V	- Validated
	VI	- Validation Incomplete
	T	- Tuned (Fitted) to Integral Data
	ID	- Insufficient Data
Technical Adequacy	1 to 7	- Defined in Sec. 1, Table 1-I

The Committee's perspective on physics or "physical processes" is discussed in Sec. 1.3.7. The Committee perspective on the "Order of Model" is also discussed in Sec. 1.3.7. When evaluating the validation status, the Committee assigned a classification of "Validation Incomplete" if any of the following were judged to be true: (1) data are available but have not been fully utilized, (2) the empirical nature of the model is not considered universal, even though the model has been assessed against the available data, because knowledge of the physical process or phenomenon is sufficiently uncertain, and (3) validation has been attempted but the validity of the model has not been established.

Several models related to Aerosol Transport/Retention (Severe-Accident Phenomena Group VIII in Table 2-I) and Vapor Fission Product Transport (Severe-Accident Phenomena Group IX) were not evaluated by the Committee. Evaluations were not performed because the models do not exist in the CONTAIN code and the revised CONTAIN design objectives associated with the revised severe-accident code strategy (App. E) dictate that there be no further CONTAIN model development effort related to these phenomena.

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Table C-I
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
I. Direct Containment Heating	a. Melt ejection from RPV	Melt ejection initiates the ex-vessel transient. The size of the breach and the reactor system pressure governs the melt ejection rate. The magnitude of the direct containment heating processes are directly related to the amount of melt material that is ejected into the cavity below the reactor pressure vessel (RPV).
	b. Melt oxidation by gas	Containment air (for non-inerted containments) and large amounts of steam participate in oxidation reactions with the high-temperature melt. The melt may be airborne due to sweepout or non-airborne due to settling.
	c. Melt sweepout of cavity	The dynamic pressure of blowdown gases in the reactor cavity is an important mechanism leading to melt sweepout of the cavity (dispersal) and breakup. Gas bubbles also exist in the melt. Pneumatic atomization of the melt can enhance fragmentation. The amount of sweepout is related to blowdown gas flow rates.
	d. Drop entrainment/fragmentation	Some of the melt mass ejected from the vessel will be in droplets. Both the blowdown gas and gases generated from oxidation reactions move to lower pressure compartments entraining some droplets and further fragmenting liquid. Some drops may be entrained from melt materials that have adhered to surfaces.
	e. Melt-water interaction	Several types of interactions apply. Melt-water heat transfer is a heat sink for debris energy, but a vapor source, and melt may solidify. Steam is produced and available for melt oxidation reactions. The presence of water may affect dispersal patterns. Water slugs may be produced. This process is different from a vapor explosion, since the continuum is likely vapor.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
	f. Fission product release	Fission products released from core materials to steam and water inside the RPV will be released with the blowdown gas. Melt oxidation reactions will result in further releases. Diffusive mechanisms along the concentration gradient will contribute only slightly to fission product release.
	g. Cavity pressurization	Mechanisms for cavity pressurization include gas ejection from the RPV, melt-gas heating, melt-water interactions, and melt-concrete interactions. The rate of pressurization is affected by cavity and compartment volumes and the connecting flow pathway characteristics.
	h. Melt trapping and carryover	The flow of gases (blowdown and generated) carry entrained melt from the cavity, into and through compartments, and into the containment dome; this is the process of carryover. However, some of the melt is not carried along; it is "trapped." Examples of trapping processes include impact and sticking on surfaces and deentrainment.
	i. Melt-debris-gas interaction	This process involves heating of the gas by the melt debris as debris flows through the containment atmosphere.
II. Non-energetic fuel coolant interaction	a. Melt fragmentation in water	The melt jet entering the water pool begins to break apart due to hydrodynamic forces as well as the vapor generation rate.
	b. Melt-water heat transfer	Melt immersed in water loses heat to the water as it solidifies and quenches. The heat transfer rate depends upon the excess melt temperature, water temperature, contact area, and melt velocity.
	c. Melt oxidation	The melt interacts with water to produce steam, which in turn participates in melt-water oxidation reactions with the high temperature.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
III. Molten core-concrete interaction	a. Energy generation	The melt pool releases energy due to the decay of the fission products in the molten core. This decay heat is the major heat source, which must be removed from containment.
	b. Crust formation/ freezing	As the molten pool upper surface radiatively cools or as water is added to the reactor cavity containing the corium melt, the melt pool will begin to cool and will form a crust. The stability, porosity, and permeability of this crust or "crust-like debris" will determine the coolability of the molten corium pool below it if water ingression continues or debris expulsion occurs to achieve pool quench.
	c. Heat transfer (concrete/bulk)	Heat transfer from the high-temperature melt to underlying concrete or to the upper pool surface is by convection induced by bubble agitation in the pool and at its interface. The overlying melt heats the concrete by conduction, causing concrete decomposition. Gases are generated from the concrete heating processes and the concrete surface recedes (ablates).
	d. Hydrodynamics in pool (swell/mixing)	Evolved gases from the MCCI percolate through the overlying pool as gas bubbles and slugs. The movement of evolved gases promotes mixing in the overlying pool, and causes the liquid pool level to swell. The amount of level swelling and mixing increases with increasing gas generation rates.
	e. Chemical reactions	As gas passes through the molten pool it can undergo chemical reactions as gases are reduced and metals are oxidized. In addition the gas stirring induces condensed phase chemical reactions between oxide and metals.
	f. Material properties	Material properties are generally not considered a phenomenon. However, the solidus and liquidus temperature, solids fraction and apparent viscosity of molten mixtures need phenomenological models, and are of particular importance for the MCCI.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
	g. Melt-debris spreading	The high-temperature molten "corium" mixture overlying the concrete basemat spreads laterally until either vertical surfaces are reached or the melt surface tension balances the gravitational forces inducing the lateral spreading. (Coolability is not considered since its actual existence is in question.)
	h. Fission product release	Gas evolved from concrete decomposition percolates through the overlying melt. The major release mechanism is by vapor transport carried out by bubbles through the melt. There is also some physical atomization by the bubbling process at the melt surface.
IV. Combustion	a. Ignition criteria	Ignition criteria depend upon gas composition (hydrogen, carbon monoxide, and oxygen) and whether igniters are present. High-temperature data has yet to be obtained.
	b. Mode of combustion	The decision logic for choosing which mode of combustion, (e.g., diffusion flame, hydrogen recombination, or deflagration) will occur. Nature employs a decision logic based upon physical reality. Computer models attempt to codify the scientific perception of nature's decision logic.
	c. Diffusion flame	A mode of low-speed combustion in which a standing gas flame characterizes the combustion process.
	d. Bulk spontaneous recombination	A mode of low-speed combustion (auto-ignition) that may occur should there be large and rapid increases in the temperature of the containment atmosphere, e.g., resulting from a DCH event or the passage of large concentrations of hot debris through the containment atmosphere. The auto-ignition temperature is a function of the stoichiometry of the mixture and diluent concentrations. This process can occur during diffusion flame burning, but not deflagration.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
	e. Deflagration	A mode of low-speed combustion (e.g., in contrast to detonation) in which combustion is accompanied by the vigorous evolution of heat and flame.
	f. Combustion completeness	Local completeness is the degree to which the available combustible material in a small volume (e.g., a compartment) has been consumed. Global completeness is the degree to which the available combustible material in a large volume (e.g., compartment) of containment has been consumed. The burning rate is dependent upon the completeness and speed with which the flame front propagates through the combustible mixture.
	g. Propagation in multi-compartments	It is possible for a burn to propagate from one compartment to another if a path is available and the combustible gas, oxygen, and water vapor concentrations in the adjacent compartment allow propagation.
	h. Combustion effect on fission product release	Combustion processes can affect fission product releases. For example, the temperature increases associated with combustion can vaporize compounds, change chemical state, and produce airborne fission products and the passage of vigorous flame fronts can resuspend radioactive materials.
V. Ex-Vessel Transport	a. Materials properties	Material properties are not phenomena. However, uncertainty in material properties may contribute to uncertainty in the estimates of some phenomena.
	b. Water pool phenomena	When water pools exist, either by design as in BWR suppression pools, as the result of planned operations as in operation of containment spray systems, or by accident as in piping breaks, there is a potential for gas blowdown or leakage through the pool that can markedly affect the outcomes of energy transport.
	c. Structure conduction	Heat transfer to structure via conduction is a mechanism for removing energy from the interface of the containment surface.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
	d. Structure radiation	Heat transfer to containment surfaces via radiation is a mechanism for removing energy that could otherwise affect the containment pressurization rate. Radiative transport can occur due to hot gases or fuel debris.
	e. Steam mass transfer	Gradients in concentration create a potential for mass transfer. Condensation in a stagnant environment is an example of mass transport arising from concentration differences. Boundary layer fog formation is not considered.
	f. Free and forced convection	Movements of the containment atmosphere caused by buoyant forces arising from temperature and/or density differences. Movement of the containment atmosphere caused by mechanical equipment or pressure differences, e.g., fan coolers.
	g. Thermodynamics	These are processes that involve the relationship between calculated properties (p,T) and other thermodynamic properties as well as energy and mass balances.
	i. Intercell flow model	Intercell natural circulation is the movement of atmosphere from cell to cell caused by buoyant forces arising from temperature and/or density differences. Intercell forced circulation is the movement of atmosphere from cell to cell caused by mechanical equipment (e.g., fans) or pressure differences due to gas introduction.
	j. Stratification	The layering of fluids or gases in the vertical direction. Liquid stratification occurs when hot liquid overlies a cold liquid. Gaseous stratification occurs when a lower density gas overlies a higher density gas.
VI. ESFs	a. Ice condenser	This ESF serves to limit containment over-pressure by condensing steam released from the primary system in a large ice chest. In addition, ice-condenser systems are effective in reducing through growth and deposition of fission product aerosols in gas streams passing through the ice condenser.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
b. Containment sprays		Containment sprays rapidly absorb thermal energy in the containment, thereby cooling the containment atmosphere and reducing pressure. These liquid sprays also remove aerosols, fission products hosted to aerosols, elemental iodine, and less reactive organic iodine compounds from the containment atmosphere.
c. Suppression pool		In BWR designs, this ESF serves to limit containment overpressure by condensing steam released from the primary system in a large pool of water. In addition, the pool is effective in reducing fission product aerosols in gas streams released into the pool.
d. Containment fan coolers		Fans in the system draw the containment atmosphere through the banks of finned, service-water-cooled coils. The coolers remove heat from the containment atmosphere. Because of the relatively cool surfaces and high condensation rates provided by fan coolers, substantial scrubbing of aerosols can occur.
e. PCCS for ALWRs		For the AP600 design, steam in the containment atmosphere condenses on the inside surface of the steel containment and condenses. The condensate flows downward to drains where it is directed to the in-containment refueling water storage tank. Some fraction of the airborne fission products will be removed from the containment atmosphere during the condensation process. For the SBWR design, a suppression pool, a gravity driven cooling system pool, and an isolation condenser/PCCS pool are employed. For loss of coolant events, the suppression pool absorbs the blowdown energy, the reactor is depressurized, and the gravity driven cooling system floods the reactor and the isolation condenser removes decay heat. Fission products are retained in the heat exchanger and any remaining noncondensable gases and liquid condensate are deposited in the suppression pool components. The PCCS provides long-term passive cooling using natural circulation.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
VII. Containment Failure Model		
	a. Local leakage rate	The failure mode is such that the containment pressure remains above the atmospheric pressure outside the containment. The rate of fission product release is smaller than for a gross failure but the duration of the release (considering only the available fission product inventory at the time of containment failure) will be longer.
	b. Gross failure	The failure mode is such that the containment pressure rapidly depressurizes to the atmospheric pressure outside the containment. The rate of fission product release is large for a short time but falls rapidly once the containment depressurizes to the atmospheric pressure.
VIII. Aerosol Transport and Retention		
	a. Size composition and distribution	Essentially all aerosol transport and retention processes are affected by particle composition and size distribution. For example, larger particles are more likely to settle under the influence of gravity and smaller particles.
	b. Agglomeration	Agglomeration processes, that is processes by which particles come into contact with each other, meld into a single particle of larger size, occur in several ways. These include Brownian, gravitational, and turbulent agglomeration.
	c. Deposition	Deposition is a process by which particles move from the aerosol to liquid or solid surfaces. Specific mechanics include gravitational settling, diffusional deposition, thermophoresis, and Stefan flow/diffusiophoresis. The later mechanism is defined as the migration of aerosol particles to surfaces in the flux of coolant vapor condensing on the surfaces. These processes occur naturally and also during operation of the ESFs.
	d. Steam condensation	Condensation of water vapor onto aerosols.
	e. Removal by ESFs	Condensation and deposition are processes by which aerosols are removed from the containment atmosphere by ESFs such as containment sprays, ice condensers, and suppression pools.

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
	f. Resuspension	Previously suspended material may be re-suspended if sufficient force is applied to overcome the physical processes binding them to a surface. Resuspension can occur, for example, if the underlying surface is heated or if gas moves across the surface at a sufficiently high velocity.
	g. Surface physical reactions	Physical reactions carried out on the surface of particles that either adsorb/absorb gases and other particles or react with them.
	h. Intraparticle chemical reactions	Chemical reactions transmutations that occur in the interior of particles and that can transform the composition/properties of the particles.
	i. Charge effects	Charged particles have associated force fields that affect aerosol behavior. Like charges repel and opposite charges attract.
IX. Vapor Fission Product Transport	a. Noble gas	Monatomic gases (e.g., helium, argon, krypton) that are, with limited exceptions, chemically inactive, but which are radioactive.
	b. Organic iodide source	Inorganic iodine species can react with a variety of organic compounds to produce organic iodides. Both gas-phase reactions and surface reactions may contribute to the formation of organic iodides. The nature of reactions involving organic iodides is dynamic. Processes include sorption and desorption of iodine species, desorption of organic species prior to reactions with iodine, radiation-induced formation and decomposition of organic compounds, and organic compounds containing iodine.
	c. Organic iodide retention	Organic iodides can be removed from the inventory available for release to the atmosphere by interactions with various surfaces and materials (steel components and paints).
	d. Volatile iodine	Gaseous iodine in forms such as I_2 and CH_3I . Deposition on aerosols and surfaces may be a significant process for removing gaseous iodine

from the containment atmosphere. Deposition

Table C-I (Continued)
Description of Ex-Vessel Phenomena

Topic	Ex-Vessel Phenomena	Description
		includes mass transport to the surface (absorption), revaporization from the surface (desorption), and possibly chemical reaction with the surface material.
	e. Retention by ESFs	Fission products may be removed from the containment atmosphere by physical processes inherent to the ESFs, e.g., condensation, deposition, and agglomeration.
X. Fission Product Characterization	a. Transmutation	A nuclear process in which one nuclide is transformed into the nuclide of a different element, e.g., a process of nuclear transformation.
	b. Fission product grouping	For typical reactor analysis, identifying and tracking individual nuclides is a large task and, depending on the focus of the analysis, may be unnecessary. Fission product groups are defined that represent the gross characteristics of the individual nuclides in the group and the group history is tracked.
	c. Decay heat	Heat produced by the decay of radioactive nuclides.

Table C-II
Summary of Ex-Vessel Severe-Accident Phenomena and Adequacy of CONTAIN Models

SEVERE-ACCIDENT PHENOMENA	Reference Sections	A ^{note 1}		B ^{note 2}	C ^{note 3}	D ^{note 4}	E ^{note 5}
		ST Imp	CL Imp	Know Phy.	Order Mod	Validate	Tech Adeq
I. Direct Containment Heating							
a. Melt Ejection from RPV	2.4,D.4	3	5	Q	1	V	2
b. Melt Oxidation by Gas	2.4,D.4	3	5	U(Q)	1(0)	V(T)	1 (2)
c. Melt Sweepout	2.4,D.4	3	5	Q	0	T	2
d. Drop Entrainment/Fragmentation	2.4,D.4	3	5	P	0	VI	3
e. Melt-Water Interactions	2.4,D.4	1	5	Q	CF	VI	4
f. Fission Product Release	2.4,D.4	3	0	Q	CF	ID	4
g. Melt Trapping and Carryover	2.4,D.4	3	5	Q	1	VI	2
h. Melt-Debris-Gas Heat Transfer	2.4,D.4	3	5	U	1	V	1
II. Non-Energetic Fuel-Coolant Interaction							
a. Melt Fragmentation in Water	2.4,D.4	1	5	Q	CF	ID	4
b. Melt-Water Heat Transfer	2.4,D.4	1	4	Q	CF	VI	4
c. Melt Oxidation	2.4,D.4	1	3	Q	CF	VI	4
III. Molten Core-Concrete Interaction							
a. Energy Generation	2.3,D.3	4	5	U	1	T	1
b. Crust Formation/Freezing	2.3,D.3	4	5	Q	0	VI	2
c. Heat Transfer (Concrete/Bulk) ^{note 6}	2.3,D.3	3	5	Q	1	VI	2
d. Hydraulics in Pool (Mixing/Swell) ^{note 7}	2.3,D.3	1	4	Q	1	VI	2
e. Chemical Reactions	2.3,D.3	4	5	Q	1	VI	2
f. MCCI Material Properties	2.3,D.3	4	5	Q	0	VI	2
g. Melt Debris Spreading	2.3,D.3	2	3	Q	CF	ID	4
h. Fission Product Release	2.3,D.3	4	0	Q	1	ID	4

note 1:

5 High importance
3 Moderate importance
0 Unimportant

note 2:

U Understood
Q Questionable
P Poor

note 3:

1 First-order model
0 Zeroeth-order model
CF Control function
NM No model

note 4:

V Validated
VI Validation Incomplete
T Tuned to data
ID Insufficient data

note 5: see Sec. 1, Table 1-1

note 6: Includes bulk pool, melt concrete, and coolant layer heat transfer

note 7: Includes bubble phenomena and interlayer mixing

Table C-II (continued)
Summary of Ex-Vessel Severe-Accident Phenomena and Adequacy of CONTAIN Models

SEVERE-ACCIDENT PHENOMENA (cont'd)	Reference Sections	A		B	C	D	E
		ST Imp	CL Imp				
				Know Phy.	Order Mod	Validate	Tech Adeq
IV. Combustion							
a. Ignition Criteria	2.7,D.7	2	5	U	1	V	2
b. Mode of Combustion	2.7,D.7	2	5	Q	0	VI	2
c. Diffusion Flame	2.7,D.7	2	3	Q	0	VI	2
d. Bulk Spontaneous Recombination	2.7,D.7	2	4	Q	0	ID	2
e. Deflagration	2.7,D.7	2	4	Q	0	VI	2
f. Combustion Completeness	2.7,D.7	2	4	Q	0	VP	2
g. Propagation in Multi-Compartments	2.7,D.7	2	3	Q	0	ID	5
h. Combustion Effect on FP Release	2.7,D.7	2	0	P	CF	ID	3
V. Ex-Vessel Transport							
a. Materials Properties	2.1,D.1	2	3	U	1	V	1
b. Water Pool Phenomena	2.2,D.2	3	3	U	1	VI	1
c. Structure Conduction	2.8,D.8	3	4	U	1	V	1
d. Structure Radiation	2.8,D.8	4	3	U	1	V	1
e. Steam Mass Transfer	2.8,D.8	5	5	U	1	V	1
f. Free/Forced Convection	2.8,D.8	5	3	U	1	VI	1
g. Thermodynamics	2.8,D.8	3	5	U	1	V	1
h. Intercell Flow	2.2,D.2	5	5	U	0	VI	4note 8
i. Stratification	2.2,D.2	2	4	U	0	VI	4note 8
VI. Engineered Safety Feature Thermal-Hydraulics							
a. Ice Condenser	2.10,D.10	1	5	Q	0	ID	2
b. Containment Sprays	2.10,D.10	1	5	U	1	VI	1
c. Suppression Pool							
Flow	2.9,D.9	1	5	U	1	VI	1
Vent	2.9,D.9	1	5	U	0	VI	4
d. Containment Fan Coolers	2.10,D.10	1	4	U	1	ID	1
e. PCCS for ALWR							
PWR	2.10,D.10	1	5	U	0	ID	1
BWR	2.10,D.10	1	5	Q	0	ID	2

note 8 Evaluation based upon the original CONTAIN design objectives. However, based upon the revised CONTAIN design objectives associated with the revised severe accident code strategy (Appendix E), this model is adequate.

Table C-II (continued)
Summary of Ex-Vessel Severe-Accident Phenomena and Adequacy of CONTAIN Models

SEVERE-ACCIDENT PHENOMENA (cont'd)	Reference Sections	A ST Imp	CL Imp	B Know Phy.	C Order Mod	D Validate	E Tech Adeq
VII. Containment Failure Modes							
a. Local Leakage Rate	2.2,D.2	3	5	U	0	ID	4 ^{note 8}
b. Gross Failure	2.2,D.2	4	5	U	1	V	1
VIII. Aerosol Transport/Retention							
a. Size and Composition Distribution	2.5,D.5	4	1	Q	1	ID	4
b. Agglomeration	2.5,D.5	4	1	Q	1	ID	4
c. Deposition	2.5,D.5	5	1	Q	1	ID	4
d. Steam Condensation	2.5,D.5	4	1	U	1	ID	4
e. Removal by ESFs-Suppression Pool	2.5,D.5	5	1	U	1	VI	4
Ice Condenser	2.5,D.5	5	1	Q	0	ID	2
Containment Spray	2.5,D.5	5	1	U	0	ID	4
f. Resuspension		3	1	P	Not Evaluated ^{note 9}		
g. Surface Physical Reactions		3	1	Q	"		
h. Surface Intraparticle Chemical Reactions		4	1	Q	"		
i. Charge Effects		3	1	Q	"		
IX. Vapor Fission Product Transport							
a. Noble Gas		4	1	U	Not Evaluated ^{note 9}		
b. Organic Iodide Source		4	1	Q	"		
c. Organic Iodide Retention		4	1	Q	"		
d. Volatile Iodine		4	1	Q	"		
e. Retention by ESFs		5	1	Q	"		
X. Fission Product Characterization							
a. Transmutation	2.6,D.6/Sec. 5.2	3	1	U	1	V	1
b. Fission Product Grouping	2.6,D.6/Sec. 5.2	3	1	U	1	V	1
c. Decay Heat	2.6,D.6/Sec. 5.2	3	1	U	1	V	1

^{note 9} Evaluations were not performed because the model did not exist in CONTAIN and the revised CONTAIN design objectives associated with the revised severe accident code strategy (Appendix E) discontinue further CONTAIN model development related to these phenomena.

Fig. C-1.a.
Ex-vessel phenomena schematic.

Fig. C-1.b.
Direct containment heating.

Fig. C-1.c.
Energetic FCI.

Fig. C-1.d.
Ex-vessel transport models.

Fig. C-1.e.
Non-energetic FCI.

Fig. C-1.f.
Engineered safety features.

Fig. C-1.g.
Core-concrete interactions.

Fig. C-1.h.
Fission product vapor transport and associated retention mechanisms.

Fig. C-1.i.
Aerosol transport and retention mechanisms.

Fig. C-1.j.
Combustion processes.

Fig. C-1.k.
Containment failure modes.

APPENDIX D

Detailed Review of CONTAIN Phenomenological Models

In Sec. 1.3.9., the Committee's process for reviewing the technical adequacy of the CONTAIN code was described. The Committee performed two review actions. A bottom-up review was conducted by examining the pedigree, applicability, and fidelity of the many individual phenomenological models in CONTAIN. This was accomplished by reviewing the CONTAIN code documentation and other related literature from the CONTAIN Document Database (App. B). The adequacy of each phenomenological model or correlation was assessed and classified according to the definitions presented in Table 1-I. The results of the bottom-up review of the CONTAIN phenomenological models are presented in the remainder of this appendix. For each phenomenological model, the following Committee review findings are documented.

1. Model Description and Pedigree
2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena
3. Results of Model Sensitivity Studies
4. Results of Benchmarking/Validation Studies
5. Identified Deficiencies and Options for Model Improvements
6. Importance of Model to Prediction of Dominant Phenomena
7. Technical Adequacy of Model and Documentation

References cited in the reviews are presented at the conclusion of each section or subsection, as appropriate. The section or subsection to which the references apply are clearly identified.

Table C-I (App. C) summarizes the technical adequacy of each phenomenological model reviewed by the Committee. This information is tabulated against the Committee's decomposition of ex-vessel severe-accident physiochemical phenomena. Additional columns in Table C-I also contain important information. The Committee's importance ranking for the ex-vessel phenomena relative to two figures of merit, containment source terms and containment loads, is provided. The Committee's assessment of the degree to which the physics of the associated ex-vessel severe-accident phenomena are understood by the scientific community and the order of the CONTAIN phenomenological model are also tabulated. The degree to which the physics are understood and the order of the model are directly linked to the technical adequacy categorization as defined in Table 1-I (Sec. 1).

The results of the top-down review of the applicability and fidelity of the total code are documented in Secs. 3 and 4.

D.1. Material Properties

D.1.1. Model Description and Pedigree

The materials properties routines used in CONTAIN are described in Sec. 3 of the CONTAIN manual (Ref. D.1-1). A library of physical properties for 50 standard materials that can be used in the modeling of containment systems is part of the CONTAIN code. This library provides temperature-dependent specific enthalpy, specific heat, density, viscosity, and thermal conductivity for these 50 materials that may be found in nuclear reactor containments under severe-accident conditions. Table 3-1 (Ref. D.1-1) lists the standard materials available in the CONTAIN code and the corresponding code name for

each material in the library. Viscosity functions are not included for solids, and gas densities are determined from the ideal gas law. The reader is referred to App. B (Reports - Sandia National Laboratories, Albuquerque, NM, Ref. VAL88b) for the complete listing of each correlation as coded into the CONTAIN model. The source of these properties are several [e.g., the CRC Handbook (Ref. D.1-2) and MATPRO (Ref. D.1-3)] and the various property tables for specific chemical species (e.g., water and steam from the ASME Steam Tables). Some of the properties for each material have not been revised or have not been supported since Version 1.1. These are clearly noted for the analyst in the aforementioned table. The properties for water are divided into water liquid and vapor properties with this approach; thus one must be clear as to what is being modeled. Also averaging of mixtures of properties are accomplished according to accepted procedures for thermophysical properties (by mass fraction) and transport properties (by mole fraction). One should note that the molar averaging done for viscosity and thermal conductivity of gases is a gross simplification of the actual practice as noted in Ref. D.1-4. However, such simplification does not have a significant effect on the simulation results. In addition, the dimensionless properties are given according to generally accepted definitions. Both the mixture relations and the dimensionless properties can be found in various texts on transport phenomena (e.g., Ref. D.1-4).

D.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The methods used for specifying material properties and the property values seem quite reasonable. The sources for these properties are well established from past efforts in high-temperature material properties (e.g., MATPRO). However, the CONTAIN manual notes that the standard material property library cannot be used to specify the properties for the debris species used in the DCH model within CONTAIN, nor is it needed for the properties used for the MCCI process in CORCON. In some cases, the properties in the DCH and CORCON module of CONTAIN are simpler approximations for the properties used in the CONTAIN material library; e.g., constant density or specific heat for the fuel in the DCH material properties or constant thermal conductivities and surface tensions in the CORCON material properties. In other cases, the DCH and CORCON modules of CONTAIN use property expressions with a greater level of detail; e.g., specific heat, enthalpy and phase transitions for condensed phase species used in CORCON. The Committee feels that this may result in possible inconsistencies between modules within CONTAIN, and must be checked and corrected so that a consistent properties database is used within the DCH, MCCI, and other parts of CONTAIN. SNL staff maintained that inconsistencies will not arise because a given application will not access multiple material routines. Nevertheless, it is Committee's impression that the results of CONTAIN simulations will not significantly change, but some logic of consistency will have been established. If this is determined to be too difficult to accomplish, the user should be given better advice to avoid inconsistencies. Also, the manual should indicate the precise source of mixture relations for thermophysical and transport properties.

The materials properties are located in separate subroutines or common blocks within the code and can be easily accessed and modified. A possible difficulty may be that the property routines are not in one location, but spread throughout the code software.

D.1.3. Results of Model Sensitivity Studies

No specific sensitivity studies were found in the manual.

D.1.4. Results of Benchmarking/Validation Studies

There were no specific validation studies presented in the formal documentation. However, the presentation by Dr. Ken Murata (see App. B, Presentation Materials (Sandia National Laboratories, Albuquerque, NM, First Meeting of the CONTAIN Peer Review Committee, May 24-27, 1993, Albuquerque, NM, presentation 1-11) indicated that the property routines used in CONTAIN are quite accurate (within 5-10%) for the available data on specific material compositions or the approximations made seemed acceptable for less well-known property values. The committee has made spot checks of certain properties of certain materials and has found good agreement with handbook values. This acceptability extends to some of the CORCON data. However, this is discussed in the section on MCCI behavior.

D.1.5. Identified Deficiencies and Options for Model Improvements

The possible inconsistency between CONTAIN property routines and those used for DCH and CORCON modules has been noted above in Sec. D.1.2. There is only one option, and that is for a staff member or some independent consultant to do a comparison of property routines from similar chemical species between CONTAIN, DCH models, and CORCON, determine the agreement or lack thereof, and then make these formulations consistent or eliminate the duplication. As far as the Committee is aware, this has not been done.

D.1.6. Importance of Model to Prediction of Dominant Phenomena

As long as the properties used for various materials have a consistent basis, the importance to prediction of the dominant phenomena is not large. However, if consistency has not been checked, there is no way to be sure that an inconsistency may adversely affect some simulations. Therefore, regardless of importance, consistency must be established between the various CONTAIN, DCH, and CORCON material property routines. The committee does not expect to find any surprises, but it must be done.

D.1.7. Technical Adequacy of Model and Documentation

The material properties used reflect the current state of knowledge of a first-order equation-of-state model for individual materials. The physics is well understood based on materials properties references within the CONTAIN manual and the properties have been validated by direct reference to well-known property tables. The documentation is adequate. Therefore, once possible inconsistencies are alleviated by a comparison of consistency and establishment of a common material properties database for DCH and MCCI as well as the rest of CONTAIN, it is judged to be technically adequate (Category 1).

REFERENCES

- D.1-1. "CONTAIN 1.2 Code Manual: A Computer Code for Severe Accident Analysis," Sandia National Laboratories report SAND94-2358, in preparation.
- D.1-2. R. C. Weast, editor, *CRC Handbook of Chemistry and Physics* (Chemical Rubber Publishing Company, 1984).

- D.1-3. J. K. Hohorst, editor, "MATPRO-A Library of Materials Properties for LWR Accident Analysis," EG&G Idaho, Inc. report NUREG/CR-5273 (EGG-2555), 1990.
- D.1-4. R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena* (John Wiley & Sons, Inc., 1960).

D.2. Atmosphere/Pool Thermodynamic and Intercell Flow Models

D.2.1. Intercell Flow Model

D.2.1.1. Model Description and Pedigree

The atmosphere/pool thermodynamic and intercell flow models are based on a generalized multi-compartment control volume (cell) flow path approach. The containment compartments are divided into multiple cells connected via arbitrary arrangement (through input) of flow paths.

The code solves a simplified set of "lumped-parameter" conservation of mass, momentum, and energy equations. The momentum equation neglects the spatial acceleration and the skin friction terms. It is solved for the gas/atmosphere region only; while the flow of liquid is assumed to occur by gravity in an instantaneous fashion (i.e., all liquid collect at the bottom of the lowest thermodynamic cell). The counter-current flow limitations are also ignored.

The thermodynamics equations of state are based on the ideal gas law. Fits to ASME Steam Tables are used for liquid water. The liquid phase in a saturated atmosphere can remain as suspended droplets, or can drop out either through a user flag or mechanistically as liquid water aerosols. The model allows for explicit mass and energy sources and/or sinks. This includes heat transfer to and from structures or any debris; heat from decay of fission products and chemical reactions in the atmosphere; mass and energy addition from pool boiling, film evaporation and/or atmosphere condensation (on structures, aerosols, spray droplets, etc.); and mass and energy transfer from core-concrete interactions and other user-defined sources and/or sinks.

There are two flow models available in the code to treat "regular" and "engineered vent" configurations. A "regular" flow model allows for a "single" flow path between two connected cells. An "engineered vent" allows for more flexibility in terms of multiple flow paths between two connected cells.

The flow rate in a flow path can be based on:

- (1) The inertial flow model (which includes both implicit and explicit solvers). The model, in its implicit form, allows for critical flow.
- (2) The steady-state (orifice) flow model. This model is applicable to special flow paths in the implicit flow solver and it also allows for critical flow.
- (3) The user-specified flow rate.

The body force term in the CONTAIN momentum equation is defined as (see Sec. 4.2.2 of Ref. D.2-1):

$$\Delta P_{ij} = g [\rho_i (H_i - H_1) + \rho_a (H_1 - H_2) + \rho_j (H_j - H_2)] \quad (1)$$

This definition can introduce errors in predicting natural circulation flows, and has been shown to be incapable of accurately predicting temperature and/or species stratification under simulated conditions. Specifically, within the control volume formulation of the existing system codes, large temperature and/or concentration gradients, such as those that exist under stratified conditions, produce large spurious mixing, which is not physical.

The recent modifications to the CONTAIN flow solver package proposed by Murata (Ref. D.2-2) in response to the concerns expressed by the peer review group are based upon several alternatives to the numerical approximations of $\int \rho dz$ under conditions that variations in ρ are either large or discontinuous along the flow path direction. The approximations investigated included the CONTAIN non-default option (Eq. 1), the CONTAIN default option (use of linear average density between two adjoining cells; $H_i = H_1$ and $H_j = H_2$ in Eq. 1), and the donor density formulation. The proposed approach is based on a "hybrid" of the average density and the donor density numerical approximations depending on the density difference between the cells, and the previous time-step flow direction, corrected for isothermal stratification effects.

Test implementation of the hybrid formulation showed significant improvements in simulation of intercell stratification and natural circulation effects for several test problems and a large scale experiment (Ref. D.2-3).

The lower cell and cavity models primarily deal with liquid and solid layers, and the CORCON-Mod3 has been integrated into the CONTAIN program library (as of March 28, 1994) to model core-concrete interactions. However, before activation of CORCON and after termination of CORCON calculations, the lower cell one-dimensional conduction models are used to calculate heat losses to the lower cell regions.

The lower cell conduction model is solved for multi-layers that include interaction between layers via interlayer heat transfer coefficients. Mass transfer between intermediate layers is not allowed, and the layer material can include concrete, core debris (absent before invoking CORCON and present after CORCON has been invoked), liquid pool, and gaseous atmosphere. The model also includes options for volumetric heating of the lower cell due to fission products, user-specified tables, or make-up decay heat to follow American National Standards Institute standards.

Coolant from all sources end up in the lower cell pool. This can be as a result of sprays, fans, ice condenser, or condensation on internal and boundary structures.

The CONTAIN condensation/evaporation model is used to calculate heat and mass transfer at the pool/atmosphere interface. This model is based on the formulation attributed to Collier (Ref. D.2-4), and includes the effect of diffusion of vapor through the gas-vapor layer. In using the heat and mass transfer analogy, the Grashof number is defined based on the temperature difference and not the density difference. The interlayer heat transfer coefficients are based on standard correlations in the literature. Pool boiling considers the entire boiling curve and uses the curve fits developed for CORCON computer code.

For large failure sizes, the containment failure model requires a user-defined failure location and failure size. The code appropriately calculates the blowdown rate from the containment into the adjoining reactor building or the environment using standard models (i.e., models for critical or sub-critical flow through orifices). However, the present model is inadequate for application to flow through cracks and large tortuous failure paths through concrete walls where a more detailed mechanistic model needs to be developed.

D.2.1.2. Applicability/Physical Reasonableness of Models to Prediction of Dominant Phenomena

In general, the atmosphere/pool thermodynamic and intercell flow models are based on a straightforward lumped-parameter formulation, somewhat simpler than the MELCOR models. Within the framework and limitations of the control-volume approach, the models are physically reasonable and are the backbone of the CONTAIN computer code. These models have been used in simulation of a large number of containment experiments. It has been shown that judicious nodalization and choice of model parameters can lead to adequate prediction of the general trends of the phenomena measured experimentally. Problems were noted during this peer review process, and were based on the SNL benchmarking activities for simulation of light noncondensable gas, temperature stratification, and mixing behavior, which, in turn, led to the development of revised numerical schemes by SNL (Ref. D.2-2).

D.2.1.3. Results of Model Sensitivity and Benchmarking Studies

The code has been used extensively at SNL and numerous other organizations. CONTAIN application to plant accident analyses and experimental assessments are very extensive; however, limited benchmarking of flow models against simple and known problems have been reported.

D.2.1.4. Results of Benchmarking/Validation Studies

Extensive studies have been performed in which CONTAIN results have been compared with experimental data. These include the CONTAIN simulation of HDR, NUPEC, AP600, and other related experiments (Refs. D.2-5-D.2-8).

D.2.1.5. Identified Deficiencies and Options for Model Improvements

The recent hybrid formulation of the buoyancy term (Ref. D.2-2) is based on physical and numerical arguments, which appear reasonable. However, additional application cases are needed to determine all potential pitfalls, and to confirm technical adequacy under conditions of most interest to containment analysis.

Provided the potential pitfalls can be demonstrated to be tolerable, then user guidelines should be developed and the numerical inefficiencies should be improved. For example, the so-called isothermal stratification effects are not believed to be significant for scales of interest in nuclear reactor containments (i.e., $g\rho\Delta H/P \ll 0.001$); therefore, the proposed numerical logic could be simplified by neglecting these effects.

The present control volume approach cannot be used to study mixing and stratification processes in large open volumes (intracell effects), even though the recent hybrid formulation has showed significant improvements in prediction of intercell mixing and stratification effects.

In evaluating the natural convection correlations, the Grashof number should be based on the density difference and not the temperature difference (see Refs. D.2-9 and D.2-10 for details). The choice of the characteristic length scale for the pool/atmosphere interface should be justified.

D.2.1.6. Importance of Model to Prediction of Dominant Phenomena

This is one of the most important models for application to DBA and severe-accident conditions in LWRs. The atmosphere/pool thermodynamic and intercell flow models directly impact prediction of containment pressure and temperature loads under all accident conditions, determine mixing and distribution of gases, and provide boundary conditions to other CONTAIN models such as aerosol transport and heat structure models.

D.2.1.7. Technical Adequacy of Model and Documentation

In many respects the models are approximate, and they are based on solution of a simplified form of fluid momentum equation, and do not account for liquid flow through the flow paths. For the most part, the documentation provides sufficient guidelines for the code users; however, inadequacies were noted in the present draft documentation (Ref. D.2-1). For instance, there is a very limited description of the "liquid drop-out" models in the documentation, the description of the interface between the various model elements is not very clear, and the limitations of the present hydrodynamic formulation are not described.

In general, using the recent hybrid formulation with a judicious nodalization of the problem, the intercell behavior can be reasonably predicted; however, the CONTAIN simple control volume model cannot be used in predicting intracell distributions of flow, temperature, and concentration fields, in large, open volumes. Furthermore, additional experimental validation of the revised buoyancy head formulation is needed to confirm its applicability under all conditions of interest.

Within the limitations of the control volume, lumped-parameter approximation, the intercell flow models are adequate under homogeneous and well-mixed conditions. On the other hand, these simple, zeroeth-order, lumped-parameter models are inadequate under conditions of large thermal and species stratification. The recent numerical fixes introduced in CONTAIN show promise for resolution of intercell distributions; however, the present model is inadequate for prediction of intracell effects. The containment failure model is appropriate for large failure sizes, while it is inadequate for application to flow through cracks and tortuous pathways. Overall, a finding of Category 4 is assigned to the intercell flow, stratification and containment failure models.

It should be noted that under the "revised severe-accident code strategy" (see App. E), the detailed mechanistic specification and accompanying requirements for models to be first order no longer exist. Therefore, with the exception of the identified deficiencies, the intercell flow model is acceptable within the revised severe-accident code strategy and practical constraints on a systems codes. No action to render the intercell flow model first order is recommended.

D.2.2. Water Pool Model

D.2.2.1. Model Description and Pedigree

The water pool model is partially described in Sec. 4.3 of the CONTAIN manual (Ref. D.2-1). It is used as the appropriate CONTAIN model for a source or sink of water associated with transport from ESF systems, existing as a pool layer in the CONTAIN lower cell model, as well as the destination for water film drainage off of structures within the containment, or as overflow locations from other higher water pools. Besides providing

the water inventory for the containment for open pools, it can also serve as the source of water vapor, steam, due to energy input from the core debris within the lower cell model. (It should be noted that the MCCI phenomenon is modeled totally separate as is the coolant layer that may exist for the MCCI by the CORCON module within CONTAIN.) This feature of water pools, to receive energy from core debris or other energy sources, is described in detail in Sec. 4.3 and is termed the "implicit boiling model." This is actually part of the original CONTAIN lower cell model that is less frequently used. The mass of steam produced within a time step is equal to the energy deposited due to decay heat or other energy sources into the water pool divided by the enthalpy required to raise the water from its initial enthalpy to its saturated vapor enthalpy at the control volume (compartment) pressure. Thus, the updated mass of the water pool is set equal to the initial mass plus any water added (or subtracted) from drainage or overflow minus the water boiled away. The documentation seems to indicate that this CONTAIN water pool model assumes that any pool within the containment is considered to become and remain saturated. Note that this is not correctly documented because a subcooled pool can be modeled.

D.2.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

In the initial presentation of the water pool model and in the discussion with the Committee, some confusion arose as to the equations used in the code and the approach taken. The Committee came to the conclusion that the documentation needed more clarification and this is discussed below. The water pool model is part of the lower cell model within the CONTAIN source code. It is the understanding of the Committee that the lower cell model is not extensively used for modeling of the core fuel debris that may be deposited within containment, but is used for the inventory of these water pools. The actual equations and technical approach used for a saturated boiling pool were described by Dr. Murata and seemed reasonable to the Committee. Also, the model can handle a subcooled water pool. The dominant phenomena is the steam source term from the water pool and the ability of CONTAIN to track the mass of water being added to containment compartments or draining from structures. Based on the discussion with the SNL staff, the Committee was satisfied with these attributes.

D.2.2.3. Results of Model Sensitivity Studies

No sensitivity studies were found within the manual or presented to the Committee.

D.2.2.4. Results of Benchmarking/Validation Studies

There were no specific validation studies presented in the formal documentation or in the Committee presentations. The Committee was made aware of a series of "standardized benchmark test problems" that were developed for CONTAIN and were used to check out the code. There was no specific problem for the water pool model, to our knowledge, and it seems that this would be a useful addition to the benchmark problems set. Otherwise, no validation is done specifically for this model apart from integral comparisons.

D.2.2.5. Identified Deficiencies and Options for Model Improvements

The models used for the implicit boiling pool source was not clearly documented in the CONTAIN manual. The equations used to explain the vapor source term (Eqs. 4-21 and 4-24 in the CONTAIN manual) were redundant and confusing to the reader. In

addition there is a mention of an App. K, which was absent from the documentation and appears irrelevant. After a discussion with the SNL staff, it seemed clear to the Committee that there were errors in the documentation, not in the code software, that needed corrections. The actual approach used for a saturated boiling pool, as well as a subcooled water pool, was described by Dr. Murata and seemed correct. Thus, the manual should be corrected to reflect the correct physical relations. In addition, the SNL staff should ensure that a description of the subcooled pool model is included in the CONTAIN documentation. It is not crucial for accident simulations, but seems straightforward to incorporate. Also the lack of standardized problems for the water pool model seems to be an easy addition to the CONTAIN benchmark set that should be formalized. There are situations where for deep water pools or for a large change in the containment conditions, as the containment heats up, that the water pool develops a stratified temperature distribution and the CONTAIN model becomes inappropriate. The importance of this effect is judged to be limited.

D.2.2.6. Importance of Model to Prediction of Dominant Phenomena

As long as the water pool boiling model and the water mass inventory is done properly (and documented accordingly), this phenomena does not have a high importance level for severe-accident phenomena. The Committee feels it has been done correctly, but documentation should be improved.

D.2.2.7. Technical Adequacy of Model and Documentation

The water pool model, as described by the SNL staff, reflects the current state of knowledge for a systems model and is judged to be of first order. The physics is well understood and validation of the model is possible with simple thought experiments as well as simple test problems, which should be included in the standardized benchmark set for CONTAIN. Therefore, once the documentation errors are corrected in the CONTAIN manual and a subcooled model is included into the formulation, the model is judged to be technically adequate (Category 1).

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D.3. Core-Concrete Interactions

D.3.1. Model Description and Pedigree

General Overview

In CONTAIN, the interaction of core debris with the basemat concrete is modeled by the CORCON computer code. The CORCON-Mod2 code has been operational within the CONTAIN architecture for several years; however, the newer CORCON-Mod3 version is currently being integrated into the lower cell/cavity models of CONTAIN.

The CORCON-Mod3 computer code integrates the CORCON code, with significant changes in the heat transfer models, with the VANESA code, which also includes modifications in the chemistry models.

CORCON-Mod3 models the thermal attack of core debris on concrete using a quasi-static approach consisting of the core debris pool, the concrete cavity, and the water and/or atmosphere above the debris pool. The decay and chemical reaction energy generated within the debris pool are transferred to the concrete basemat and sidewalls, as well as the overlaying water pool and/or atmosphere.

The partition of heat transfer is via corresponding thermal resistances. Concrete ablation and decomposition generates gases, molten oxides, and molten metals. These decomposition gases are reduced as result of interactions with the debris pool metallic constituents to produce H_2 and carbon monoxide gases. Both the reacted and unreacted decomposition gases eventually enter the atmosphere above the pool as sources to the CONTAIN computational cells.

Energy Generation

The core debris/concrete interaction process is driven by decay and chemical reaction heat generated in the pool. The decay heat includes contributions from actinides, decay products, and irradiated structural material (Ref. D.3-1). During a relatively short period, chemical reaction energy from zirconium oxidation may be predicted to greatly exceed the decay heat contribution.

The decay heat is scaled to a large PWR core at equilibrium burnup (3,320 MW(t) and 33,000 MWD/MTU) based on Sandia ORIGIN calculations. The decay heat is approximated by contributions from 27 elements (excluding noble gases), which were found to account for nearly all of the energy production in the ORIGIN calculations. The initial core inventory of fission products is assumed to be proportional to core operating power, as specified through user input. In addition, it is assumed that the specific decay power (W/g-atom) associated with each of the 27 elements is a simple function of time after scram (up to 240 hours) based on the ORIGIN results, which is tabulated and then used for interpolation or extrapolation to other times.

Crust Formation and Freezing

This model is based on CORCON-Mod2 where a quasi-steady one-dimensional analysis is performed that assumes the heat generation rate equals the heat loss rate. Crust is assumed to begin to form when the local interface temperature is calculated to fall below the solidus temperature. Crust thickness is determined by matching the energy generation rate with the net heat loss rate.

Using a one-dimensional conduction model, CORCON-Mod3 treats liquid layers, solid layers, and liquid layers with solid crust. The model does not account for crust history. This is problematic, because during the calculations the crust may appear and disappear in a single time step. In addition, the model for crust growth and its evolution is not correct, especially in the presence of water; crust breakup upon interaction with water and crust instability are not considered.

In the absence of water, these modeling uncertainties are not expected to have a significant impact on the overall model predictions.

Bulk Pool Heat Transfer

The melt pool is considered to be composed of several metal and oxide layers in a stratified configuration, with well-defined interfaces. The CORCON-Mod3 model considers interlayer heat transfer as well as heat transfer at pool boundaries. Empirical correlations reported in the literature are used for calculation of heat transfer by convection (with and without gas flow) from the top, bottom, and radial boundaries of the molten pool.

The heat transfer to the bottom interface of the melt pool, where gas bubbles evolving from the interaction of the melt and concrete can be injected, is based on the Kutateladze correlation.

The heat transfer to liquid layers (except for the upper most layer) within the melt pool is based on a correlation by Greene. The heat transfer from the upper most layer (adjacent to containment atmosphere or coolant) is based on a modified Kutateladze correlation, adjusted for area enhancement to account for increased surface area due to agitation as derived by Farmer. The heat transfer from the radial boundaries of the melt pool is based on natural convection correlations.

At low gas velocities, the heat transfer in the molten pool is based on natural convection correlations. In CORCON-Mod3, the natural convection is imposed by choosing the greater Nusselt numbers based on natural convection and for bubble enhancement. In the lower limit, a conduction limit is imposed on the Nusselt number based on natural convection.

Melt-Concrete Heat Transfer

In CORCON-Mod2, for a horizontal surface, a pseudo-film-boiling model based on the concept of Taylor instability was used; this model is still an option in CORCON-Mod3. In this model, for surfaces having an angle of inclination larger than 30 degrees, a laminar or turbulent film model based on Reynolds analogy is used. An iterative procedure is required to solve for the heat transfer coefficient on a surface with an angle of inclination larger than 30 degrees. Surfaces with angle of inclination less than 15 degrees are assumed to behave like horizontal surfaces. Radiation heat transfer is also included in the model. The model will yield a lower heat loss rate from the pool for a given opacity of the environment. This discrepancy will become important at high temperatures.

The use of gas film flow path length in calculating heat and mass transfer is not supported by the laboratory data reported in the literature.

In addition to the original stable gas film model of CORCON-Mod2, a new model based on intermittent contact of debris pool and concrete surface is included as an option in CORCON-Mod3.

The slag film model allows for intermittent pool concrete contact, using the model proposed by Epstein. The Epstein's model is implemented by treating the transient slag layer growth and removal process as a heat transfer resistance in series with the pool convective heat transfer. The slag heat transfer coefficient is then approximated by:

$$h_s = 0.41 h_p .$$

The code assumes a lower limit of $1000 \text{ W/m}^2\text{-K}$, which is based on conduction through 1 mm of slag. Even though the lower limit is not expected to be reached unless a crust is present, actual code applications showed that the limit was reached without the presence of a crust. The code documentation does not discuss the impact of this assumption.

The code does not allow a transition from the original stable film model to the new slag film model. This transition could have been accomplished via a simple gas velocity criterion. In addition, user guidance on the choice of the model options is not provided.

Coolant Layer Heat Transfer

The standard correlations for nucleate boiling, film boiling, maximum heat flux, and minimum heat flux are used in the CORCON model within CONTAIN. However, instead of rederiving the boiling curve for each set of conditions, an empirical fit of the boiling curve as a function of pressure for water is used in the calculations. The radiative energy contribution to the heat transfer is also included.

The effect of gas injection on film boiling is based on the correlation proposed by Greene. This correlation is based on small temperature differences of about 100 K and thus its applicability to reactor conditions is not justified or traceable in the CORCON-Mod3 documentation (Refs. D.3-1 and D.3-2). Another condition that can alter the standard boiling curve is the effect of subcooling of the coolant layer. Although this is well established for certain geometrical shapes (horizontal or vertical plates and spheres), superposition of the combined effects of gas injection and liquid subcooling are not based on experimental evidence, and do not seem physically reasonable. Also the effect of this gas injection and liquid subcooling on the minimum film boiling temperature and heat flux is not referenced or justified.

Probably the largest difficulty with the current coolant layer heat transfer model is what it does not address:

1. There is no model to account for the passage of the molten fuel as a jet or a series of jets from the failed RPV through the coolant layer to the cavity floor; even a parametric model of this sort is needed to address the impact of melt quenching in the absence of energetic FCI and is already part of MELCOR in the FDI package.

2. If the molten fuel does reach the cavity floor as a molten pool it will continue to quench at its surface, and the current model does not properly treat the growth of the crust; i.e., neither the properties of the crust are properly accounted for or is the thermal inertia of the crust growth considered and both can affect the physical reasonableness of MCCI calculations.

3. With the presence of a molten pool and an MCCI the present model does not have the potential for enhancement of the coolant heat transfer at the melt-crust-coolant interface by the dynamic action of crust breakup, water ingress, and possible local melt quenching and debris production. The committee is well aware that this is an area of major uncertainty and that the MACE program is still aimed at addressing it; however, it is not clear to us why a parametric model could not be used to address the impact of such processes on the overall containment response.

Bubble Phenomena

Bubble behavior affects heat transfer and interlayer mixing within the molten debris pool. The terminal velocity of the bubbles is calculated for different bubble shapes (i.e., spherical, ellipsoidal, and spherical cap bubbles) using the correlations/models available from the literature.

Changes resulting from variations in chemistry, pressure, temperature, and composition are accounted for; however, coalescence or breakup of bubbles has not been considered. Chosen bubble size is not substantiated with experiments. Froth formation at the pool free surface and at the layer interfaces has not been considered.

Overall the model is adequate but there may be substantial error in calculated void fractions, which in turn will affect the convective heat transfer coefficient.

Interlayer Mixing

The CORCON-Mod2 assumed the existence of mixture layers; however, it lacked models for mixing between the various layers of the debris pool. Models are now in CORCON-Mod3, which include the effects of mixing between molten layers within the debris pool. If this option is activated, mixing can occur instantaneously (within one time step). The code can currently model two types of mixture layers, a layer of light oxide with suspended metal drops or a layer of metals with suspended heavy oxide drops. In addition, single layers can also be formed (stratified) due to the de-entrainment mechanism. This is one of the most important modeling aspects in terms of CORCON-Mod3 predictions of core-concrete interactions. Under most severe-accident conditions, CORCON-Mod3 predicts substantial periods of stratification (layers never mix completely).

The entrainment model is solely based on one set of experimental data (i.e., Greene's experiments). Two conditions are given for the onset of entrainment: (1) the ratio of layer densities must be less than 3, and (2) the bubble volume must be greater than a prescribed bubble volume for interface penetration (Refs. D.3-1 and D.3-2). These conditions are applicable for single spherical bubbles and low gas flow rates. The limitations of the entrainment criteria are not clearly documented (Refs. D.3-1 and D.3-2). In addition, the validity range of the entrainment correlations is not discussed. Greene in his documentation of the entrainment correlation has stated that the correlation may not be applicable to other flow regimes. In addition, the critical volume for penetration in the code is higher than the value reported in Greene's paper by $(4.91/3.9)^{3/2}$. The reason for this difference is not provided in the documentation (Ref. D.3-2).

The de-entrainment mechanism is analyzed by observing the behavior of single spherical droplets in a semi-infinite medium. The drag coefficients for the liquid droplets are given as a function of a droplet Reynolds number (in the range of 0.2-200). The

experimental observations revealed that beyond a certain critical velocity, droplet oscillations may occur. For multiple droplets interacting with the debris pool, the drag coefficient and oscillation criteria may be different than that of a single spherical particle in a semi-infinite medium. CORCON-Mod3 does not consider the effects of particle coalescence and inter-particle interactions as they rise through the molten pool. The documentation does not mention the relevance of the particle time constant or whether particles can achieve their respective terminal velocity during their flight through the debris pool layers (due to the finite depth of the pool layer).

These issues were outlined as part of an earlier review of the CORCON-Mod3 Users' Manual (Ref. D.3-3).

Chemical Reactions

The primary objectives of the chemistry modeling in the CORCON-Mod3 module of CONTAIN, as indicated by the Sandia staff (Dr. Powers) in a presentation to the committee (see App. B, Presentation Materials (Sandia National Laboratories, Albuquerque, NM, First Meeting of the CONTAIN Peer Review Committee, May 24-27, 1993, Albuquerque, NM, presentation 1-19), is to provide estimates of the generation rates of :

Combustible Gases (within a deviation of 25% from the actual amounts)

Aerosols (within a factor of 2 to 3 of the actual amounts)

in this order of importance. CORCON-Mod3 incorporates VANESA for chemistry calculations, but the chemistry models of the erstwhile CORCON-Mod2 and the VANESA codes have not been fully integrated into one single set of models or package. The computational philosophy is not based on dynamical reaction kinetics equations, rather, the computations are carried out by use of the following scheme:

1) Material compositions at a given instant of time (or within a small time interval) are estimated by use of Equilibrium Chemistry models (in VANESA part of CORCON-Mod3) applicable to a multiphase but otherwise homogeneous system. This requires first a compilation of the possible materials, their phasic conditions, possible reactions among them, and the free energies and the activity coefficients associated with the reactions at the specified temperature. Next, the functional for the total free energy is constructed, and is minimized, by use of optimization techniques, and corresponding phasic concentrations of the materials present are obtained.

2) These equilibrium calculations are followed by a computational time step in CORCON-Mod3 (external to VANESA) in which the gases, vapors, and aerosol particles can flow or diffuse and escape, and the melt/debris/gas-vapor (the melt) may cool (or heat up). The state of the melt at the end of the time step is thus known, but this state may not be consistent with the new physico-chemical conditions at the end of the time step. Thus a new equilibrium calculation (step 1 above) is performed to obtain material compositions consistent with the new physico-chemical conditions.

The computational scheme thus consists in repetition of the above two steps, with some specified time steps over the total time interval of interest.

Since there is not sufficient information available on high-temperature chemistry (activity coefficients, reaction rates) of complex melts of the type envisaged, the CORCON-Mod3/VANESA approach is reasonable. The package does represent a significant advance

over CORCON-Mod2 in that a wider range of species is considered (for example, uranium, aluminum, silicon, and calcium have been included). Further, reactions not only between gases and condensed phases, but also those among the condensed phases (that is, intra-condensed phase reactions) are considered. Options are provided for control (incorporation or suppression) of coking reactions (the reactions that lead to formation of condensed phase carbon; suppression of this reaction leads to generation of large amounts of methane and ethane). The computed results are, however, uncertain, and even within the limitations of the chosen approach, these are sensitive to the assumptions that include:

a) *Use of ideal chemistry.* There has been an attempt by the SNL staff to use non-ideal chemistry, and they have made considerable progress in compiling a list of activity coefficients. This list is not complete, and at present it appears that only an activity coefficient model (a subregular solution model) for the metallic phases and a "partial" activity coefficient model (an associated solution model) for the oxide phase have been implemented. Thus, the gas/vapor phase interactions with the condensed phase species are still treated with ideal chemistry assumptions, a constraint that would warrant future investigations.

b) *Zirconium form and reactions.* Zirconium can react strongly with gases, and in particular, it can be quite effective in reducing CO_2 to CO and H_2O to H_2 , both of which are combustible. The computed results regarding the generation of these gases are thus dependent on assumptions made regarding the form of zirconium (as partitioned between metal and oxide forms) in the initial melt as it exits from the core and interacts with the concrete. Note that CORCON-Mod3, in an improvement over CORCON-Mod2, does allow interactions among condensed species. Thus, zirconium reaction with, for example, SiO_2 , can lead to rapid oxidation of zirconium to ZrO_2 , and the assumptions regarding the form of zirconium in the initial melt may be less of a concern.

c) *Particle formation rates.* Mechanistic calculation of gas(vapor) to particle conversion poses a very difficult and challenging problem. VANESA attempts this, but it appears that in actual calculations this attempt is abandoned, and the aerosol formation rates (and size/composition distributions) are either based on empirical estimates, or the very experimental data that the code was supposed to predict.

Further, incorporation of additional condensed phase reactions is most likely needed; e.g., SiC, U_3O_8 , and other species to cover a wider range of chemical specie evolution. It is possible that the lack of additional species (e.g., SiC) is the reason that coking is observed in CORCON-Mod3 calculations. The documentation needs to clarify why CORCON and VANESA chemistry models have not been integrated into a single set of models. The addition of the condensed phase chemistry models is a positive development. However with the condensed phase chemistry option activated, the equilibrium model leads to reaction of most of the zirconium content of the melt within the first time step, provided zirconium is initially present in large quantities in the pool (greater than a few percent). This leads to an early escalation of chemical reaction heat and the melt temperature, as discussed in Ref. D.3-4. Numerical problems have also been observed with the code when the metallic species are nearly depleted from the pool.

Material Properties

CORCON-Mod3 calculates thermophysical properties over a large range of temperatures. The modeling of thermophysical data remains largely unchanged from CORCON-Mod2.

The phase diagrams include data built in for the three concrete types, while other concrete types the code requires user values for the liquidus and the solidus temperatures.

The phase diagrams for metallic mixtures consist of simple fits for chromium, iron, and nickel liquidus and solidus temperatures. The presence of zirconium, silicon, etc., which could substantially reduce the melting temperature in the metal phase, is currently ignored. In CORCON-Mod3 a new option is included for the user to provide the solidus temperature of the metallic phase, and the code in turns adds 10 K for the liquidus temperature.

The phase diagrams for oxidic mixtures (pseudo-binary system) are based on an ideal solution for solid phase, while the recent ACE experiments clearly showed eutectic interactions in the oxide mixtures. A much faster reduction in solidus temperature expected with concrete addition (at 10-20% concrete, mixture solidus temperature falls to that of concrete). The user can select a parametric value of solidus temperature to represent eutectic interactions. A better representation of recent experimental observations is desirable. The phase diagrams between the in-vessel and ex-vessel severe-accident codes may not necessarily be consistent.

Melt Spreading

CORCON-Mod3 allows the radius of the debris pool to be specified as a function of time. The simple model for melt radius variations with time incorporated in the code is believed to be appropriate for comparison with experimental data where the melt spreading can be measured. However, in the event of an actual accident scenario, the progression of the melt radius with time is not known, and the present model is too limited to be of much use. The code manual (Ref. D.3-1) should provide some guidance or perhaps implement a simple model for the melt spreading rate. Simple melt spreading models have been developed and are available in the open literature.

Fission Product Release

CORCON-Mod3 models releases of fission products from the melt-concrete pool via a combination of CORCON/VANESA calculations. The fission product vapors (from the chemical reactions described previously in this section) are converted to aerosol particles in the rising gas/vapor bubbles, and are transported to the pool surface from where they enter the containment environment. The bubble transport, and hence the aerosol transport, is affected by the pool thermal-hydraulics. The calculation of vapor to particle conversion is difficult scientifically and CORCON-Mod3 (VANESA) eventually uses empirical, integral experiment based estimates of the particle size/composition distribution. Thus, the fission product release modeling is based on a mix of mechanistic calculations and empiricism.

D.3.2. Applicability/Physical Reasonableness of Models to Prediction of Dominant Phenomena

In general, the models implemented in the CORCON-Mod3 computer code are reasonable and have been shown to be capable of predicting the trends observed in recent experiments (Refs. D.3-4 and D.3-5).

D.3.3. Results of Model Sensitivity Studies

A number of sensitivity calculations have been performed with CORCON-Mod3 for several recent experiments, and are documented in Ref. D.3-6. For the SURC-1

experiment, the largest sensitivities were observed for the ablation temperature, melt pool temperature, and use of the condensed phase chemistry model.

For the ACE-L6 sensitivity calculations (Ref. D.3-6), the choice of the slag or film model was seen to have a larger sensitivity than the SURC-1 calculation. Similarly, the interlayer mixing sensitivity calculation resulted in a larger difference than the SURC-1 calculation. The condensed phase chemistry sensitivity calculation resulted in smaller differences, but the code did not exhibit the unphysical oscillatory behavior that was observed in the SURC-1 calculations (Ref. D.3-6).

In general for both sets of sensitivity studies, the most readily observable result was the numerical problems that exist for the chemistry model. The base case calculation for SURC-1 predicted an artificial generation of iron, which has been observed to affect the gas release. The use of the condensed phase chemistry model resulted in numerical instabilities for the SURC-1 calculation and the presence of zirconium in trace amounts for the entire ACE-L6 calculation, which affects the cumulative gas release. Also, the use of the mixing model for the SURC-1 sensitivity calculation resulted in numerical instabilities which are attributed to the chemistry model.

For both experiments investigated, the use of the slag or film model was found to have a large effect on the outcome of the calculations, in agreement with earlier results reported in Ref. D.3-5.

The initial melt pool temperature sensitivity calculations showed the role that viscosity plays in the heat transfer correlation. For an initially high melt pool temperature, the heat transfer was an order of magnitude higher than the sensitivity calculation with a lower initial melt pool temperature. These differences are accounted for by the differences in the pool viscosity at the two temperatures.

The time step and the geometry nodalization were relatively insensitive for the calculations presented in (Ref. D.3-6). Similarly, changes in the liquidus and solidus temperature did not have a large effect on the results.

D.3.4. Results of Benchmarking/Validation Studies

The CORCON-Mod3 code has been used to simulate most of the available test data for core-concrete-interaction experiments (Ref. D.3-5). These include SURC-1 through SURC-4, ACE-L6 and L8, ISP-30 (BETA V5.1), SWISS-2, and MACE-ST. An independent experimental assessment of CORCON-Mod3 concluded the following (Refs. D.3-4 and D.3-6):

- (1) The CORCON-Mod3 prediction of concrete erosion for the one-dimensional experiments was found to be reasonable; however, the study found that the code underpredicted concrete erosion distances for the two-dimensional experiments.
- (2) The code consistently underpredicted the melt layer temperatures, and qualitatively, in many cases, the code did not predict the melt pool temperature behaviors that were observed in the experiments.
- (3) The code prediction of aerosol concentrations were observed to be relatively reasonable, usually predicting the experimental data within an order of magnitude. However, the predicted release of certain individual species

differed from the observed experimental results by many orders of magnitude.

- (4) The use of the condensed phase chemistry model in a well-mixed heterogeneous pool in presence of zirconium resulted in unreasonably large increases in the melt pool temperature in the first time steps. This is due to the chemical equilibrium assumption of the CORCON chemistry model.

D.3.5. Identified Deficiencies and Options for Model Improvements

The modeling deficiencies identified by this review and options for improvement of these models are listed below:

- (1) The model for crust formation and freezing does not account for crust history. This is problematic, since during the calculations the crust may appear and disappear in a single time step. In addition, the model for crust growth and its evolution is not correct especially in the presence of water; crust breakup upon interaction with water and crust instability are not considered. The thermal inertia of the crust should be included in the energy balance equation for the crust to alleviate the observed problems. The issue of crust breakup and crust stability remains uncertain experimentally; however, it is important to develop a model that incorporates these mechanisms as the experimental database increases.
- (2) The present melt-concrete heat transfer model does not allow a transition from the original stable film model to the new slag film model. This transition can be implemented via a simple gas velocity criterion.
- (3) The coolant layer heat transfer model is limited to heat transfer from the pool surface (assumed to be represented by a flat plate). The model does not treat the potential for crust breakup, water ingress, debris fragmentation, quench, debris dryout, and remelt. Debris coolability, both as a result of an overlying water pool or during melt spread under water, remain uncertain; nevertheless, at least in a parametric sense, models need to be provided for the users to scope the expected range of phenomenological uncertainties.
- (4) The melt spreading model is not mechanistic. Models have been proposed and are available in the literature. Melt spreading is an important issue impacting severe accidents for reactors involving large floor areas (i.e., BWRs and advanced LWRs).

Other modeling deficiencies and suggested improvements will be discussed in Sec. D.3.7.

D.3.6. Importance of Model to Prediction of Dominant Phenomena

The CORCON-Mod3 is one of the most important models for prediction of thermal and radiological loads resulting from interaction of core debris with concrete basemat following failure of the reactor pressure vessel.

Core-concrete interactions directly impact containment pressure, temperature, and aerosol loading, and determine the penetration of basemat leading to fission product release

to the environment. Containment failure due to direct contact by the molten core debris is also an important issue for BWRs with MARK-I containments.

D.3.7. Technical Adequacy

In summary, the CORCON-Mod3 code has incorporated a number of improvements since the release of the earlier version of the code (CORCON-Mod2). These include:

- (1) Full integration of the VANESA model into CORCON-Mod3 to model the effects of aerosol generation and radionuclide releases.
- (2) Addition of a slag film model as the boundary between the molten core and concrete during the intermittent core-concrete contact.
- (3) Improvement of the bubble phenomena to account for the entrainment between immiscible liquid layers and enhanced rate of heat transfer.

Notwithstanding the problems identified earlier, the model documentation (Refs. D.3-1 and D.3-2), for the most part provide sufficient information for the code users. The following is a summary of findings for the specific code models:

Energy Generation: The approach for calculation of decay and chemical heat production appears reasonable. The technical adequacy of this model is classified as Category 1.

Crust Formation and Freezing: The model does not account for crust history; therefore, during calculations the crust may appear and disappear in a single time step. In addition, the model for crust growth and its evolution is not correct, especially in the presence of water; crust breakup upon interaction with water and crust instability are not considered. The technical adequacy of this model is classified as Category 2.

Bulk Pool Heat Transfer: The heat transfer processes within the pool remain uncertain, and many models are available in the literature; however, none of these models have been found to be able to predict the experimental measurements adequately. This is a complicated problem, and it is not expected that a universally accepted model can be developed that will capture the physics observed in the experiments; therefore, it appears that adequate dials are built into the present CORCON models so that parametric studies can be performed over the expected range of uncertainties. The technical adequacy of this model is classified as Category 2.

Melt-Concrete Heat Transfer: The use of gas film flow path length in calculating heat and mass transfer is not supported by the laboratory data reported in the literature. The code does not allow a transition from the original stable film model to the new slag film model. Here again, it is not expected that a universally accepted model can be developed that will capture the physics observed in the experiments; therefore, it appears that adequate dials are built into the present CORCON models so that parametric studies can be performed over the expected range of uncertainties. The technical adequacy of this model is classified as Category 2.

Coolant Layer Heat Transfer: The use of nucleate boiling and critical heat flux correlations applicable to water boiling on a solid, flat surface to heat transfer from a molten pool/solid debris to an overlying coolant layer remains in question. The effect of gas injection on film boiling is based on the correlation proposed by Greene. This correlation

is based on a small temperature difference of about 100 K, and its applicability to reactor calculations is not established. Superposition of combined effects of gas injection and liquid subcooling is not based on experimental evidence. The correlation for effect of gas barbotage on minimum film boiling temperature is not justified. The technical adequacy of this model is classified as Category 2.

Bubble Phenomena: Overall the model is adequate but there may be substantial error in calculated void fractions which in turn will affect the convective heat transfer coefficient. The technical adequacy of this model is classified as Category 2.

Interlayer Mixing: This is one of the most important modeling aspects in terms of CORCON-Mod3 predictions of core-concrete interactions. The models for the entrainment of liquid droplets by the rising gas bubbles and the de-entrainment mechanism are based on single particles which may prove to be rather too simplistic. The experimental basis of this model is very weak (solely based on one set of experiments). The effects of gas flow rate, interface conditions (i.e., waviness), and particle interactions and coalescence are not included in these models. The technical adequacy of this model is classified as Category 2.

Chemical Reactions: Overall, the model is evolving in the correct direction; however, the potential limitations of the equilibrium chemistry model needs to be assessed. The modeling of non-ideal solution chemistry is not yet operational. Furthermore, the chemistry package needs additional condensed phase chemical reactions for SiC, U_3O_8 , and other species. Lack of additional chemical reactions may be the reason for prediction of coking reaction in CORCON. The technical adequacy of this model is classified as Category 2.

Material Properties: The material properties for the most part are adequate. They should be updated to reflect the recent experimental database (Refs. D.3-1 and D.3-5) The technical adequacy of this model is classified as Category 2.

Melt Spreading: The simple model for melt radius variations with time incorporated in the code is believed to be appropriate for comparison with experimental data where the melt spreading can be measured. However, in the event of an actual accident scenario, the progression of the melt radius with time is not known, and the present model is too limited to be of much use. The technical adequacy of this model is classified as Category 4.

Fission Product Release: The fission product release modeling is based on a mix of mechanistic calculations (amount released and transport) and empiricism (size/composition distribution of particles). The technical adequacy of the overall release calculations is, therefore, classified as Category 4.

REFERENCES

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- D.3-2. D. R. Bradley and D. Powers, "CORCON-Mod3 Models and Correlations," Sandia National Laboratories letter report, February 17, 1993.

- D.3-3. H. Esmaili, R. Vijaykumar, and J. Ptacek, "Review of the CORCON-Mod3 User's Manual," Energy Research, Inc., report ERI/NRC 92-1105, November 1992.
- D.3-4. J. Ptacek and H. Esmaili, "Experimental Assessment of the CORCON-Mod3 Computer Code," Energy Research, Inc., report ERI/NRC 9205, June 1993.
- D.3-5. J. E. Brockmann, R. O. Griffith, and D. R. Bradley, "CORCON-Mod3 Validation Study," Sandia National Laboratories report SAND93-0295, 1993.
- D.3-6. J. Ptacek and H. Esmaili, "Sensitivity Analysis of the CORCON-Mod3 Computer Code," Energy Research, Inc., report ERI/NRC 9208, June 1993.

D.4. Direct Containment Heating

D.4.1. Melt Ejection From Reactor Pressure Vessel

D.4.1.1. Model Description and Pedigree

Single-Phase Debris Discharge

The single-phase discharge of debris from the vessel is assumed to obey Bernoulli's equation, with a user-defined discharge coefficient multiplying the breach area. The breach is always assumed to be at the bottom of the vessel, so that discharge from the vessel is always complete.

Two-Phase Discharge

The onset of gas blowthrough is predicted using the Gluck correlation (Ref. D.4-1). Once blowthrough has occurred, separated flow of the two phases is assumed to occur: the melt is assumed to obey Bernoulli's equation, as above, and the gas discharge is modeled as choked flow of an ideal gas. The flow quality is predicted using a correlation developed by Pilch and Griffith especially for the purpose (Ref. D.4-1).

Hole Ablation

Hole ablation is calculated assuming that all of the heat transferred to the vessel as the melt flows through the breach goes into melting steel. The heat transfer rate is estimated using a standard flat plate heat transfer coefficient, modified to allow for "transpiration cooling" of the boundary layer during ablation and for incomplete contact of the orifice by melt during the two phase discharge (Ref. D.4-2).

The RPV models are only available when the cavity entrainment models are used, otherwise the user must specify the debris ejection rate explicitly.

D.4.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Single-Phase Discharge

This is the standard treatment of liquid discharge from a vessel under pressure. The effects of solid debris in the lower head are not explicitly allowed for in the model. The presence of solid debris could affect the effective orifice area and the discharge rate, in addition to the mass of debris discharged from the lower head. However, the discharge coefficient and flow path area can be used to scope the effect of solid debris on the discharge rate. In view of the uncertainty in the understanding of the effects of solids in the debris, such a parametric approach is justified.

Two-Phase Discharge

The correlation used for gas blowthrough is appropriate for both the reactor vessel and experimental geometries. The flow quality correlation was developed by Pilch and Griffith specifically for the reactor geometry as there were no correlations available in the literature applicable to this geometry.

Similar remarks on the effects of solid debris in the lower head to those in the on single-phase discharge above apply. In addition it is noted that if the breach is above the bottom of the lower head (i.e., an off-center discharge), then incomplete discharge of the debris in the lower head may occur. In view of the uncertainty in the debris available for discharge and in the location of the breach, it is appropriate to scope such variations by varying the debris mass input to the code.

Hole Ablation

Heat conduction within the vessel is neglected, which appears to be justified in view of the rapid predicted ablation rates and the agreement with experiment. The use of a flat plate heat transfer correlation for an orifice geometry is questionable and complete contact of the orifice boundary by the melt would be more in keeping with the separated flow assumption used in calculating the two-phase discharge; however, the reported agreement of the model with experiment (Ref. D.4-2) justifies its use.

D.4.1.3. Results of Sensitivity Studies

No relevant results were reported to the Committee.

D.4.1.4. Results of Benchmarking/Validation Studies

Single-Phase Debris Discharge

No relevant results were reported to the Committee.

Two-Phase Discharge

The Gluck correlation for gas blow through is a fit to experimental data over the relevant parameter range (Ref. D.4-1). When compared to the SURTSEY IET-9 data, the correlation predicted blowthrough much earlier than the 0.3 s measured in the test (Ref.D.4- 3).

The correlation developed by Pilch and Griffith for the quality of the two-phase discharge has been compared with the available experimental correlations for discharges from horizontal pipes (Ref. D.4-1). The available experimental correlations included those of: Schrock et al., Smoglie and Reimann, Reimann and Khan, and Yonomoto and Tasaka, as presented in Ref. D.4-1. The agreement between the Pilch and Tarbell correlation and the experimental correlations was good.

Hole Ablation

Pilch and Tarbell have compared the hole ablation model with the observed ablation in the HIPS-2C and HIPS-3J experiments (Ref. D.4-2) and showed that the predictions agree with the measurements to within the accuracy of the data.

D.4.1.5. Identified Deficiencies and Options for Model Improvements

The gas blowthrough model has been found to significantly underpredict the observed time to blowthrough in the SURTSEY IET-9 test. Further analysis would be required to determine the reason for this discrepancy; the effect of an error in the predicted timing of gas blowthrough on containment pressurization is not known. Sensitivity

calculations are required to determine the importance of the failure to accurately predict the blowthrough time in the SURTSEY IET-9 experiment.

D.4.1.6. Importance of Model to Prediction of Dominant Phenomena

The mass of debris discharged from the vessel can have a significant effect on containment pressurization and on the amount of fission product aerosol formed during HPME. As debris dispersal is likely to occur on a short time scale compared to the time scale for the interaction of the debris with the atmosphere, the discharge rate is likely to be of less importance.

D.4.1.7. Technical Adequacy

Where the phenomena are understood adequate first-order models are incorporated in the code. Where the phenomena are uncertain, there is sufficient flexibility in the modeling to scope the importance of the effects. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

D.4.2. Melt Oxidation by Gas

D.4.2.1. Model Description and Pedigree

The model allows for the oxidation of zirconium, aluminum, chromium, and iron to form ZrO_2 , $AlO_{1.5}$, $CrO_{1.5}$, and FeO , respectively. The metals are reacted in the above order, first with oxygen then with steam. The reactions with zirconium, aluminum, and chromium are assumed to go to completion. The reaction of steam with O_2 is also assumed to go to completion but the reaction of iron with steam is limited by the equilibrium of the iron, FeO , H_2O , H_2 system. The heat of reaction is added to the debris in all cases. The oxidation of metals by steam results in the production of hydrogen, which can either be added to the gas inventory in the containment or can be immediately recombined with oxygen in the cell (if present).

The rate of oxidation of the metals is limited by mass transfer in the gas and within the debris droplets. Mass transfer in the gas phase is estimated using a standard correlation for drops, based on a heat and mass transfer analogy (Ref. D.4-4). Mass transfer in the drop is treated as a linear approximation to the conduction problem in a stagnant sphere, chosen to give the correct time to oxidize half of the metal in the drop. The gas and drop side rates are combined by taking the root sum square of the time scales for the gas and drop side processes to represent the time scale for the combined process.

The oxidation of metals is allowed to occur in both the airborne debris and in non-airborne debris (NAD). In the latter case, the user must input a length scale to represent the size of the debris for the mass transfer model.

D.4.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The important chemical reactions and physical processes are accounted for in the model.

The estimated mass transfer rate in the drops and its combination with the gas side transport are both very approximate. However, the drop side processes are probably not important and the models are adequate to scope the size of the effect.

The NAD model is parametric in that the user must decide the length scale of the deposited debris for heat and mass transfer processes. In the case of a large, dry containment, the NAD is likely to make only a small contribution to the overall debris oxidation. In addition, the model has been fitted to the SURTSEY experiments, and with the chosen length scale of 1 cm gives good agreement with the measured hydrogen production. A methodology is presented in Ref. D.4-5 for scaling this value up to the reactor plant. Heat transfer between NAD and structures is neglected. This omission could potentially lead to overprediction of the oxidation of the NAD and this could be important (Ref. D.4-5); however, this effect will have been allowed for to some extent in choosing the optimum length scale to fit the experimental data and the possible magnitude of the effect can be scoped by turning the NAD model off.

The debris and associated carrier gas is assumed to be well mixed with the atmosphere in any cell through which it passes; no allowance is made for possible plume effects. Due to the entraining nature of turbulent plumes the well-mixed assumption is probably reasonable.

D.4.2.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.4.2.4. Results of Benchmarking/Validation Studies

Predictions of hydrogen production during the SURTSEY LFP, WC, and IET tests have been compared with the measured values (Ref. D.4-6). With the recommended DCH parameter values, good agreement is obtained with the experimental data.

D.4.2.5. Identified Deficiencies and Options for Model Improvements

The neglect of heat transfer between NAD and structures may lead to overprediction of the oxidation of NAD and consequently may contribute to overprediction of hydrogen production. Switching the model on and off allows the magnitude of the effect to be scoped.

D.4.2.6. Importance of Model to Prediction of Dominant Phenomena

The chemical energy resulting from the oxidation of the metals and the subsequent release of energy from any combustion of hydrogen generated during the oxidation are major contributors to the pressurization of the containment during DCH.

D.4.2.7. Technical Adequacy

The basic physical processes are understood and appropriate models are in place, with the possible exception of heat transfer between NAD and structures. The technical adequacy of this model is classified as Category 1 for airborne debris and Category 2 for NAD. The documentation should include advice to the user on how to estimate the required particle size for the NAD model for plant calculations.

D.4.3. Melt Sweepout

D.4.3.1. Model Description and Pedigree

The actual breakup of melt to form droplets is discussed in Sec. D.4.4 and melt trapping on structures is discussed in Sec. D.4.8; neither of these processes is considered here. What is considered is the transport of melt drops by the flowing gas.

The debris is modeled as a number of fields of two types. First, different types of debris can be included in the calculations each with its own mean particle size, initial composition, mass, and temperature. Second, each type can have a number of generations that allows the code to follow the thermal and chemical evolution of debris released over a period of time.

The transport of debris between cells is accomplished by adjusting the gas density input to the flow solver to allow for the presence of the debris. Slip between the debris and the gas is allowed and is a user input constant, which can be different for each containment cell and for each debris type. A choked flow rate is also calculated and the minimum of the choked and unchoked flows is used.

D.4.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The provision of two types of debris field allows a wide range of discharge scenarios to be modeled in some detail. The general methodology of the incorporation of debris transport into the implicit flow solver is at the appropriate level; however, a few of the details of the implementation may warrant further investigation.

The recommended values for the slip factors were obtained by fitting to the SURTSEY experiments (Ref. D.4-6). However, at the reactor scale the debris will have more time to accelerate to the gas velocity, suggesting that lower slip ratios may be necessary; a sensitivity could determine if this is an important issue.

No check is carried out to determine what fraction of a given type of debris can be levitated out of the cavity by the gas flow; this will not be a significant issue for high flow rates.

For choked flow the gas velocity is assumed to be equal to the sound speed in the absence of debris (Ref. D.4-7). In the limit of slip approaching unity, this could over predict the gas and debris flows out of the cavity by a factor of up to 4-5 (compared to the usual equation for homogeneous, frozen choked flow).

D.4.3.3. Results of Sensitivity Studies

A number of sensitivity studies have been reported, which include variation of the slip ratio in the containment subcompartments. It is reported in Ref. D.4-8 that the variation of the slip ratio in the subcompartments has little effect upon the results for the scenarios considered.

A sensitivity study on the slip ratio could determine whether it is an important parameter at reactor scale, and hence, whether any further analysis is required to confirm or improve the extrapolation from the SURTSEY data.

D.4.3.4. Results of Benchmarking/Validation Studies

Analysis of the SURTSEY LFP, WC, and IET tests indicates that good agreement is obtained for all experiments if the slip ratio in the cavity is set to 5, whereas it is set to 1 everywhere else. This suggests that the debris may only lag significantly behind the gas for a short while after the discharge and may therefore be of less importance at reactor scale.

D.4.3.5. Identified Deficiencies and Options for Model Improvements

A sensitivity study should be performed to determine the importance of the cavity slip ratio at reactor scale in order to confirm the adequacy of the recommended value determined from the SURTSEY experiments.

The ability of the gas flow to levitate the particles out of the cavity should be investigated at the lowest pressures and flow rates of interests.

The choked flow model should be made consistent with established homogeneous choked flow models in the limit slip = unity (e.g., Ref. D.4-9).

D.4.3.6. Importance of Model to Prediction of Dominant Phenomena

The sweepout of debris from the cavity can be of great importance to the pressurization of the containment as it can determine how much oxidant contacts the debris other than that contained in the blowdown gas from the RPV.

D.4.3.7. Technical Adequacy

The basic phenomenology is understood in outline though the precise details of the cavity flow patterns are not known. A parametric model is in place and the parametric nature of the user input slip factors is justified in view of the lack of understanding of the detailed flow processes.

The documentation with regard to debris transport is confusing in places (note: the appropriate sections have been expanded in the recently revised documentation and the resultant explanations are clear and concise), and the various DCH updates need to be incorporated into the manual in an easily understandable form.

The technical adequacy of this model is classified as Category 2.

D.4.4. Drop Entrainment/Fragmentation

D.4.4.1. Model Description and Pedigree

Five models are available for determining the rate of entrainment of debris in the gas flow in the cavity: three forms of the Whally-Hewitt correlation (Refs. D.4-10 through D.4-12), the Levy correlation (Ref. D.4-13), and the Tutu correlation (Ref. D.4-14). The user is left to define a multiplier for the rate correlation and the surface area over which entrainment takes place. Some guidance is provided on the choice of values and the user is advised to consult the original references.

Six models are provided for the entrained fraction of the debris in the cavity: the Levy correlation (Ref. D.4-13) and five versions of the Tutu-Ginsberg correlation (Refs.

D.4-15 and 16) (Surry no cavity structures, Surry skirt only, Surry all cavity structures, Zion, Watts-Bar). Again the user is referred back to the original references for guidance on the use of the correlations.

There is also an option to have the entrainment time calculated. However, if this time is calculated separately (or input by the user) and the dispersal fraction option is used, then the dispersal rate (if used) will be overwritten, if necessary, to achieve the specified dispersal fraction in the specified time.

The size of the entrained debris drops is determined by using a user-input, critical Weber number (which defaults to 12 if not specified by the user) to estimate the maximum stable drop size, based on the average gas velocity in the cavity (or the cavity exit velocity). The mass median diameter is set to one half of the maximum diameter and the geometric standard deviation defaults to 2, unless specified by the user.

Considerable flexibility is provided in the modeling by allowing the user to input the entrainment rate and fraction, determine the timing of the entrainment, and set the sizes of the entrained particles.

D.4.4.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The entrainment rate and fraction correlations were derived from small-scale, isothermal experiments. As such, the tests could not represent all of the physical processes involved in high-pressure melt ejection from a reactor cavity. Nor could all of the dimensionless groups pertaining to the processes that were represented in the experiments be kept within the required range at once. For example, a common choice in the experiments was whether to have the Froude number in range and the Kutateladze number out of range or vice versa. Crudely one might expect the former case to result in a reasonable representation of the liquid geometry, but a poor representation of entrained particle sizes and vice versa for the latter case. In addition, nearly all of the scaled cavity experiments used central discharges from the RPV; recent experiments have shown that the results can be sensitive to the discharge angle, with some angles being much more dispersive than a central discharge (Refs. D.4-17 and 18). The use of correlations based on such experiments to extrapolate from the SURTSEY tests to the reactor is therefore questionable.

There is some advice provided on the choice of multiplier and surface area for the entrainment rate correlations though the user is advised to consult the original references. In fact it is not obvious what to use for the entrainment area; recent experiments show that the melt discharged before gas blow through can rebound off the end wall of the cavity and meet the gaseous discharge head on part way down the cavity, resulting in massive fragmentation of the liquid (Ref. D.4-18). Whether such transient breakup of the liquid is important is not clear.

Cavity conditions such as final hole size in the RPV, gas flow rate from the vessel, and blowdown time are required for the entrainment correlations and are estimated in side calculations for this use. There is no mention of any check in the code that these values are consistent with the values produced in the main calculation.

Using a critical Weber number to determine particle size implies that the size is inversely proportional to the square of the velocity (taken to be the average gas velocity in the cavity or the cavity exit velocity). In particular this implies that the size should decrease strongly as the gas discharge rate is increased. Such behavior is not evident in the

experiments. Indeed it is not known if there is sufficient time for unstable fragments to break up in the cavity. Whether such unstable fragments could be transported out of the cavity at reactor scale is not known. However it raises the possibility that the predictions of oxidation and heat transfer to the atmosphere may be pessimistic at high discharge rates. Also the use of an average cavity gas velocity may not be justified in view of the large inhomogeneities in velocity that have been observed in some of the experiments (Ref. D.4-19).

D.4.4.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.4.4.4. Results of Benchmarking/Validation Studies

The models discussed above are new to the CONTAIN code. However a preliminary analysis of the SURTSEY IET-9 experiment has been performed (Ref. D.4-20). The results are encouraging with the predictions of peak dome pressure and temperature and peak cavity pressure being in the right ballpark. More detailed parameters, such as particle size, which could yield information on individual models, were not compared with data.

D.4.4.5. Identified Deficiencies and Options for Model Improvements

The dispersal models consist of correlations which are based on isothermal, simulant experiments, which may not adequately represent the phenomena under reactor accident conditions. Several of the correlations, including the Whalley-Hewitt and Levy correlations, should be tuned to the available experimental data and then applied to plant calculations to confirm scaling behavior of the extrapolation from the experiments to the plant.

The experimental data do not support the use of a critical Weber number criterion to predict the particle size. It remains to be determined if unstable fluid particles have time to break up in the cavity and whether one can estimate the effect on DCH if the particles do not break up.

D.4.4.6. Importance of Model to Prediction of Dominant Phenomena

The entrained mass of debris determines the energy that is potentially available for transfer to the atmosphere, and the particle size determines the rate of transfer to the atmosphere. Therefore, these models are extremely important to the prediction of containment pressurization.

D.4.4.7. Technical Adequacy

The detailed physics of the cavity processes is poorly understood. Therefore, though modeling deficiencies have been identified, the set of models provided, together with the flexibility afforded to the user, is probably the best that can be done at present. An alternative approach and more mechanistic approach to modeling debris entrainment is incorporated in the CORDE code (Ref. D.4-21). To significantly improve upon the modeling in the code would require considerable effort and success could not be guaranteed. The technical adequacy of this model is classified as Category 3. The

documentation should be adequate when the various pieces have been consolidated into a single document.

D.4.5. Melt-Water Interactions

D.4.5.1. Model Description and Pedigree

There are no models in the code specifically designed to deal with the interactions of melt with water during a high-pressure discharge into the cavity. However, the boiling of water by the debris can be studied parametrically by the user specifying a time-dependent source of water to the cavity atmosphere.

D.4.5.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The method of treating heat transfer is parametric and, as such, does not model the actual heat transfer processes between the debris and the water. Not all of the water in the cavity may interact with the debris. If the cavity contains a lot of water, much of it may be expelled as a slug due to the pressurization resulting from the interaction of a fraction of the water with the debris. The mass of water will influence the time to accelerate the slug out of the cavity, which, in turn, will affect the time for melt-water interaction in the cavity and the coherence of the debris and steam discharges from the cavity. There is no model of water slug ejection in the code.

Energetic FCIs are still poorly understood and are not modeled.

Fission product release during melt-water interactions is poorly understood and is not modeled. This is probably a small contributor to the source term (Ref. D.4-22), especially for the less energetic interactions.

D.4.5.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.4.5.4. Results of Benchmarking/Validation Studies

According to Ref. D.4-23, steam spikes have been successfully represented using the parametric method referred to in Sec. D.4.5.1 above, though no reference is given.

D.4.5.5. Identified Deficiencies and Options for Model Improvements

There is no model for the ejection of water slugs from the cavity, and the interaction of the user-defined amount of water with the debris can only be treated in a parametric fashion, which does not represent the actual heat transfer processes between the melt and the water.

Simple, parametric models of the above phenomena are incorporated in the CORDE code (Ref. D.4-21). More detailed modeling would be required to determine the appropriate values for the parameters in such a model. An assessment of the best parameters to use could be based on the use of more detailed steam explosion codes, such as CHYMES (Ref. D.4-24), TEXAS (Ref. D.4-25), THIRMAL (Ref. D.4-26), or IFCI (Ref. D.4-27).

D.4.5.6. Importance of Model to Prediction of Dominant Phenomena

This phenomenon is obviously important to cavity pressurization. It is also important to containment pressurization as interaction with a small amount of water may give higher pressures than dry DCH, whereas interaction with sufficient water could quench the debris and lead to a relatively benign dispersal of the debris around the containment.

D.4.5.7. Technical Adequacy

The occurrence and extent of energetic FCIs is still poorly understood and there are no features in the code to model such phenomena.

Less energetic interactions are better understood but there are no features in the code to predict processes such as water slug ejection from the cavity. Heat transfer and oxidation can be represented using features akin to control functions but without capturing the essential physics of the process.

Fission product release during melt-water interactions is poorly understood, not modeled, and probably not important.

The technical adequacy of the overall melt-water interaction model is classified as Category 4. There is no documentation describing how to use the code to represent melt-water interactions.

D.4.6. Fission Product Release

D.4.6.1. Model Description and Pedigree

There are no models in the code specifically designed to estimate fission product release during high-pressure melt ejection. The phenomenon can be represented parametrically by the user specifying source tables of fission products and aerosols to the cavity.

D.4.6.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The release of fission products during high pressure melt ejection can occur by two mechanisms: mechanical fragmentation of the melt and vaporization from the melt. The former may depend upon the mass of debris ejected, the driving pressure for the discharge from the vessel, the geometry of the cavity, the discharge angle, the composition of the melt (including the amount of dissolved gas in the melt), etc. The latter will depend on factors such as the mass of melt ejected, the composition of the melt (including the amount of dissolved gas in the melt), the composition of the atmosphere into which the melt is discharged, etc. For instance, the vaporization of many species is likely to be sensitive to the oxygen potential of the system, just as it is for in-vessel and core-concrete releases.

In view of the likely sensitivity of the fission product releases to the conditions of the discharge it is difficult to extrapolate from experimental data to provide the necessary input for CONTAIN calculations. To allow for the above effects would require a code equivalent to the VANESA code used to predict the releases during core-concrete interactions.

D.4.6.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.4.6.4. Results of Benchmarking/Validation Studies

Not applicable as there is no model in the code to benchmark or validate. However, there is a considerable amount of data on aerosol production during melt ejection from the SNL SPIT, HIPS and SURTSEY experiments (Refs. D.4-28 through 34). These data could be used in model development and/or validation.

D.4.6.5. Identified Deficiencies and Options for Model Improvements

There is no model for fission product release in the code and no tool available to provide the necessary data to use fission product and aerosol source tables to represent the phenomenon.

D.4.6.6. Importance of Model to Prediction of Dominant Phenomena

Brockmann (Ref. D.4-29) extrapolated the results of the SPIT and HIPS tests, based on melt mass alone, to suggest that the DCH aerosol release is of the same order as the in-vessel release.

The ejected melt is likely to have released most of its iodine and cesium along with much of its tellurium in-vessel. The main fission product release during DCH is therefore likely to consist mainly of ruthenium (if it sees sufficiently oxidizing conditions), tellurium (if there is any left in the ejected melt), and some of the more refractory materials, such as barium and strontium species.

D.4.6.7. Technical Adequacy

The understanding of the processes by which fission products are released from the melt during high-pressure melt ejection is questionable. The releases can only be represented in the code by user input of the releases via the fission product and aerosol source tables. The technical adequacy of this model is classified as Category 4. There is no user guidance advising how to estimate the data required to use the fission product and aerosol source tables to represent fission product release during the DCH.

D.4.7. Melt Trapping and Carryover

D.4.7.1. Model Description and Pedigree

The rate at which particles are trapped can be set by the user, or one of three models can be used: GFT, the gravitational fall time of the particles; TFI, the time to first impact and fall; or TOF/KU, time of flight/Kutateladze criterion.

The GFT model is self-explanatory. The debris particles are assumed to fall with the terminal velocity of a sphere. The velocity is calculated from a quadratic expression, which tends to the Stokes velocity at low Reynolds numbers, and at high Reynolds number Re tends to $1.85 \cdot N_D^{0.5}$, which is close to the value of $1.73 \cdot N_D^{0.5}$ recommended in Ref. D.4-35, where N_D is the Best number.

In the TFI model the debris is assumed to undergo a single impact, without sticking, before falling under gravity to the floor. The distance to first impact is user defined. The velocity to the first impact is calculated using a turbulent jet model (see, e.g., Ref. D.4-36) for the flow of the gas/debris mixture to the point of impact (unless the structure convection velocity is greater). The initial velocity of the jet is that calculated by the flow solver for the nominated flow path.

In the TOF/KU model the debris may impact two structures before falling (or being carried on the gas flow) to the floor. At each of the structures, the code determines whether the debris will stick to the structure or be re-entrained into the gas flow and borne off to the next structure. The debris is assumed to stick to the structure if the Kutateladze number is less than a critical value, which defaults to 10 unless a value is input by the user (Ref. D.4-37). The velocity to the first impact is estimated using the jet model described above. If the debris sticks, the trapping rate is determined from the time of flight to the first structure (as long as it exceeds the settling time). If it is re-entrained, it is borne by the gas to the second structure with the convective velocity pertaining to the structure. If it sticks, the trapping rate is determined by the time of flight to the second structure (as long as it exceeds the settling time). If it is re-entrained again, it deposits on the floor and the user can choose if it falls at the gravitational settling speed or at the structure convective velocity. In this case, the trapping rate is determined by the time of flight to the second structure plus the time to deposit on the floor.

D.4.7.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Given the wide range of geometries that must be addressed by this model it is appropriate that the user be given a number of options to allow him to tailor the model to his/her needs.

The calculated gravitational settling velocity is appropriate, so long as there is not a strong overall upflow in the cell.

The jet model for calculating the time to first impact is the best, simple model available, though its accuracy near to the source is questionable. Sensitivity studies are therefore likely to be required in some circumstances. The user-defined distance to the point of the jet at which turbulent entrainment is fully established should be used with caution, as any value other than the calculated default will result in a discontinuity in velocity when the critical distance is reached.

The critical value of the Kutateladze number at which re-entrainment occurs can depend upon the geometry, so sensitivity studies on this parameter are advisable. Outgassing from concrete is not modeled but its effect may be bounded by setting the critical Kutateladze number to zero.

D.4.7.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.4.7.4. Results of Benchmarking/Validation Studies

Analysis of SURTSEY tests generally supports the models (Refs. D.4-38 and 39).

In DCH-1 only 16% of the dispersed mass was found to be trapped on the upper head. The TOF/KU model predicted no sticking, implying that the gravitational fall time

dominated the trapping rate. This is supported by the good agreement between the predicted and measured dome pressures (Ref. D.4-38).

In DCH-2 60% of the dispersed mass adhered to the dome. The TOF/KU model predicted trapping on first impact, which is confirmed by the much better agreement obtained from the time of flight to first impact than from a similar calculation using the gravitational fall time (Ref. D.4-38).

In IET-9 the debris carryover was under estimated by a factor of 4 in the blind calculation, but this was due mainly to the use of a slip ratio of 5 everywhere. For IET-10 an open calculation was performed with slip = 2 in the cavity and 1 everywhere else (as recommended) and the disagreement in the carryover was reduced to less than a factor of 2. The predicted peak containment pressure was in good agreement with the measured values for both tests (Ref. D.4-39).

D.4.7.5. Identified Deficiencies and Options for Model Improvements

No deficiencies or options for improvements were found.

D.4.7.6. Importance of Model to Prediction of Dominant Phenomena

The trapping of debris on structures effects the time available for the debris to interact with the atmosphere and is therefore important to the oxidation of, the heat transfer from and the release of fission products from the debris.

The trapping of the debris also determines the distribution of the debris and consequently the decay heat around the containment.

D.4.7.7. Technical Adequacy

The basic physics of trapping and carryover are understood in outline, though the details for all possible geometries are not known. First-order models are in place for the important phenomena, which capture the essence of the processes. Ample flexibility is provided in the modeling for the user to adapt the models to suit his/her needs. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

D.4.8. Melt Debris-Gas Heat Transfer

D.4.8.1. Model Description and Pedigree

Debris-gas convective heat transfer was calculated using the Ranz and Marshall correlation for forced convection over a sphere (Ref. D.4-4).

A simple grey body law is used to estimate debris to atmosphere thermal radiation, with a user-defined multiplier that defaults to 1.

The atmosphere-to-structure thermal radiation model is that used for non-DCH calculations and has a provision for the user to override the calculated emissivity of the atmosphere.

A grey body law is also used for the debris to structure thermal radiation model. Again there is a user-defined multiplier, which is recommended be kept close to the default value of 0 in view of the likely high opacity of the airborne debris. The surface area for this term is the minimum of the total surface area of all debris particles and the total surface area of all structures in the cell.

D.4.8.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The convective heat transfer model is the appropriate model recommended by Bird, Stewart, and Lightfoot (Ref. D.4-4) for spherical particles. The choice of flow velocity is not crucial due to the square-root dependence of the Nusselt number on this parameter.

The gas to structure thermal radiation model makes no allowance for the presence of airborne debris (including DCH aerosols). However, the user can override the atmosphere emissivity in order to estimate the likely importance of this effect.

The thermal radiation models are essentially parametric as the user must estimate the effective emissivity of the atmosphere in the presence of airborne debris particles. This could more easily be done within the code, where the time-dependent airborne concentration, size distribution, and composition of the debris particles are readily available.

D.4.8.3. Results of Sensitivity Studies

Thermal radiation sensitivity studies have been performed for Surry and Bellefonte plant calculations as well as for SURTSEY IET-1 calculations (Ref. D.4-36). It was concluded that atmosphere to structure heat transfer can be an important mitigation effect, but that the results are fairly insensitive to reasonable variations in the user-defined thermal radiation multipliers.

Also see subsection D.8.2 on structure radiation.

D.4.8.4. Results of Benchmarking/Validation Studies

See subsection D.8.2 on structure radiation.

D.4.8.5. Identified Deficiencies and Options for Model Improvements

The user-defined multipliers for the thermal radiation models could be more easily estimated in the code where the time-dependent airborne concentrations, size distributions, and compositions of the debris are readily available.

There is no model for heat transfer from NAD to structures which will result in an overprediction of the heat transfer from the NAD to the gas.

D.4.8.6. Importance of Model to Prediction of Dominant Phenomena

Heat transfer from the debris to the gas is the direct cause of much of the pressurization of the containment during DCH.

In addition, the transfer of heat from the debris and the atmosphere to the heat sink structures can be an important mitigating effect.

D.4.8.7. Technical Adequacy

The heat transfer processes involved in DCH are reasonably well understood, with the exception of the effect of airborne debris on the atmosphere emissivity and heat transfer from NAD to structures.

First-order models are in place for the important phenomena, with the exception of the parametric treatment of the effect of airborne debris on the atmosphere emissivity via the user-defined thermal radiation multipliers and heat transfer from NAD to structures. The technical adequacy of this model is classified as Category 1. The documentation is adequate.

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D.5. Aerosol Behavior

D.5.1. Size and Composition Distribution

D.5.1.1. Model Description and Pedigree

The intracell size and composition distribution of aerosols are calculated from the set of ordinary differential equations:

$$\begin{aligned} \frac{d}{dt} Q_{\ell k}(t) = & \frac{1}{2} \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} \left(\bar{\beta}_{ij\ell}^{(1a)} Q_{jk}(t) Q_i(t) + \bar{\beta}_{ij\ell}^{(1b)} Q_{ik}(t) Q_j(t) \right) \\ & - \sum_{i=1}^{\ell-1} \left[\bar{\beta}_{i\ell}^{(2a)} Q_i(t) Q_{\ell k}(t) - \bar{\beta}_{i\ell}^{(2b)} Q_{\ell}(t) Q_{ik}(t) \right] \\ & - \frac{1}{2} \bar{\beta}_{\ell\ell}^{(3)} Q_{\ell}(t) Q_{\ell k}(t) - Q_{\ell k}(t) \sum_{i=\ell+1}^m \beta_{i\ell}^{(4)} Q_i(t) \\ & + \bar{G}_{\ell k}^{(1)} Q_{\ell}(t) - \sum_{i=1}^{N_i} \left[\bar{G}_{\ell i}^{(2)} Q_{\ell k}(t) - \bar{G}_{\ell-1,i}^{(2)} Q_{\ell-1,k}(t) \right] + \bar{G}_{\ell-1,k}^{(3)} Q_{\ell-1}(t) \\ & + \bar{S}_{\ell k}(t) - Q_{\ell k}(t) \sum_{j=1}^{N_{sr}} \bar{R}_{j\ell}(t) \end{aligned} \quad (1)$$

with appropriate initial conditions. Here, $Q_{\ell k}$ is the mass concentration (kg/m^3) of the species k in the ℓ the section (size bin), and β s are two-fold integrals on the agglomeration kernels ($\text{m}^3/\text{s}\cdot\text{kg}$). G represent gas to particle conversion (condensation/evaporation, s^{-1}), S are the source terms ($\text{kg/m}^3\cdot\text{s}$), and R are the removal (deposition, s^{-1}) terms. The derivation of this equation has been discussed in the open literature (Ref. D.5-1). The following constraints apply to the Eq. (1):

- The aerosol material density is assumed to be the same for all components.
- The aerosol shape is independent of aerosol composition and shape factors are independent of size.
- The suspension medium is air of a fixed composition.
- The degree of turbulence is fixed in the simulation.
- Deposition rates do not depend on composition.

D.5.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

For a mixed aerosol one wishes to calculate the extended aerosol distribution function. Following the development in Ref. D.5-2:

$$n(v_1, v_2, \dots, v_N; m_1, m_2, \dots, m_N, t) dv_1 dv_2 \dots dv_N dm_1 dm_2 \dots dm_N,$$

which is the number of aerosol particles that contain a volume, v_p to v_p+dv_p , and mass, m_p to m_p+dm_p , of species p ($1 \leq p \leq N$). The total volume of the aerosol particle will be:

$$v = \sum_{p=1}^N v_p$$

and the total mass:

$$m = \sum_{p=1}^N m_p$$

Note that the conventional distribution function for the total volume, regardless of its constituents, is:

$$N(v, t) = \int dv_1 \int dv_2 \dots \int dv_N \int dm_1 \int dm_2 \dots \int dm_N \\ n(v_1, v_2, \dots, v_N; m_1, m_2, \dots, m_N, t) \delta\left(v - \sum_{p=1}^N v_p\right)$$

One can also define other useful reduced distribution functions. For example, if $M_p(v, t)$ is the total volume of species p per unit volume of space that resides in particles whose own volume lies in the range, v to $v+dv$, then we have:

$$M_p(v, t) = \int dv_1 \int dv_2 \dots \int dv_p v_p \dots \int dv_N \int dm_1 \int dm_2 \dots \int dm_N \\ n(v_1, v_2, \dots, v_p, \dots, v_N; m_1, m_2, \dots, m_N, t) \delta\left(v - \sum_{p=1}^N v_p\right)$$

Similarly for the mass fraction, $M_p(m, t)$. Such quantities are useful for they give a measure of the concentration of a particular species in a given particle of volume, v , or mass, m .

Using a shorthand notation:

$$n(v_1, v_2, \dots, v_N; m_1, m_2, \dots, m_N, t) = n(\mathbf{v}, \mathbf{m}, t)$$

and:

$$\int dv_1 \int dv_2 \dots \int dv_N = \int d\mathbf{v},$$

the general dynamic equation (GDE) for a well-mixed spherical multi-species aerosol is written as:

$$\begin{aligned}
& \frac{\partial}{\partial t} n(\mathbf{v}, \mathbf{m}, t) + R(\mathbf{v}, \mathbf{m}, t) n(\mathbf{v}, \mathbf{m}, t) + \sum_{p=1}^N \frac{\partial}{\partial v_p} [I_p(\mathbf{v}, \mathbf{m}, t) n(\mathbf{v}, \mathbf{m}, t)] \\
& = \frac{1}{2} \int_0^\infty d\mathbf{v} \int_0^\infty d\mathbf{w} \int_0^\infty d\mathbf{q} \int_0^\infty d\mathbf{s} n(\mathbf{u}, \mathbf{q}, t) n(\mathbf{w}, \mathbf{s}, t) K(u, q|w, s) \prod_{p=1}^N \delta(v_p - u_p - w_p) \delta(m_p - q_p - s_p) \\
& \quad - n(\mathbf{v}, \mathbf{m}, t) \int_0^\infty d\mathbf{u} \int_0^\infty d\mathbf{q} K(u, q|\mathbf{v}, \mathbf{m}) n(\mathbf{u}, \mathbf{q}, t) + S(\mathbf{v}, \mathbf{m}, t),
\end{aligned} \tag{2}$$

where

$$q = \sum_{p=1}^N q_p$$

and

$$s = \sum_{p=1}^N s_p$$

Note that spatial homogenization or averaging has been introduced, and deposition at the boundaries is accounted for by the deposition/removal terms as substitutes for the diffusive and the body force terms. Also, in proceeding from the spatially nonuniform case to the homogenized case, the nonlinear agglomeration terms are averaged in a manner that is not clearly understood.

The terms of Eq. (2) have the following meanings. The second term on the left-hand side describes the losses due to settling and deposition. These can be due to gravitational settling and various diffusive mechanisms. In general, such processes are functions of the total volume, v , of the particle, which determines the drag, and the total mass, m , which determines the force in the case of gravitational settling. The third term on the left-hand side describes condensation with $I_p(\mathbf{v}, \mathbf{m}, t)$ being the condensation rate for species p . This term affects the total volumes and masses of species p by either the accretion or evaporation of material which is residing in the atmosphere in the form of vapor. Since there can be several types of vapor species, the net effect will be the sum over all species present. The nature of $I_p(\mathbf{v}, \mathbf{m}, t)$ will depend on the type of growth law involved. It is most likely that the growth law will depend only on the total volume of the particle. However, it could also be envisaged that the vapor-solid interaction might depend on the material near the surface in which case I_p would be sensitive to the individual values of v_p . Further, the first term on the right-hand side describes the rate at which coagulation creates particles of individual volumes $\mathbf{v}$ and masses $\mathbf{m}$. $K(u, q|w, s)$ is the coagulation kernel for particles of total volume, u , masses, q , coalescing with particles of total volumes, w , and masses, s . The delta functions are present to ensure conservation of volume and mass in a collision. We note that an opportunity exists here to allow for nonconservation of volume, due say to some packing effect. It would only be necessary to rewrite the delta function as $\delta(v_p - a(u_p + w_p))$ where a is somewhat greater than unity and must be derived experimentally. Of course the mass must always be conserved. The

second term on the right-hand side describes the rate at which particles are removed from (v, m) due to coagulation. Finally, the last term is an independent source.

It should be noted that CONTAIN uses a simplified version of Eq. (2) by setting $R(v, m) = R(v)$, $I_p(v, m) = I_p(v)$, and $K(u, q|w, s) = K(u|w)$, i.e., dependence on total particle volume (or mass) only. In general such an assumption is unjustified. However, if the densities of the materials involved do not differ substantially, then the error in making the above assumption (using some average density) should not be too large and may well be overshadowed by the other assumptions made such as spherical particles and spatial homogeneity.

As an example of the general equation, let us assume that we have a two species aerosol, which can be described by the distribution function $n(v_1, v_2, m_1, m_2, t)$. From Eq. (2) we find:

$$\begin{aligned} & \frac{\partial}{\partial t} n(v_1, v_2, m_1, m_2, t) + R(v_1, v_2, m_1, m_2, t) n(v_1, v_2, m_1, m_2, t) \\ & + \frac{\partial}{\partial v_1} [I_1(v_1, v_2) n(v_1, v_2, m_1, m_2, t)] + \frac{\partial}{\partial v_2} [I_2(v_1, v_2) n(v_1, v_2, m_1, m_2, t)] \\ & = \frac{1}{2} \int_0^{v_1} du_1 \int_0^{v_2} du_2 \int_0^{m_1} dm'_1 \int_0^{m_2} dm'_2 n(u_1, u_2, m'_1, m'_2, t) n(v_1 - u_1, v_2 - u_2, m_1 - m'_1, m_2 - m'_2, t) \\ & \quad K(u_1 + u_2, m'_1 + m'_2 | v_1 + v_2 - u_1 - u_2, m_1 + m_2 - m'_1 - m'_2) \\ & \quad - n(v_1, v_2, m_1, m_2, t) \int_0^\infty du_1 \int_0^\infty du_2 \int_0^\infty dm'_1 \int_0^\infty dm'_2 \\ & \quad K(u_1 + u_2, m'_1 + m'_2 | v_1 + v_2, m_1 + m_2) n(u_1, u_2, m'_1, m'_2, t) + S(v_1, v_2, m_1, m_2, t). \end{aligned} \quad (3)$$

For simple forms of the removal and agglomeration terms, this equation can be solved analytically. A comparison of such results with the results obtained from the CONTAIN Eq. (1) would provide insights into the effects of assuming same densities for all species.

Aerosol particles in postulated accidents, as well as the validation experiments, can be electrically charged (because of radiation and tribological effects), nonspherical, and be chemically reactive. The particles can also adsorb/desorb gases and they can be resuspended. Equation (1) does not account for these effects. There is an attempt in CONTAIN, similar to that in other nuclear aerosol codes, to account for nonspherical particles by use of "shape-factors" γ and χ for agglomeration and deposition, respectively. But these factors are ad-hoc, and they neither have a good pedigree nor a good basis. These are also used in a somewhat inconsistent manner throughout the code.

D.5.1.3. Results of Model Sensitivity Studies

The fidelity of Eq.(1) to the more detailed Eq.(2) has not been studied, and also the role of the neglected phenomena is not sufficiently well understood (some progress could be realized by studying simple and tractable situations, such as Eq.(3). Still, Eq. (1)

represents a major improvement on equations used in other similar nuclear accident analysis codes.

D.5.1.4. Results of Benchmarking/Validation Studies

Equation (1) has given a fair simulation of aerosol distribution of the suspended aerosol mass in LACE (Ref. D.5-3). Good data on controlled experiments on mixed aerosols are, however, sparse, and it is possible that Eq. (1) has not been sufficiently tested as some of the apparently good comparison of the simulation with the data could have been fortuitous (because of compensating errors from the rate process models or ex-post-facto adjustments).

D.5.1.5. Identified Deficiencies and Options for Model Improvements

While the limitations of Eq. (1) are apparent (neglect of density, charge, shape, and species effects), any efforts towards use of improved equations will entail major time commitments and expenditures.

D.5.1.6. Importance of Model to Prediction of Dominant Phenomena

Use of a correct equation is crucial to the source term calculations. Equation (1) is an approximation to the correct equation for multispecies aerosols. The correct equation is known. Its numerical solution, however, would be quite challenging. Also, the rate process data base needed for solving the correct equation is limited. Also, the containment loading is affected by condensation of steam on particles.

D.5.1.7. Technical Adequacy of Model and Documentation

Equation (1) could be reasonably good for scenarios where the inherent approximations are justified. But, without recourse to the analysis with the more general equations or availability of data from controlled experiments on mixed aerosols that challenge Eq. (1) fully, it is not possible to regard this equation as technically adequate for all situations of interest.

Equation (1) is stated quite clearly in the document. The nature of the approximations, however, should be described more fully. In view of the approximations the equation does not converge to the general multicomponent equation as the number of the bins is increased.

Rather than using Eq. (1), a model based upon Eq. (2), with further inclusion of charge, shape, and species effects, is needed for a realistic description of aerosol behavior. The technical adequacy of the model based upon Eq. (1) is classified as Category 4.

D.5.2. Agglomeration:

D.5.2.1. Model Description and Pedigree

CONTAIN uses the expressions:

Process	Model (Expression), $\beta = \beta_B + \beta_G + \beta_T$; (m^3 / s)	Pedigree (Reference)
Brownian	$\beta_B = 2\pi(D_{p,i} + D_{p,j})(\gamma_i d_{p,i} + \gamma_j d_{p,j}) / F$	Ref. D.5-4 γ are ad-hoc
Gravitational	$\beta_G = \varepsilon(d_{p,i} / d_{p,j}) \frac{\pi}{4} (\gamma_i d_{p,i} + \gamma_j d_{p,j})^2 v_{s,i} - v_{s,j} $ where, the collisional efficiency ε is $\varepsilon(d_{p,i} / d_{p,j}) = \frac{3}{2} \frac{(d_{p,i} / d_{p,j})^2}{(1 + (d_{p,i} / d_{p,j}))^2} \quad , \quad d_{p,i} \leq d_{p,j}$	Ref. D.5-5 γ are ad-hoc
Turbulent	$\beta_T = \sqrt{\beta_{T,1}^2 + \beta_{T,2}^2}$ $\beta_{T,1} = \sqrt{\frac{\pi \varepsilon_T}{120 \nu}} (\gamma_i d_{p,i} + \gamma_j d_{p,j})^3$ $\beta_{T,2} = \frac{0.04029 \rho_g^{1/4} \varepsilon_T^{3/4}}{\mu^{5/4}} (\gamma_i d_{p,i} + \gamma_j d_{p,j}) \times$ $\left \frac{\rho_{p,i} C_{m,i} d_{p,i}^2}{\chi_i} - \frac{\rho_{p,j} C_{m,j} d_{p,j}^2}{\chi_j} \right $	Ref. D.5-6 γ are ad-hoc

The code takes:

$$C_{m,i} = 1 + N_{Kn,i} \left[1.37 + 0.4 \exp(-1.1 / N_{Kn,i}) \right] ,$$

which is slightly different from

$$C_m = 1 + N_{Kn} \left[1.257 + 0.4 \exp(-1.1 / N_{Kn}) \right]$$

taken in the deposition calculations. Also, the diffusion coefficient is

$$D_{p,i} = \frac{k_B T C_{m,i}}{3\pi d_{p,i} \mu \chi_i}$$

and the nondimensional interpolating factor F is given as

$$F = \frac{d_{p,i} + d_{p,j}}{d_{p,i} + d_{p,j} + 2g_{i,j}} + \frac{8(D_{p,i} + D_{p,j})}{\bar{v}_{i,j}(d_{p,i} + d_{p,j})},$$

where

$$g_{i,j} = \sqrt{g_i^2 + g_j^2}; \quad g_i = \frac{1}{3d_{p,i}\ell_i} |(d_{p,i} + \ell_i)^3 - (d_{p,i}^2 + \ell_i^2)^{3/2}| - d_{p,i}; \quad \ell_i = \frac{8D_{p,i}}{\pi v_i}$$

$$\bar{v}_{i,j} = \sqrt{v_i^2 + v_j^2}; \quad v_i = \sqrt{\frac{8k_B T}{\pi m_{p,i}}}.$$

In the above, N_{Kn} is the Knudsen number. Other nomenclature is explained in the code manual. The Brownian agglomeration is effective for small particle (diameters <1.0 microns), while the gravitational agglomeration is effective for larger particles.

D.5.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Agglomeration is a mass conserving but number reducing process that shifts particle distribution towards larger sizes (that is, the mean particle size increases). The larger particles diffuse (to the surfaces) more slowly, but they settle (on the floors) more rapidly; they also offer comparatively smaller surface area for condensation/reactions. For any dense aerosol (number concentration > 10^7 /cm³), accurate modeling of agglomeration is essential to good predictive abilities. The CONTAIN models are reasonable, but there are many limitations that are discussed below.

D.5.2.3. Results of Model Sensitivity Studies

CONTAIN sensitivity studies (Ref. D.5-7) have shown that that the calculated (suspended aerosol mass, etc.) results are strongly dependent on the values chosen for the various quantities in the agglomeration models.

D.5.2.4. Results of Benchmarking/Validation Studies

The use of the models, in conjunction with Eq. (1), has given a fair simulation of aerosol distribution in several large scale experiments. Good data on controlled experiments on mixed aerosols are however sparse. For mixed aerosols, there have been no separate-effect tests for the individual agglomeration models and the models must be regarded as unvalidated.

D.5.2.5. Identified Deficiencies and Options for Model Improvements

Information on agglomeration kernels of multicomponent aerosols is practically nonexistent. CONTAIN uses single species expressions, both because of this reason, and also because the CONTAIN GDE, Eq. (1), cannot treat the density dependence of particles. Of the three kernels of the table, the Brownian kernel can be regarded as the better established (it is an interpolator expression that compares well with the results based on numerical solutions of the Boltzmann equation, Ref. D.5-8). The gravitational kernel of the table is not correct in its functional dependence; reasons are discussed extensively in the open literature. Indeed better models are available. There are questions of a generic nature

about the Safman-Turner kernel, as modeling of turbulence remains beset with difficulties. Thus, there are two problems: (1) a limited scientific database for mixed aerosols, and (2) that CONTAIN uses an incorrect model for gravitational agglomeration (see Refs. D.5-2 and D.5-9 through 13 for models that better capture the true physics).

D.5.2.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct agglomeration models is crucial to source term calculations.

D.5.2.7. Technical Adequacy of Model and Documentation

For a single-component, spherical aerosol, the CONTAIN model for Brownian agglomeration is adequate, while that for gravitational agglomeration is inadequate (it does not capture known physics as captured by models available in the literature). The adequacy of the turbulent agglomeration model cannot be ascertained (it may or may not be adequate as the scientific basis of turbulence modeling is still not firm). For mixed-component aerosols that the CONTAIN approximate GDE seeks to model, none of the three agglomeration models is adequate. First, the CONTAIN GDE does not display fidelity to correct models where they are available (e.g., the Brownian agglomeration model). Second, there is only very limited information (theoretical/experimental) in the literature on gravitational/turbulent agglomeration of mixed aerosols. Some available theoretical results (Ref. D.5-9) do indicate, however, that the mixed aerosol agglomeration process can be significantly different from those of single component aerosols. The technical adequacy of this model is assessed as Category 4.

D.5.3. Deposition

D.5.3.1. Model Description and Pedigree

For a particle of diameter d_p and density ρ_p , for deposition velocities (m/s) CONTAIN uses the expressions:

Process	Model (Expression) $R = R_{diff} + R_s + R_{therm} + R_{dep}; (1/s)$	Pedigree (Ref.)
Brownian	$v_{diff} = \frac{k_B TC_m}{3\pi\mu d_p \Delta}, \quad R_{diff} = \frac{A_{wall} v_{diff}}{V_{chamber}}$	assumed standard
Gravitational	$v_s = \frac{\frac{1}{6} \pi d_p^3 \rho_p g C_m}{3\pi\mu d_p \chi}, \quad R_s = \frac{A_{floor} v_s}{V_{chamber}}$	assumed standard

Thermophoresis	$v_{\text{therm}} = \frac{1.5\mu C_m (C_l N_{Kn} + k_{\text{gas}} / k_p) \nabla T}{\chi \rho_{\text{gas}} T (1 + 3C_m N_{Kn}) (1 + 2C_l N_{Kn} + 2k_{\text{gas}} / k_p)}$ $R_{\text{therm}} = \frac{A_{\text{wall}} v_{\text{diff}}}{V_{\text{chamber}}}$	Ref. D.5-14
Stefan flow /diffusiophoresis	$v_{\text{dep}} = \left[\frac{\gamma_1 \sqrt{M_w}}{\gamma_1 \sqrt{M_w} + \gamma_2 \sqrt{M_{w,NC}}} \right] \left[\frac{\dot{m}_{\text{tr}}}{\rho_w A_{\text{as}}} \right], \quad R_{\text{dep}} = \frac{A_{\text{wall}} v_{\text{dep}}}{V_{\text{chamber}}}$	Ref. D.5-15

The nomenclature is explained in the code manual. The Brownian deposition is effective for small particle (diameters <1.0 microns), while the gravitational settling is effective for larger particles. The thermophoretic velocity is significant for large temperature gradients, while the stefan flow/diffusiophoresis is important in condensing conditions. The dynamic shape factor χ accounts for nonspherical particle effects .

D.5.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Deposition reduces particle number as well as mass from the suspension, and it is the most important natural removal process. The CONTAIN models for diffusive and gravitational settling are appropriate for a single-species spherical aerosol in a stagnant atmosphere. Both the shape factor $\chi \geq 1$ and the boundary layer thickness parameter $\Delta \sim 10^{-5}$ m are, however, empirical, and subject to question. It is not clear as to why the particles are assumed nonspherical only with respect to settling (the factor χ is used in some places, and not in others. It is also not clear as to why this factor should be the same for the gravitational settling and the diffusive motion). Note that the diffusion layer thickness can be adjusted to account for the enhanced deposition in a well-mixed environment. No similar adjustment is prescribed for the gravitational settling.

There are several questions regarding the thermophoretic and Stefan flow/diffusiophoresis models. As discussed below, these models are not adequate, first the rate expressions, and then the manner in which the homogenization is carried out (to convert the spatially dependent aerosol general dynamic equation to the homogenized equation).

D.5.3.3. Results of Model Sensitivity Studies

CONTAIN sensitivity studies (Ref. D.5-7) have shown that the calculated (suspended aerosol mass, etc.) results are strongly dependent on the values chosen for the various quantities in the deposition models.

D.5.3.4. Results of Benchmarking/Validation Studies

The use of the models, in conjunction with Eq. (1), has given a fair simulation of aerosol distribution in several large-scale experiments. Good data on controlled experiments on mixed aerosols are, however, sparse.

D.5.3.5. Identified Deficiencies and Options for Model Improvements

To elucidate the calculation of deposition velocities, it is useful to note that without agglomeration and condensation, the single-species aerosol dynamic equation for a monodisperse aerosol is simply the continuity equation (the development below is from Williams and Loyalka):

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

where $\mathbf{J}$ is the particle current caused by the various mechanisms:

$$\mathbf{J} = \mathbf{J}_c + \mathbf{J}_d + \mathbf{J}_T + \mathbf{J}_D + \mathbf{J}_e + \dots$$

and

$$\mathbf{J}_c = \mathbf{v} n, \quad \mathbf{J}_d = -D \nabla n, \quad \mathbf{J}_T = \mathbf{v}_T n, \quad \mathbf{J}_D = \mathbf{v}_D n, \quad \mathbf{J}_e = \mathbf{v}_e n$$

are, respectively, the convective, diffusive, thermophoretic, diffusiophoretic, and external force induced currents. In the above $\mathbf{v}$ is the convective (hydrodynamic, or mean mass) velocity, D is the particle diffusion coefficient, $\mathbf{v}_T$ is the thermophoretic velocity, $\mathbf{v}_D$ is the diffusiophoretic velocity, and $\mathbf{v}_e$ is the velocity of the aerosol induced by external forces (for example gravity). Here $n(\mathbf{r}, t)$ is the particle concentration at $(\mathbf{r}, t)$. Note that the diffusive and other currents are calculated with respect to the hydrodynamic current.

To develop basic correlations for the deposition currents and deposition rates, one considers the steady-state or time-averaged equation:

$$\nabla \cdot \mathbf{J} = 0 \tag{2}$$

subject to appropriate boundary conditions. The complete solution would require calculation of the velocity, U , and temperature and molecular concentrations (for $\mathbf{v}_T$ and $\mathbf{v}_D$) from the Navier-Stokes and/or Boltzmann equations for the gas. These latter may be coupled to the particle equations. Boundary conditions associated with Eq. (2) may be specified as:

$$n(\mathbf{r}) = 0, \quad \mathbf{r} \in \partial s^+,$$

where ∂s^+ indicates an extrapolated surface of the body at which the particle concentration essentially vanishes. Also, far away from the body, at the edge of the concentration boundary layer, we assume that the particle concentration has some specified value, n_∞ :

$$\lim_{|\mathbf{r}| \rightarrow \infty} [n(\mathbf{r})] = n_\infty.$$

Equation (2) then is solved for $n(\mathbf{r})$ and $\mathbf{J}$. The deposition rate, j (#/time), is obtained from:

$$j = - \int \mathbf{J}(\mathbf{r}) \cdot d\mathbf{S},$$

where $d\mathbf{S}$ is the surface element. Note that the local deposition rate coefficient, $k(\mathbf{r})$ (cm/s), also referred to as the deposition velocity, V_d , is defined as:

$$k(\mathbf{r}) = - \frac{1}{n_\infty} (\mathbf{J} \cdot \mathbf{e}_s) = \left| -D \frac{1}{n_\infty} \nabla n \cdot \mathbf{e}_s \right|,$$

where $\mathbf{e}_s$ is a unit vector normal to the surface of the body at the point, $\mathbf{r}$, directed into the gas. Thus:

$$j = n_\infty \int k(\mathbf{r}) dA.$$

Actually, the particle continuity equation is no different from an equation we might have written for convective mass transfer or deposition of molecular species (except that instead of thermophoresis we would have thermal diffusion, etc.). Also, it is similar to the energy equation of the Navier-Stokes equations. To further clarify, the heat and mass transfer analogies, we note that the energy equation is:

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{J}_q = 0,$$

where T is the temperature, ρ is the mass density, C_p is the heat capacity, and $\mathbf{J}$ is the energy (heat) current:

$$\mathbf{J}_q(\mathbf{r}, t) = \rho C_p \mathbf{v} T(\mathbf{r}, t) - k \nabla T(\mathbf{r}, t).$$

The heat flux at the wall is given by:

$$\mathbf{J}_q = [-k \nabla T(\mathbf{r}) \cdot \mathbf{e}_s(\mathbf{r})] \quad ; \quad \mathbf{r} \in \partial S$$

with the heat transfer coefficient defined as:

$$h = \frac{J_q}{\Delta T} = \frac{J_q}{T_\infty - T(0)}$$

We consider typical flow problems for which we can assume constant properties. Introducing the definitions:

$$\hat{u} = \frac{\mathbf{v}}{U_\infty}, \quad \hat{\mathbf{r}} = \frac{\mathbf{r}}{L}, \quad \hat{n} = \frac{n}{n_\infty}, \quad \hat{T} = \frac{T - T(0)}{T_\infty - T(0)}$$

and retaining only the convective and diffusive (conductive) parts, we can write the steady state particle continuity and energy equations as (with Pe as the Peclet Numbers):

$$\hat{u} \cdot \hat{\nabla} \hat{n} = \frac{1}{Pe} \hat{\nabla}^2 \hat{n}$$

and

$$\hat{u} \cdot \hat{\nabla} \hat{T} = \frac{1}{Pe_{th}} \hat{\nabla}^2 \hat{T},$$

and we have the similarity in the solutions. Such similarity, while it holds between the continuity equation with diffusion and the energy equation, does not hold between the continuity equation with thermophoretic/Stefan flow motion and the energy equation. For the development of a correct expression for the thermophoretic deposition velocity one needs to consider solution of the continuity equation with convection, diffusion and the thermophoresis all together. In this case the boundary layer structure is more complicated, as one must deal first with the bulk convective/thermophoretic flow, then a thermophoretic/diffusive flow in a buffer layer, and finally the diffusive flow near the surface. Details of how such calculations are carried out are discussed in the Chapter 7 of Ref. D.5-2, as well as Ref. D.5-16.

It should also be noted that the respective Brock and Waldmann expressions for thermophoresis and Stefan flow/diffusiophoresis while still useful, are not the state of the art. The cited references (Refs. D.5-17 and 18 and Refs. D.5-19 through 22) report results of recent research that show that thermophoresis and diffusiophoretic motions have very complex dependence on intermolecular and gas surface interaction laws not captured by the Brock and Waldmann expressions.

D.5.3.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct deposition models is crucial to source term calculations.

D.5.3.7. Technical Adequacy of Model and Documentation

The models used are simple to implement. But it appears that the effect of mixing (hydrodynamics) is not appropriately accounted for in the models, whether it be Brownian or gravitational, or thermophoretic and Stefan flow/diffusiophoretic where the boundary layer structure is even more complex. Also, there has not been validation of the models for mixed aerosols using separate effect experimental data.

The models are stated quite clearly in the document. There could have been a more thorough description of their applicability and validity. The manual should refer to recent work on thermophoresis and Stefan flow/diffusiophoresis to indicate that the CONTAIN models would need to be refined. The technical adequacy of this model is classified as Category 2 for Brownian and gravitational deposition, and Category 4 for thermophoretic and Stefan flow/diffusiophoretic deposition.

D.5.4. Steam Condensation/Evaporation

D.5.4.1. Model Description and Pedigree

For a particle of diameter d_p , for condensation/evaporation rate (kg/s), CONTAIN uses either the expression (see Eq. 7.6 in the CONTAIN manual, used in the fixed grid calculations)

$$\frac{dm}{dt} = \frac{4\pi r(SSAT - 1)}{\left[\frac{M_w h_{lg}^2}{k_{gas} RT^2} + \frac{1}{\rho_{sat} \mathfrak{D}} \right]} \quad (3)$$

or the expression (see Eq. 7.7 in the manual, used in the moving grid calculations)

$$\frac{dm}{dt} = \frac{2\pi d_p \rho_w \left[\frac{Q_s}{Q_{eq}} - a_w \exp \left[\frac{4\sigma M_w}{RT \rho_w d_p} \right] \right]}{\frac{\rho_w}{Q_{eq} \mathfrak{D}} + \frac{h_{lg} \rho_w}{k_{gas} T} \left[\frac{M_w h_{lg}}{RT} - 1 \right]}, \quad (4)$$

where dm/dt is the mass condensation/evaporation rate (kg/s) on particles of mass m , r is the particle radius (m), $SSat$ is the supersaturation ratio, M_w is the molecular weight of water (kg/kg Mol), h_{lg} is the latent heat of vaporization (J/kg), k_{gas} is the gas thermal conductivity (J/m s K), R is the universal gas constant (J/kg Mol K), T is the temperature (K), ρ_{sat} is the saturated steam density (kg/m³), and $\mathfrak{D}$ is the steam diffusivity (m²/s). Also d_p is the particle diameter (m), ρ_w is the density of water (kg/m³), a_w is the activity of water, and σ is the surface tension (N/m). Q_s is the actual steam concentration (kg/m³) and Q_{eq} (kg/m³) is the equilibrium steam concentration. Both of these expressions essentially derive from the work of Mason, Ref. D.5-23 [the manual cites Byers, Ref. D.5-24, for the Eq.(3) and due to an oversight Reidel should be Pruppacher and Klett, Ref. D.-25) for Eq. (4)]. SNL staff should check if Eq. (4) is really what is being used in the code. Pruppacher and Klett have a different equation in which the vapor diffusivity and the gas thermal conductivity are modified to account for the Knudsen effects. If the code used the original Pruppacher-Klett equation, then SNL should document the values of the accommodation coefficients that were used.

D.5.4.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

It would appear that $Q_{eq} = \rho_{sat}$ and $SSat = Q_s / Q_{eq}$. Thus both Eqs. (3) and (4) can be cast, respectively, into the forms:

$$\frac{dm}{dt} = \frac{2\pi d_p \left[\frac{Q_s}{Q_{eq}} - 1 \right]}{\left[\frac{M_w h_{lg}^2}{k_{gas} R T^2} + \frac{1}{\rho_{sat} \bar{D}} \right]} \quad (5)$$

and

$$\frac{dm}{dt} = \frac{2\pi d_p \left[\frac{Q_s}{Q_{eq}} - a_w \exp \left[\frac{4\sigma M_w}{RT \rho_w d_p} \right] \right]}{\frac{1}{Q_{eq} \bar{D}} + \frac{M_w h_{lg}^2}{R k_{gas} T^2} - \frac{h_{lg}}{k_{gas} T}} \quad (6)$$

Both these expressions are then essentially the same, except for an additional term in the denominator of the expression (6). The expression (6) includes the solute effects through a_w and the Kelvin effect through the exponential term. It is known that the fixed grid does not work well for condensation, but the manual does not clarify as to why the expression (5) is needed at all. The different forms in which Eqs. (3) and (4) are used, and the nomenclature is unnecessarily confusing. Note that for all practical situations the last term in the denominator of (6) is small, and one essentially has for the condensation rate,

$$\frac{dm}{dt} = \frac{2\pi d_p \left[\frac{Q_s}{Q_{eq}} - a_w \exp \left[\frac{4\sigma M_w}{RT \rho_w d_p} \right] \right]}{\frac{1}{Q_{eq} \bar{D}} + \frac{M_w h_{lg}^2}{R k_{gas} T^2}} \quad (7)$$

The Eq. (7) is applicable to the growth of large spherical particles ($d_p \geq 1.0 \mu m$).

D.5.4.3. Results of Model Sensitivity Studies

CONTAIN sensitivity studies in regards to the dependence of the calculated results (suspended aerosol mass, etc.) on the model parameters have not been reported. Reference D.5-26 suggests, however, that the calculations would be quite sensitive to parameters in the condensation models.

D.5.4.4. Results of Benchmarking/Validation Studies

The use of the models, in conjunction with Eq. (3), has given a fair simulation of aerosol distribution in several large-scale experiments. Good data on controlled experiments on mixed aerosols are sparse, however, and it is possible that the model has not been sufficiently tested as some of the apparently good comparison of the simulation with the data could have been fortuitous (because of compensating errors from several processes or ex-post-facto adjustments).

D.5.4.5. Identified Deficiencies and Options for Model Improvements

A generalization of the Mason equation for all particle sizes is available in the literature (see Refs. D.5-2 and 19). This generalized equation is:

$$\bar{u} = 4\pi \bar{a} D \rho_s (S-1) \frac{f_c(Kn_c) f_h(Kn_h)}{\frac{LD}{\lambda} \rho_s \frac{L m_v}{k T_\infty^2} f_c(Kn_c) + f_h(Kn_h)}, \quad (8)$$

where the various quantities are defined in the original paper and in Ref. D.5-2. The factors f_c and f_h account for the noncontinuum corrections. The activity and the Kelvin effects are simply included in this equation by replacing $S-1$ by

$$S - a_w \exp \left[\frac{4\sigma M_w}{RT \rho_w d_p} \right]$$

In the CONTAIN notation, the Eq.(8) then simply becomes:

$$\frac{dm}{dt} = 2\pi d_p \frac{\left[\frac{Q_s}{Q_{eq}} - a_w \exp \left[\frac{4\sigma M_w}{RT \rho_w d_p} \right] \right] f_c(Kn_c) f_h(Kn_h)}{\frac{M_w h_{fg}^2}{Rk_{gas} T^2} f_c(Kn_c) + \frac{1}{Q_{eq} \bar{\Theta}} f_h(Kn_h)} \quad (9)$$

This equation should then be preferred over the Eq. (7) for calculations of growth of particles of all sizes. Its implementation in CONTAIN would be a trivial matter (note that the Eqs.(13-28) in Pruppacher and Klett also have Knudsen corrections, obtained by a variant of the somewhat less accurate but reasonably good Fuchs boundary sphere method). In particular note that Eq. (8) could be written as:

$$\frac{dm}{dt} = 2\pi d_p \frac{\left[\frac{Q_s}{Q_{eq}} - a_w \exp \left[\frac{4\sigma M_w}{RT r_w d_p} \right] \right]}{\frac{M_w h_{fg}^2}{Rk'_{gas} T^2} + \frac{1}{Q_{eq} \bar{\Theta}'}} \quad (10)$$

where

$$k'_{gas} = k_{gas} / f_h(Kn_h), \quad \bar{\Theta}' = \bar{\Theta} / f_c(Kn_c) \quad (11)$$

The restriction on the number of aerosol size classes that may be used has, on occasion, prevented converged solutions from being obtained when modeling some large-scale experiments, including condensation onto airborne aerosols (Refs. D.5-27 and 28). The code should be generalized to allow any number of size classes to be used; one approach is described in Ref. D.5-29. The implementation of the Kelvin effect model was found to be inconsistent with the assumption of a uniform composition within a size class. One approach to overcoming the inconsistency is described in Ref. D.5-30.

D.5.4.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct condensation model is crucial to source term calculations.

D.5.4.7. Technical Adequacy of Model and Documentation

The model used is simple to implement. It needs to be extended to all size ranges. This can be accomplished in a very straightforward manner. The model should be modified to allow use of more size classes and the implementation of the Kelvin effect model should be made consistent with the assumption of a single composition in each size class.

The model is stated quite clearly in the document. There could have been a more thorough description of the model's application range and validity.

The technical adequacy of this model is classified as Category 4.

D.5.5. Removal by Engineered Safety Features

D.5.5.1. Model Description and Pedigree

The CONTAIN manual does not explain the incorporation of aerosol removal terms (due to ESFs) in the Eq. (1) very clearly, and from the pages 7-22 to 7-31 one can only surmise as to how these removal terms may have been incorporated. For example on page 7-22 it is indicated that "These sources (that is, the term S in Eq. D.5.1.1 (1)) may include aerosol removal by other models (for example, ESF's)." What follows on pages 7-23 to 7-31 does not make explicit the connection of these removal terms with the source term, rather the removals are discussed in terms of a Dep_{df} (deposition decontamination factor), Eq. (7-15) and collection efficiencies, E, Eq. (7-16)-(7-25). One suspects that a more natural relationship of the removal by the ESFs is with the R terms in Eq. D.5.1.1 (1), and in the following we will make this assumption.

Fan Cooler: It appears that the CONTAIN uses the formulation:

$$\frac{dQ_{fk}(t)}{dt} = -RQ_{fk}(t),$$

where the removal coefficient R (1/s) is expressed as

$$R = \left[\frac{\gamma_1 \sqrt{M_w}}{\gamma_1 \sqrt{M_w} + \gamma_2 \sqrt{M_{w,NC}}} \right] \left[\frac{\dot{m}_{tr}}{\rho_w A_{as}} \right] \frac{A_{as}}{V_{cooler\ cell}}.$$

Containment Spray: We surmise that the model used for removal is:

$$\frac{dQ_{fk}(t)}{dt} = - \left(\int dV_{drop} \frac{\pi d_{drop}^2}{4} \epsilon |v_{s,drop} - v_{s,p}| n_{drop}(V_{drop}, t) \right) Q_{fk}(t),$$

where d_{drop} is the drop(spray) diameter (m), $v_{s,\text{drop}}$ is the drop settling velocity (m/s), $v_{s,p}$ is the particle settling velocity (m/s), ϵ (or E, in CONTAIN nomenclature) is the collisional (collection) efficiency (dimensionless), and $n(V_{\text{drop}},t)dV_{\text{drop}}$ is the number of drops of volume V_{drop} in unit volume (m^3). One has

$$\frac{dQ_{\epsilon k}(t)}{dt} = -RQ_{\epsilon k}(t),$$

where the removal coefficient R (1/s), assuming the drops to be monodisperse, and $v_{s,p} \ll v_{s,\text{drop}}$, is expressed as

$$R = \frac{\pi d_{\text{drop}}^2}{4} \epsilon v_{s,\text{drop}} n_{\text{drop}}(t),$$

and $n_{\text{drop}}(t)$ is the number of drops of the diameter d_{drop} in a unit volume ($\#/\text{m}^3$) at time t . The models used for the collisional efficiency are noted below. In some cases these expressions are interpolated.

Models for the Collisional Efficiency ϵ

Process	Model (Expression)	Pedigree (Reference)
Interception	$\epsilon_{l,\text{viscous}} = \frac{3}{2} \left(\frac{d_p}{d_{\text{drop}}} \right)^2, \epsilon_{l,\text{potential}} = 3 \left(\frac{d_p}{d_{\text{drop}}} \right)$	Ref. D.5-5: This expression for efficiency in the potential flow regime neglects boundary layer effects around the spray drop. If boundary layer effects are included, the functional form of the equation is changed and the predicted efficiencies are much lower than the estimates produced by the equation shown here (Ref. D.5-31).

	<p>For viscous flow</p> $\varepsilon_{ll,v} = 0, \quad N_{st} \leq 1.214$ $\varepsilon_{ll,v} = \left[1 + \frac{0.75 \ln(2N_{st})}{N_{st} - 1.214} \right], \quad N_{st} > 1.214$ <p>where N_{st} is the Stokes Number. And for Potential Flow</p>	Ref. D.5-5
Inertial	$\varepsilon_{ll,p} = 0, \quad N_{st} \leq 1/12$	
Impaction	$\varepsilon_{ll,v} = \left[\frac{N_{st}}{N_{st} + 1/2} \right]^2, \quad N_{st} \geq 0.2$ <p>linear interpolation is used for $N_{st} \in (1/12, 0.2)$,</p>	

<p>Brownian diffusion</p>	$\varepsilon_B = \frac{4D_p}{v_{s,drop} d_{drop}} \left(2 + 0.6 N_{Re,drop}^{1/2} N_{Sc,p}^{1/3} \right)$ <p>where D_p is the particle diffusion coefficient. The details of the derivation are as follows:</p> $\frac{v_{deposition} d_{drop}}{D_p} = N_{Sh}$ $\Rightarrow R = v_{deposition} \pi d_{drop}^2 n_{drop}(t) = \frac{D_p}{d_{drop}} N_{sh} \pi d_{drop}^2 n_{drop}(t)$ <p>Since, by definition of ε_B</p> $R = \frac{\pi d_{drop}^2}{4} \varepsilon_B v_{s,drop} n_{drop}(t)$ <p>it follows that:</p> $\varepsilon_B = \frac{4D_p}{v_{s,drop} d_{drop}} N_{Sh}$ <p>The Sherwood Number is taken to be:</p> $N_{Sh} = \left(2 + 0.6 N_{Re,drop}^{1/2} N_{Sc,p}^{1/3} \right)$	<p>Is based on a standard formula on convection-diffusion to spheres.</p>
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<p>Thermophoresis</p>	$\varepsilon_T = \frac{4C_{th}}{v_{s,drop}d_{drop}} \left(2 + 0.6N_{Re,drop}^{1/2} N_{Pr,gas}^{1/3} \right) (T_{gas} - T_{drop})$ <p>where,</p> $C_{therm} = \frac{1.5v_{gas}C_m(C_tN_{Kn} + k_{gas}/k_p)}{\chi T(1 + 3C_mN_{Kn})(1 + 2C_tN_{Kn} + 2k_{gas}/k_p)}$ <p>The derivation is as follows: Writing the thermophoretic velocity as,</p> $v_T = -K \frac{v_{gas}}{T} \nabla T$ <p>and the heat current as,</p> $J_q = -k_{gas} \nabla T = N_{Nu} \frac{(T_{gas} - T_{drop})k_{gas}}{d_{drop}}$ <p>one obtains, on eliminating ∇T,</p> $v_{deposition} = v_T = \frac{v_{gas}}{d_{drop}} K \frac{(T_{gas} - T_{drop})}{T} N_{Nu}$ $\Rightarrow R = v_{deposition} \pi d_{drop}^2 n_{drop}(t)$ $= \frac{v_{gas}}{d_{drop}} K \frac{(T_{gas} - T_{drop})}{T} N_{Nu} \pi d_{drop}^2 n_{drop}(t)$ <p>Since, by definition of ε_B</p> $R = \frac{\pi d_{drop}^2}{4} \varepsilon_T v_{s,drop} n_{drop}(t)$ <p>it follows that:</p> $\varepsilon_T = \frac{4v_{gas}}{v_{s,drop}d_{drop}} K \frac{(T_{gas} - T_{drop})}{T} N_{Nu}$ <p>we take:</p> $N_{Nu} = \left(2 + 0.6N_{Re,drop}^{1/2} N_{Pr,gas}^{1/3} \right)$	<p>Is based on a combination of a standard formula on convection-conduction to spheres and thermophoretic velocity. But the derivation is flawed as the boundary layer structure is more complicated, as discussed in conjunction with deposition on structures.</p>
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Stefan flow/ diffusiophoresis	$\epsilon_{df} = \frac{4C_{df}}{v_{s,drop} d_{drop}} \left(2 + 0.6 N_{Re,drop}^{1/2} N_{Sc,p}^{1/3} \right) \ln \left[\frac{P_g - P_{v,d}}{P_g - P_2} \right]$ <p>where,</p> $C_{df} = D_v \frac{\sqrt{M_1}}{\gamma_1 \sqrt{M_1} + \gamma_2 \sqrt{M_2}},$ <p>The derivation is similar to that for thermophoresis.</p>	Is based on a combination of a standard formula on convection-diffusion to spheres and Stefan/flow and diffusiophoretic velocity. But the development is flawed as the boundary layer structure is more complicated, as discussed in conjunction with deposition on structures.
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Ice Condenser: The condenser is modeled as a chamber of adjoining cells. Models of the Sec. D.5.3 for deposition on structures are used.

Suppression Pool: Models from the SPARC and the VANESA codes have been adopted. The manual does not contain full descriptions of these models, and it also appears that not all of the SPARC models have been implemented. For consistency, it would be appropriate to rewrite the models in the CONTAIN framework.

Note that for sprays, the Brownian diffusion is effective for removal of small particle (diameters <1.0 microns), while the interception and impaction are effective for larger particles. The sprays could also lead to an increase in the supersaturation in the containment. The thermophoretic and stefan flow/diffusiophoresis could be important in condensing conditions.

D.5.5.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The models are reasonable, but have the same kinds of limitations as discussed in the Secs. D.5.2 through D.5.4.

D.5.5.3. Results of Model Sensitivity Studies

CONTAIN sensitivity studies have shown that that the calculated (suspended aerosol mass, etc.) results are strongly dependent on the values chosen for the various quantities in the ESF models. For example, for sprays the removal is sensitive to the chosen drop diameter and the collisional efficiency models (Ref. D.5-7).

D.5.5.4. Results of Benchmarking/Validation Studies

There has been no extensive application of CONTAIN to simulate actual ESF experiments, at least as far as reports in the open literature are concerned.

D.5.5.5. Identified Deficiencies and Options for Model Improvements

Generally the observations of the Secs. D.5.1-4 apply. Since some of the ESF geometries (e. g., ice condensers) or flows (suppression pool) can be complex, the use of a homogenized aerosol dynamic equation may not always be justifiable.

D.5.5.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct removal models is important to source term calculations.

D.5.5.7. Technical Adequacy of Model and Documentation

The models used are simple to implement. But it is not clear that all of them are technically adequate, or the state of the art.

The technical adequacy of suppression pool aerosol removal model is classified as Category 4.

The technical adequacy of the ice-condenser aerosol removal model is classified as Category 2.

The technical adequacy of containment spray aerosol removal model is classified as Category 4.

The technical adequacy of the PCCS aerosol removal model is classified as Category 2.

The models, and in particular, their integration into the dynamic equation, are not stated adequately in the manual. The documentation needs to be improved.

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D.6. Fission Product Behavior

D.6.1. Model Description and Pedigree

Overall, fission products are not treated mechanistically or in detail in the CONTAIN code. There has been, however, an NRC-sponsored research effort underway at ORNL on a computer program **TRENDS** (Transport and **RE**tention of Nuclides in Dominant Sequences), wherein the focus has been on defining and solving the basic set of rate equations. The Committee was asked to review the suitability of incorporating the **TRENDS** program elements in CONTAIN. With the issuance and (apparent) adoption of the revised severe-accident code strategy and its associated revised design objectives and targeted applications for CONTAIN (see App. E), the **TRENDS** evaluation became less germane to the CONTAIN peer review. Thus, the **TRENDS** review is presented as "Other Review Findings" in Sec. 5.2.

D.6.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

See Sec. 5.2.

D.6.3. Results of Model Sensitivity Studies

See Sec. 5.2.

D.6.4. Results of Benchmarking/Validation Studies

See Sec. 5.2.

D.6.5. Identified Deficiencies and Options for Model Improvements

See Sec. 5.2.

D.6.6. Importance of Model to Prediction of Dominant Phenomena

See Sec. 5.2.

D.6.7. Technical Adequacy of Model and Documentation

See Sec. 5.2.

D.7. Combustion

D.7.1. Ignition Criteria

D.7.1.1. Model Description and Pedigree

For ignition to occur within a cell, the effective hydrogen mole fraction must exceed 7%; the effective hydrogen mole fraction is equal to the actual hydrogen mole fraction plus 0.541 times the carbon monoxide mole fraction. This expression is derived from the 7%/13% ignition criteria for hydrogen/carbon monoxide alone, respectively, using Le Chatelier's mixing rule, which states that a mixture of limiting mixtures is itself a limiting mixture.

In addition, the oxygen mole fraction must exceed 5% in the cell before combustion can commence.

The final condition to be met is that the diluent mole fraction should not exceed 55%. The diluent is taken to be the steam and carbon dioxide in the atmosphere together with 79% of any nitrogen in excess of that required to form air out of the available oxygen in the cell.

All of the above can be overwritten by the user on input.

D.7.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The ignition criteria are approximate fits to experimental data. They are a reasonable representation of the conditions under which ignition can occur in the presence of igniters for the limited range of conditions of the experiments (e.g., initial pressure = 1 bar, initial temperature between 20 and 100°C). However, ignition is not guaranteed under these conditions and the user is advised to vary the criteria in order to determine their importance to a particular scenario.

In the absence of igniters, the possible ignition sources will be less well characterized. In plant studies the initial conditions may well lie outside those used for the experiments (especially the temperature and pressure) and the atmosphere may contain more inhomogeneities. In addition the geometry is likely to be more complex.

Due to the variety and complexity of the containments that may be studied as well as the somewhat stochastic nature of ignition (if the ignition sources are not well characterized), it is appropriate that the user be left to vary the criteria parametrically to assess the various possibilities. Such sensitivity studies are extremely important as, in many cases, the default criteria give the lowest hydrogen concentration for which a burn may occur; a more energetic burn could occur if the combustible gas were allowed to concentrate further.

Some advice is given to guide the user in the choice of parameter ranges for sensitivity studies but it does not go far enough, especially in view of the nonconservative nature of the default values.

D.7.1.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.7.1.4. Results of Benchmarking/Validation Studies

The ignition criteria are themselves derived from experimental data. The Lawrence Livermore data indicate that ignition occurs, in the presence of igniters, in dry hydrogen-air mixtures at between 6 and 8% hydrogen (Refs. D.7-1 and 2). For hydrogen-air-steam mixtures, the variation is greater with ignition occurring at hydrogen concentrations greater than 7% (Refs. D.7-1 and 2). Whether the atmosphere is initially stagnant or circulating can make a significant difference.

The Whiteshell data indicate that ignition occurs when the oxygen concentration exceeds 5% in hydrogen-steam-air mixtures (Ref. D.7-1). The variability was quite low in this case.

The Whiteshell data also indicate that ignition occurs in hydrogen-steam-air mixtures for mixtures with less than approximately 55% steam (Ref. D.7-1).

D.7.1.5. Identified Deficiencies and Options for Model Improvements

Some advice is given to guide the user in the choice of parameter ranges for sensitivity studies but it does not go far enough, especially in view of the nonconservative nature of the default values. Some idea of the maximum hydrogen concentration that could build up before ignition is likely to occur, for a given ignition source strength, would be very useful.

D.7.1.6. Importance of Model to Prediction of Dominant Phenomena

The ignition criteria determine the conditions for a burn to occur and in particular the amount of hydrogen in the cell when combustion commences. The ignition criteria are therefore very important to containment pressurization.

As combustion is likely to result in the revaporization/resuspension of deposited fission products the ignition criteria will also effect the source term via the size, timing, and frequency of any burns

D.7.1.7. Technical Adequacy of Model and Documentation

For well-characterized igniters in well-mixed, relatively featureless volumes, the ignition criteria are reasonably well understood for low initial temperatures and pressures. For much higher temperatures, the BSR model can be used.

For poorly characterized ignition sources in more complex geometries or with initial conditions outside of those studied in the experiments, ignition takes on a more stochastic nature. This is appropriately treated in the code by allowing the user the freedom to perform sensitivity studies on the criteria.

Some advice is given to guide the user in the choice of parameter ranges for sensitivity studies but it does not go far enough, especially in view of the nonconservative

nature of the default values. This concern is being addressed in the preparation of the final version of the manual.

The technical adequacy of this model is classified as Category 2.

D.7.2. Mode of Combustion

D.7.2.1. Model Description and Pedigree

The code determines which form of combustion will take place, depending on the conditions in a given cell and the parameter values chosen by the user for the different combustion options.

The combustion modes available in the code are: deflagration, DFB, and BSR. The conditions under which a deflagration is modeled by the code are discussed in subsection D.7.1 above.

Bulk spontaneous recombination is intended for use if the temperature in a cell reaches the auto ignition temperature, e.g., during DCH or in a source room during hot hydrogen injection. BSR is modeled if either the gas temperature in the cell exceeds a critical value (default = 773 K) or the debris temperature and mass concentration (during DCH) exceed critical values (defaults are 773 K and 1 kg/m^3 , respectively). Bulk spontaneous recombination is allowed to occur during diffusion flame burning, but not during a deflagration.

The diffusion flame model is included to allow the continuous burning of incoming fuel. This option is activated in the following circumstances. First, an ignition source must be present, i.e., either igniters are present or the BSR criteria are met. Second, the temperature of the incoming gas must exceed a user-specified threshold (default = 1000 K). Third, there must be sufficient oxygen in the receiving cell (default = 5%). Also the diluent mole fraction must be below a critical value (default = 55%). The mass flow of the incoming gas must be above a threshold value (default = 0 kg/s). Finally, the diluent to combustible mole fraction in the incoming gas must be below a critical value (default = 9.0).

D.7.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The important burning modes are represented by first- or zeroth-order models, with the exception of detonations. Due to the multi-dimensional nature of detonations it would not be appropriate to attempt to represent them in a lumped-parameter code such as CONTAIN. It is worth noting that in spray de-inerting burn experiments in the SURTSEY facility, when the sprays were activated, "detonation conditions" were attained, but only a slow deflagration ensued (Ref. D.7-3).

The ignition criteria for deflagrations are discussed in subsection D.7.1.

The ignition criteria at high temperature are not known. It is therefore important to have the facility in the code to allow the hydrogen to burn during high-temperature events, such as DCH, even if the low-temperature ignition criteria are not met. The BSR model provides a parametric way of achieving this. The default value of the threshold temperature is in the range of reported minimum autoignition temperatures, though the minimum

autoignition temperature is a function of the combustible gas and diluent concentrations (Ref. D.7-1), which is not allowed for in the code.

Similarly the diffusion flame model provides a parametric method of deciding whether the hydrogen should burn continuously as it enters the cell. The default values for the flame stability criteria may not be appropriate for all calculations and the user is referred to several papers for ideas on how to estimate some of the parameters (Refs. D.7-4 through 7).

D.7.2.3. Results of Sensitivity Studies

In Ref. D.7-8 it is noted that forcing a hydrogen burn to take place in Surry plant calculations of DCH resulted in pressure rises 2-3 bars higher than with the default burn criteria, which predicted that combustion was steam inerted.

D.7.2.4. Results of Benchmarking/Validation Studies

Deflagrations are discussed in subsection D.7.1.

Experimental data indicate that the auto-ignition temperature can be considerably higher than the default value of 773 K used in the code for the initiation of BSR and is a function of combustible and diluent concentrations.

D.7.2.5. Identified Deficiencies and Options for Model Improvements

If simple models exist to estimate the criteria for diffusion flame burning, they should be included in the code.

D.7.2.6. Importance of Model to Prediction of Dominant Phenomena

It is estimated in Refs. D.7-8 through 10 that hydrogen combustion during DCH can be a major contributor to containment pressurization, if it occurs. The mode of combustion can effect the burn completeness and therefore the pressurization due to the burn. For example if hydrogen produced during DCH burns but the pre-existing hydrogen in the containment does not, then the pressurization can be significantly less than if all the hydrogen burns; this might be represented in CONTAIN calculations as the difference between diffusion flame burning and bulk spontaneous recombination.

The choice of burn mode is therefore important to containment pressurization and thermal loading and consequently also to fission product revaporization.

D.7.2.7. Technical Adequacy of Model and Documentation

The choice of burn mode is uncertain and this is reflected in the parametric way in which the choice is made in the code. The user is pointed to relevant literature for guidance in setting the parameters. If simple methods exist for estimating some of the parameters, it would make more sense to implement them in the code where the necessary variables are readily available for the computations. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

D.7.3. Diffusion Flame

D.7.3.1. Model Description and Pedigree

The diffusion flame model allows continuous burning of incoming combustible gases to be modeled parametrically, by the user specifying the fraction of the incoming fuel to be burned.

In addition to burning the incoming combustible gases, the code allows for the combustion of hydrogen and carbon monoxide that are entrained into the DFB jet from the surrounding atmosphere. This is not a mechanistic model; rather, it is assumed that sufficient oxygen is entrained to burn the user-specified fraction of the incoming combustible gas plus the hydrogen and carbon monoxide that must also be entrained in order to supply the required oxygen. The entrained gases are not allowed to exceed their inventories in the cell in which combustion is taking place.

The inflows from all other cells are treated separately when checking if DFB should take place and some inflows may burn while others do not. On the other hand, user input source tables to a given cell are combined into a single source before the DFB criteria are applied, so that a high steam input rate into a cell may preclude the diffusion flame burning of a combustible gas source to that cell.

D.7.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Given the uncertainty in the details of diffusion flame burning in the complex geometry of a reactor containment and in the presence of hot core debris, it is reasonable that the magnitude of the effect be estimated using the parametric model provided in the code.

D.7.3.3. Results of Sensitivity Studies

No relevant studies were presented to the Committee.

D.7.3.4. Results of Benchmarking/Validation Studies

The results from the SURTSEY IET-6 direct containment heating experiment "indicate that the hydrogen produced by the steam/metal reactions during the HPME burned as it entered the upper dome, but the pre-existing hydrogen did not undergo global combustion even though dispersed molten debris represented a significant ignition source" (Ref. D.7-11). In this test the pre-mixed hydrogen was below the flammability limit and so did not burn, though the hot gas jet carrying the debris did. This gives qualitative support to the diffusion flame model, which can represent such behavior given appropriate values of the user-defined threshold parameters. Similar behavior is reported in other tests in the IET series, where various combinations of plume combustion and/or pre-mixed hydrogen combustion are possible (Ref. D.7-12).

D.7.3.5. Identified Deficiencies and Options for Model Improvements

Neither deficiencies nor needed improvements were noted.

D.7.3.6. Importance of Model to Prediction of Dominant Phenomena

The DCH IET experimental data indicate that in some cases it is possible that the hydrogen produced during DCH may burn, whilst the pre-existing hydrogen in the containment may fail to burn. In this case the burning of the DCH hydrogen may still make a significant contribution to the pressure rise (if there is a significant amount of unoxidized metal in the melt at the time of vessel failure), though not as large a contribution as when all of the hydrogen in the containment burns.

D.7.3.7. Technical Adequacy of Model and Documentation

Though the basic physics of diffusion flames is understood the detailed behavior in the complex geometry of a reactor containment and in the presence of hot core debris is uncertain. A parametric model is provided in the code and enables the user to bound the magnitude of the effect that diffusion flame burning would have on containment pressurization. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

D.7.4. Bulk Spontaneous Recombination

D.7.4.1. Model Description and Pedigree

Two models are available to the user: the hydrogen recombination model and the bulk spontaneous recombination model. The former is a control function model, the latter a parametric model.

The hydrogen recombination feature allows hydrogen produced during DCH to be recombined with oxygen in the time step in which it is produced, providing there is enough oxygen in the cell. This feature can be turned on or off by the user.

The bulk spontaneous recombination model allows all of the hydrogen in a cell to burn at a user-defined rate, providing a set of user-specified criteria are met (see subsection D.7.2). The user is informed that the SENKIN code can be used to provide an estimate of the recombination rate.

D.7.4.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The hydrogen recombination model is similar to the diffusion flame model when applied to a DCH situation, except that it does not burn combustible gas entrained into the plume with the oxygen required to burn the DCH hydrogen, nor does it have the parametric freedom to choose the fraction of hydrogen which is burned.

During DCH the hot debris particles lofted into the atmosphere provide a possible ignition source for pre-existing hydrogen in the containment. Due to the heating effect of the airborne debris, the hydrogen may ignite even if the atmosphere composition is such that it does not satisfy the ignition criteria at low temperature. The conditions under which the pre-existing hydrogen will burn (and the extent of any such burn) are uncertain. The parametric model provided allows the user to bound the magnitude of the effect.

The pessimism in the upper bound on the pressurization provided by the BSR model may be reduced by using the SENKIN code to estimate a finite rate of recombination.

D.7.4.3. Results of Sensitivity Studies

In Surry plant calculations (Ref. D.7-10), it was found that BSR (with a conservative burning rate) increased the maximum pressure attained by about 20-30%, even though much of the burning occurred on a time scale too slow to affect the predicted peak temperature.

D.7.4.4. Results of Benchmarking/Validation Studies

No relevant studies were presented to the Committee.

D.7.4.5. Identified Deficiencies and Options for Model Improvements

If the use of the SENKIN code allows significant a reduction to be made in the pessimism of the BSR calculation (relative to an instantaneous burn) then fits to SENKIN calculations should be considered for inclusion in the CONTAIN code.

D.7.4.6. Importance of Model to Prediction of Dominant Phenomena

If much of the clad is oxidized before vessel failure, there will be a considerable amount of hydrogen in the atmosphere into which the debris is discharged. The fate of this "pre-existing" hydrogen has a significant effect on the pressurization resulting from DCH. If much of the pre-existing hydrogen burns during DCH, it can significantly increase the peak pressure attained and raise the peak temperature, which may in turn increase any fission product revaporization that may occur.

D.7.4.7. Technical Adequacy of Model and Documentation

The phenomenon of hydrogen recombination during DCH is not fully understood. Parametric models are provided in the code that enable the user to bound the effect on containment pressurization. If the SENKIN code allows significant reductions to be made in the degree of pessimism in the predicted bounds then fits to SENKIN calculations should be considered for inclusion in CONTAIN. The technical adequacy of this model is classified as Category 2. The documentation is adequate.

D.7.5. Deflagration

D.7.5.1. Model Description and Pedigree

The rate of combustion is determined by dividing the amount of combustible gas to be burned (see subsection D.7.6) by the burn time. The burn time is determined by dividing the burn length by the flame speed. The burn length is a user-input parameter, which defaults to the cube root of the cell volume if not specified.

The flame speed is determined using correlations derived from experiments (Ref. D.7-13). The data used to derive the correlations were taken from the VGES, FITS, and NTS experiments (Refs. D.7-14 through 16, respectively). The experiments were performed in a premixed hydrogen-steam-air atmosphere. The correlations give the flame speed as a function of the hydrogen and steam concentrations.

The correlations are generalized to include carbon monoxide in CONTAIN by replacing the hydrogen mole fraction by the combustible gas mole fraction, which is

defined as the hydrogen mole fraction plus 0.541 times the carbon monoxide mole fraction (where 0.541 is the parameter derived from the ignition criteria). The correlations are further generalized to allow for diluents other than steam by replacing the steam mole fraction by the diluent mole fraction, which is set to the sum of the steam and carbon dioxide mole fractions plus 0.79 times the excess nitrogen mole fraction (this is the diluent as defined by the ignition criteria).

Two versions of the correlation are available: one for laminar flames and one that allows for the turbulence generated by the containment sprays.

The user may input a constant flame speed to be used in place the value calculated within the code.

D.7.5.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The correlations are reasonable fits to the experimental data, though there is considerable scatter in the data.

The correlations apply to the relatively simple geometry of the vessels used for the experiments. Reactor containments have more complex geometries and there is no allowance in the correlations for effects such as flame acceleration around objects. Due to the large variety in containment geometries it is not practical to allow for geometrical effects in the code. The provision of sufficient flexibility for the user to perform sensitivity studies is therefore reasonable. However, some advice to the user on how to choose the parameter ranges for sensitivity studies is needed.

The correlations account for only two levels of turbulence: no turbulence or turbulence caused by operation of the containment sprays. Other sources of turbulence exist in the containment during severe accidents, notably jets and/or plumes of hot gas (possibly carrying entrained debris). Such sources must be investigated by using the input option to override the calculated burn rate in order to perform sensitivity studies. Advice to the user on how to estimate parameter ranges for sensitivity studies is needed.

The burn parameters are not updated to allow for the input of combustible gas to the cell during the burn. The obvious case where this may be of concern is during DCH when combustion is likely to occur and the hydrogen source rate is likely to be high; however, in this case the BSR and DFB models can be used which do not suffer from the above drawback.

D.7.5.3. Results of Sensitivity Studies

As steam levels in the containment are likely to be high during a severe accident in a water reactor, the predicted flame speed will be low. As turbulence can increase the flame speed, a sensitivity calculation was carried out for a large dry PWR containment with version 1.03 of the code in which the flame speed was increased by a factor of 10 (Ref. D.7-17). As a result of the reduction in the time available for heat transfer to the structures the increase in flame speed resulted in an increase of almost 20% in the predicted pressure rise.

D.7.5.4. Results of Benchmarking/Validation Studies

The correlations are themselves derived from experimental data in which there is considerable scatter. Even when the data are grouped with respect to hydrogen

concentration, steam concentration and turbulence level and an attempt is made to remove the length-scale effect, there is still considerable scatter in the data. As a result Wong states that the equations for flame speed correlate the data to within + or - 40%, but that this figure is significantly reduced if slow flames (less than 2 m/s) are omitted from the comparison (Ref. D.7-13).

Pong has compared HECTR 1.8 calculations with the experimental data for 12 NTS tests with bottom ignition and quiescent atmospheres (Ref. D.7-18). As the combustion correlations in CONTAIN 1.2 are taken from HECTR 1.8, the comparison gives useful information on the modeling in the CONTAIN code. Pong found that the predicted pressures agreed well with the measurements though the estimated pressure rise times were always shorter than the measured values (by factors of less than 10% in one case, up to factors of 3 or 4 in other cases). In view of the sensitivity of plant calculations to the burn time (noted in subsection D.7.5.3 above), the under prediction of the burn time may result in significant pessimism in some plant calculations.

Pong also reports analyses of two of the VGES experiments with HECTR 1.8 (Ref. D.7-18). The chosen experiments had no obstacles in the vessel to accelerate the flame. The pressure rise times were under estimated by an order of magnitude and the pressure rises were over estimated by more than 50% in both cases. The longer pressure rise time in the experiments seems to be due to the time taken for the flame to accelerate to its steady state value. Such an effect may be less important in the much larger volume of a reactor containment, but a proper scaling argument is required to confirm this.

Comparison of CONTAIN 1.12+C110V calculations with four of the hydrogen-steam-air combustion experiments conducted at the University of Pisa is reported in Ref. D.7-19. The predicted burn time is in reasonable agreement with the measurements except for the case with high hydrogen concentration (17%) and low steam concentration (10%) which under predicted the burn time by a factor of about 4.

D.7.5.5. Identified Deficiencies and Options for Model Improvements

User advice is required on the choice of parameter ranges for sensitivity studies to assess the possible effects of turbulence and obstacles on the flame speed and consequently on containment pressurization.

Further assessment is required of the discrepancies between the predicted and measured pressure rise times for various NTS, VGES, and Pisa experiments to determine the implications for plant calculations. Such a study would provide useful information for the specification of parameter ranges for sensitivity studies as discussed previously.

D.7.5.6. Importance of Model to Prediction of Dominant Phenomena

The flame speed determines the burn time and therefore the time available for heat transfer to the structures before the peak pressure is attained. The flame speed correlations can have a significant affect on the peak pressurization and can also affect the peak temperature.

D.7.5.7. Technical Adequacy of Model and Documentation

The deflagration models provide a reasonable starting point for the analysis of low-speed combustion in the containment. However, the effects of turbulence and obstacles on

the flame speed are uncertain and not allowed for in the code (with the exception of spray induced turbulence). There is adequate flexibility in the code to allow sensitivity studies to be performed to assess the effects by varying the flame speed, but the user is provided with no advice on the choice of parameter ranges for such studies. The technical adequacy of this model is classified as Category 2.

D.7.6. Combustion Completeness

D.7.6.1. Model Description and Pedigree

In the absence of any diluent, the combustion completeness rises linearly from zero at a combustible gas concentration of 4.2057% to complete combustion at 7.4845% in a quiescent atmosphere and from 0 at a combustible gas concentration of 3.6535% to complete combustion at 7.1454% for an atmosphere with sprays on.

For both quiescent and turbulent atmospheres, the combustion completeness is reduced in the presence of a diluent by a factor of $\exp(a)$, where a is given by

$$a = X_d(-4.1966 + 3.3985 X_d) ,$$

where X_d is the mole fraction of diluent, as defined in subsection D.7.5 above.

The above correlations are derived from the experimental data from the NTS (Ref. D.7-16), VGES (Ref. D.7-14), Whiteshell (Ref. D.7-20), ACUREX (Ref. D.7-21), and FITS (Ref. D.7-15) test series.

D.7.6.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The combined experimental data from the above tests indicate that it is reasonable to assume that combustion completeness rises linearly from 0 at about 4% hydrogen to 1 at about 7-8% hydrogen in dry atmospheres (Refs. D.7-1 and D.7-13). The data also indicate that the presence of steam has little effect below concentrations of 30-40%, but can greatly reduce the combustion completeness as the inerting concentration (55%) is approached (Ref. D.7-13). The exponential function used for the effect of steam exhibits this behavior, of being close to unity for low steam concentrations and falling to less than 0.1 by the time the steam concentration reaches 55%. The correlations therefore reasonably represent the data.

Wong has compared the correlations (which he produced) with the data (Ref. D.7-13). He shows that the correlation for the case of spray-induced turbulence reproduces most of the data to within + or - 20%. The correlation for quiescent atmospheres also predicts the NTS and ACCUREX data to within about + or - 20%, but it tends to over-predict the combustion completeness in the VGES and Whiteshell experiments by factors of up to 2.

The experiments used to generate the correlations only had hydrogen concentrations up to 20%, so there is no guarantee that they will maintain their accuracy at higher concentrations.

The experiments used to generate the correlations all had well-mixed atmospheres. Recent, small-scale (0.5 m^3) experiments at the University of Pisa have compared combustion in well-mixed and steam-stratified atmospheres (Ref. D.7-18). The results

indicate that stratification has little effect at low steam concentrations but significantly increases the efficiency of the burn for steam concentrations approaching the inerting limit, by increasing the combustion completeness.

The experiments were all conducted in air-steam-hydrogen atmospheres and have been generalized to include mixtures of hydrogen and carbon monoxide for the combustible gas and mixtures of steam, carbon dioxide, and nitrogen for the diluent, using the same linear combinations of concentrations as used for the ignition criteria. The rationale behind the use of the same combinations of combustible gases and diluents for the ignition criteria and the combustion completeness is not evident from the literature provided for the review, especially as different combinations of the combustible gases are required for propagation in different directions (upwards, downwards, and sideways--see subsection D.7.7).

D.7.6.3. Results of Sensitivity Studies

As the energy released to the atmosphere is proportional to the amount of gas burned, the magnitude of the effect of incomplete combustion on the current burn is usually evident without performing code calculations, especially for rapid burns, which give little time for heat transfer to structures.

D.7.6.4. Results of Benchmarking/Validation Studies

Because the combustion completeness correlations in CONTAIN are the same as those in HECTR 1.8, comparisons of the latter with experiment provide support for the modeling in CONTAIN.

Pong compared HECTR version 1.8 with 12 NTS experiments with bottom ignition and quiescent atmospheres (Ref. D.7-18). Good agreement between calculated and measured peak pressures is reported, indicating that the predicted combustion completeness is probably reasonable, unless there were compensating errors, which is unlikely.

Pong also compared HECTR 1.8 calculations with two VGES experiments that did not have any obstacles inside the test vessel (Ref. D.7-18). Once the appropriate flame speed had been incorporated into the calculation, the predicted pressure rise agreed well with the measurements, thereby supporting the model of combustion completeness.

O'Mahoney and Neill report a comparison of CONTAIN 1.12+C110V with four of the experiments in the small-scale facility at the University of Pisa (Ref. D.7-19). For three of the four tests, the predicted completeness is in reasonable agreement with the data, but in the fourth the completeness is over-estimated by a factor of 4. In the latter case, the hydrogen concentration was low (7.22%) and the atmosphere was nearly inerted by the high steam concentration (48%). In the experiment there appear to have been a succession of small burns that left most of the hydrogen unburned. This indicates that there is a large uncertainty in the combustion completeness, at least for mixtures that are only just flammable.

D.7.6.5. Identified Deficiencies and Options for Model Improvements

Because there can be considerable uncertainty in the combustion completeness, Wong advocates the use of sensitivity studies to determine the consequences of the uncertainty. Some advice to the user is required in the manual on reasonable parameter ranges to use for sensitivity studies.

D.7.6.6. Importance of Model to Prediction of Dominant Phenomena

As the energy input to the atmosphere is proportional to the amount of hydrogen burned, this phenomenon is of considerable importance to containment pressurization and heatup and, consequently, may also affect the amount of airborne fission products in the containment.

D.7.6.7. Technical Adequacy of Model

There is considerable scatter in the experimental data, indicating a degree of uncertainty in the current understanding of combustion completeness. The process is represented by correlations that capture the major trends in the data but necessitate the use of parametric sensitivity studies to take account of the uncertainty in the data. The model is therefore zeroeth order and its adequacy is assessed to be Category 2.

The documentation adequately describes the model but fails to provide advice to the user on reasonable parameter ranges to use for sensitivity studies.

D.7.7. Propagation in Multi-Compartments

D.7.7.1. Model Description and Pedigree

For the burn to propagate into another cell, the mole fraction of diluent (as defined in subsection D.7.1) must be less than a critical value, which can be user defined but defaults to 55% if not specified (Ref. D.7-22). Similarly the oxygen mole fraction in the cell must exceed a user-specified value which defaults to 5% (Ref. D.7-23).

In addition the combustible mole fraction must exceed a critical value. The critical values can be user specified or can be left to default to 4.1% for upward propagation, 6% for horizontal propagation, and 9% for downward propagation (Ref. D.7-24). The mole fraction of combustible gas is defined to be the mole fraction of hydrogen plus a fraction of the mole fraction of carbon monoxide, where the fraction is 0.328 for upward propagation, 0.435 for horizontal, and 0.600 for downward.

The relative heights of the cells are specified by the user and may be different to the heights specified for the flow solver.

If the conditions for propagation are met in a cell adjacent to the burn cell then the burn will propagate to the adjacent cell after a time delay which is a user-specified fraction of the burn time in the burn cell. The delay fraction defaults to 0.5 if not specified.

D.7.7.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The critical mole fractions of the combustible gas quoted above apply to hydrogen. Coward and Jones (Ref. D.7-24) also list the corresponding values for carbon monoxide as 12.5%, 13.5%, and 15.0%, respectively. Using Le Chatelier's mixing rule implies that the combustible mole fraction must be the hydrogen mole fraction plus a fraction of the carbon monoxide mole fraction, where the required fractions for upward, horizontal, and downward propagation are as given in the subsection above.

The correlations capture the major trends in the experimental data, but there is considerable scatter in the data. The user must therefore perform sensitivity studies in order to properly interpret the results of any calculations.

If combustion occurs in one or more cells then the pressurization of that cell or cells will result in gas flowing into adjacent cells that are not burning. Such flows are likely to be energetic and will generate a certain amount of turbulence in the downstream cells. The effect of this turbulence on the burn rate in the downstream cells is not modeled in the code.

In addition the gas flowing from burning to nonburning cells carries with it a mixture of burnt and unburnt gases in the code model. The introduction of burnt gases will reduce the concentration of fuel in the downstream cells, which may effect the occurrence, rate, and completeness of burns in those cells.

D.7.7.3. Results of Sensitivity Studies

Pong demonstrates the effect of forcing combustion products into downstream cells with a HECTR calculation of combustion in a chain of cells (Ref. D.7-18). Each cell has an initial concentration of 7% hydrogen and the ignition limit is assumed to be 6%. Combustion is assumed to start at the far end from the flowpath in an end cell of the chain. For the chosen geometry the burn never propagates out of the first cell as the combustible concentration in the next cell falls below 6% before the burn reaches the flowpath. When a simple model to track the flame front is used, and only unburnt gases flow to the downstream cell until the front reaches the connecting flowpath, the burn is shown to propagate through the chain of seven cells.

Pong also compares a two cell calculation with the flame tracking model (Ref. D.7-18). In this case the initial conditions are such that combustion propagates to the second cell in both calculations. The flame tracking model is shown to predict a peak pressure which is 6% higher and a peak temperature that is 300 K higher than the CONTAIN model.

D.7.7.4. Results of Benchmarking/Validation Studies

Experiments on flame propagation in a series of several cells have been performed in the Battelle model containment (Ref. D.7-25). The results show that vent flow induced turbulence in the downstream cells can lead to pressures approaching the Adiabatic, Instantaneous, Isochoric, Complete (AIIC) combustion limit. CONTAIN 1.1 calculations which do not model this effect were found to under estimate the pressure rise by a factor of 2. However, when the burning rate calculated by a more mechanistic code was used in CONTAIN, much better agreement with the measured pressurization was obtained.

D.7.7.5. Identified Deficiencies and Options for Model Improvements

In order to model propagation in compartmentalized geometries adequately it is necessary to include a flame front tracking model, such as that developed for HECTR, in the code. It is also necessary to develop a strategy to allow for vent path flow induced turbulence. This could be achieved by performing side calculations of such effects using specialized codes and feeding the calculated burn rate into CONTAIN, as advocated in Ref. D.7-25. Alternatively simplified models of turbulence generation (e.g., for specific geometries, such as jets) and its effect upon flame speed could be incorporated into the CONTAIN code.

D.7.7.6. Importance of Model to Prediction of Dominant Phenomena

For compartmentalized geometries the processes of combustion have been shown to determine whether or not burns occur in adjacent cells and cases have been found where associated processes can double the pressure rise. Combustion propagation is therefore very important to pressurization in compartmentalized containments. As it can also significantly effect the peak temperature it may have an effect on revaporization (and also resuspension due to induced flows and associated turbulence) of fission products.

D.7.7.7. Technical Adequacy of Model and Documentation

The basic physics is understood, though the generation of turbulence in complex geometries and its effect on burn rate are not known in detail. Thus, the overall knowledge of the physics is questionable. The model does not represent two of the most important processes in propagation (segregation of burnt and unburnt gases by the flame front and vent flowpath induced turbulence). Its adequacy is therefore assessed to be Category 5. The documentation is adequate.

D.7.8. Effect of Combustion on Fission Product Release

D.7.8.1. Model Description and Pedigree

The targeted host and release mechanism in the code could be used to represent some aspects of the effect of combustion on fission products. This feature allows fission products to be hosted on aerosols, on structure surfaces, in the gas, and in water pools. The fission products can be released from their hosts at user-specified rates and accepted by other user-specified hosts. The release rates can have an Arrhenius temperature dependence with the constants specified by the user. The constants could be set to release the iodine from aerosols and structure surfaces at high temperatures and host them on the gas, thus representing the conversion of iodine to more volatile forms during combustion.

The alternative is to use the source tables to provide a control function representation of the phenomena.

D.7.8.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

Experiments indicate that the amount of iodine converted to the vapor phase depends upon a number of factors, such as, the amount of steam in the atmosphere (Refs. D.7-26 and 27) and the concentration of airborne cesium iodide (Refs. D.7-26, D.7-28, and 29 and maybe also the amount of water condensed on the cesium iodide (Ref. D.7-27). None of these factors is currently allowed for in the targeted host and release mechanism.

D.7.8.3. Results of Sensitivity Studies

Valdez (Ref. D.7-30) has performed a sensitivity study on the amount of cesium iodide converted to elemental iodine for a TMLB' accident scenario in the Surry PWR, using the CONTAIN code. A small breach in the reactor is assumed. The results indicate that the effect of a hydrogen burn on the amount of iodine released from the reactor containment is at most a factor of four and can be beneficial or detrimental, depending on whether the containment sprays operate, respectively.

D.7.8.4. Results of Benchmarking/Validation Studies

No relevant studies were presented to the Committee.

D.7.8.5. Identified Deficiencies and Options for Model Improvements

There is no model in the code to predict the extent of the conversion of cesium iodide to elemental iodine during a hydrogen burn. A simple correlation to estimate the extent of conversion was proposed by Weber and Beahm (Ref. D.7-31). Further work would be required to allow for the possible effect of water condensed on the cesium iodide.

D.7.8.6. Importance of Model to Prediction of Dominant Phenomena

Valdez has estimated that combustion could effect the iodine source term by a factor of up to a few, though the effect could be scenario dependent and only a single scenario (TMLB') has been investigated for the Surry PWR. The effect on the source term is therefore rated as having an importance level of 3 (see Table C-II, column A).

The feedback effect of the fission products on the thermal-hydraulics is likely to be small (though the caveats in the following subsection should be noted) and is therefore rated as having an importance level of 0 (see Table C-II, column A).

D.7.8.7. Technical Adequacy of Model and Documentation

Though the targeted host and release mechanism could be used to qualitatively represent the conversion of cesium iodide to more volatile forms, there is no mechanistic model to estimate the extent of the conversion for the relevant range of atmospheric conditions. Though models for some aspects are described in Refs. D.7-28 and 29, the processes are still poorly understood on the whole. As control functions are available to represent the processes that are not modeled, the adequacy of the model is assessed as Category 3.

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D.8. Heat and Mass Transfer

D.8.1. Structure Conduction

D.8.1.1. Model Description and Pedigree

Heat transfer through solid structures to an ultimate heat sink by conduction is one of the major mechanisms for energy loss from the containment. CONTAIN considers this mechanism of heat loss in a one-dimensional fashion (Sec. 10.4 of the CONTAIN manual, Ref. D.8-1). Any structure within the containment or acting as a boundary to the containment can be subdivided into control volumes of one-dimensional slabs of material (steel, concrete, paint, or any other prescribed material) through which energy can pass from a higher surface temperature (or ambient temperature with a prescribed or calculated heat transfer coefficient) to a lower surface temperature (or ambient temperature with a prescribed heat transfer coefficient). In general this energy transfer process occurs under the constraint of constant mass.

If the material being heated by fission product decay heat through atmospheric convection or radiative transfer is concrete, then it can decompose, releasing gaseous decomposition products. The CONTAIN model includes an outgassing model for the release of water vapor and carbon dioxide gases from the heated concrete. Both evaporable and chemically bound water vapor are considered to be released due to excessive heating. The gas release model used within the CONTAIN formulation is not completely mechanistic in that it does not model explicitly the transport (i.e., diffusion) of these gases within the porous concrete internal structure. Rather, the temperatures within the heated concrete solid (i.e., temperatures of these individual control volumes) are numerically computed and once the temperature exceeds the appropriate values for evaporable water release, or chemically bound water vapor or carbon dioxide release, and the proper amount of decomposition energy is absorbed for the control volume, then outgassing occurs. It is as if the concrete at these particular temperatures has very large values of heat capacity, where the integral of this large heat capacity over these transition temperature equals the decomposition enthalpy. Thus the enthalpy of decomposition is preserved without the need to calculate the rate of transport of these gases through the porous structure. The outgassing model is defined in greater detail in a SNL document (Ref. D.8-2). The choice of considering if the concrete can be heated and then decomposed is determined by the analyst as user input.

D.8.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

From the documentation within the CONTAIN manual in Sec. 10.4, the heat conduction model developed seems quite reasonable. The Committee saw no particular problems with the conduction heat transfer model. In fact it found it to be quite versatile and well documented. In the Committee's opinion it is quite applicable for the complete range of one-dimensional problems one would encounter in containment analysis. The concrete outgassing model included with the conduction package is also considered to be a reasonable model for gas release from heated concrete. Its applicability is quite extensive given its assumptions as long as the concrete oxide constituents have not begun to melt.

D.8.1.3. Results of Model Sensitivity Studies

No specific sensitivities were found in the manual.

D.8.1.4. Results of Benchmarking/Validation Studies

There were no validation or benchmarking calculations presented in the CONTAIN manual. Dr. Ken Murata did discuss validation exercises for the conduction model as part of the "standardized test problems" developed for CONTAIN. The Committee was made aware of these test problems as part of the initial CONTAIN presentations.¹ It is the opinion of the Committee that these standardized test problems constitute a reasonable set of validation and benchmark numerical/physical tests, but should be more formally made available for the user or auditor for comparison and comment. The Committee is aware that the CONTAIN staff regularly uses these standardized test problems as informal routine checks for the CONTAIN code modules as they may be modified for CONTAIN updates.

D.8.1.5. Identified Deficiencies and Options for Model Improvements

The concrete outgassing model included in the conduction heat transfer model needs to be referenced to specific data comparisons rather than just comparisons to other more sophisticated models; e.g., SLAM or USINT. Benchmark data exists as part of the early materials testing and severe-accident research at SNL; e.g., concrete ablation or heating work by T.Y.Chu or J.Muir. This was mentioned in the SNL staff presentations, but this should become part of the more formal "standardized test problems" that the CONTAIN group ought to develop.

D.8.1.6. Importance of Model to Prediction of Dominant Phenomena

The conduction model is an important part of the heat loss mechanism to cold walls and as such must be checked relative to standard problems or test data as modifications are made or materials added, or as part of the code maintenance efforts.

D.8.1.7. Technical Adequacy of Model and Documentation

The conduction heat transfer model represents the current state of knowledge and is judged to be of first order. The knowledge of the physics of the process is well known and validation of the conduction portion of the model has been benchmarked relative to more fundamental analyses. We feel the outgassing model could be more directly compared to data; e.g., the data generated at SNL by T.Y.Chu and J.F.Muir. The technical adequacy of this model is classified as Category 1.

D.8.2. Structure Radiation

D.8.2.1. Model Description and Pedigree

If the gas temperature in containment rises to high values due to gas combustion or due to energy transfer from the surface of an ex-vessel molten corium pool or debris, then radiation heat transfer would become a significant heat transfer mechanism. The radiation heat transfer model in CONTAIN is described in Sec. 10.3 of Ref. D.8-1, along with the associated corrections for a participating gas (composed primarily of water vapor, carbon monoxide, or carbon dioxide) and the debris radiation heat transfer model for direct

¹ K. C. Rentzsch, "CONTAIN Standard Test Problems, Updated and New Problems," Presentation at the Second Meeting of the CONTAIN Peer Review Committee held August 23-26, 1993, Albuquerque, New Mexico.

containment heating conditions. In CONTAIN, the analyst can choose from two radiative heat transfer models: the net enclosure model and the simple radiation model. The former model allows for simultaneous calculation of radiative heat transfer between the compartment (control volume) atmosphere (which can include aerosols or corium debris), all heat structures, and the upper boundary of the compartment below, as gray surfaces or gases with known average properties.

The major limitation of such a model is that only the inner surfaces of the structures facing the compartment atmosphere can be included in such an analysis. The latter model considers the direct radiative heat transfer between the compartment atmosphere and the heat structures (inner and outer surfaces of the structure if both are within the compartment), and between the atmosphere and upper layer of the compartment below. This latter model is recommended for use with the direct containment heating model because it is consistent with the additional direct radiative transfer models for corium debris to atmosphere and debris to structure heat transfer. A separate model consistent with the simple radiation model allows for radiative energy transfer from a lower compartment to inner heat structure walls.

Both of these radiation models can account for the optical properties of the atmosphere based on the emissivity of water vapor, carbon monoxide, or dioxide; i.e., the Cess-Lian correlation when water vapor is the dominant participating gas species, or the Modak correlation when the other two gases are significant species in the atmosphere. The presence of aerosols can be accounted for by a simple parametric model or by considering the aerosol cloud emissivity due to the aerosol mass loading. The presence of corium fuel debris due to high-pressure melt ejection must also be considered separately. This consideration is not straightforward and the CONTAIN model includes a parameter KMX, which allows the analyst to alter the atmosphere properties with the debris present. The CONTAIN manual does a reasonable job of explaining this uncertainty and warning the user of the possible effects.

D.8.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The radiation model is clearly state of the art and the Committee sees no specific weaknesses in the models used and feels that once the analyst picks either model, the CONTAIN formulations are internally consistent. However, the one area of uncertainty is the interaction of the dispersed corium fuel debris and its radiative properties with the normal considerations for radiative energy transfer within the compartment and its structures. The corium fuel debris would come out as a cloud of hot particles and it seems that the interaction of these particles and the surrounding atmosphere is complex enough to make this mode of heat transfer highly uncertain; e.g., radiative self-shielding could reduce this form of energy transfer to a cloud surface phenomena. The CONTAIN staff must recognize that the approach to this radiative transfer analysis may have to rely on parametric studies to determine the proper (or reasonable) values for the DCH radiative properties.

D.8.2.3. Results of Model Sensitivity Studies

No sensitivity studies were presented in the CONTAIN manual and there was limited discussion in the formal SNL presentations.

D.8.2.4. Results of Benchmarking/Validation Studies

The same comments mentioned for the conduction heat transfer model are quite applicable here; i.e., validation studies for the radiative model were not part of the formal

documentation nor were they extensively discussed in the presentations to the Committee. However, there were some "standardized test problems" on radiation heat transfer modeling as part of the package discussed with the Committee at a CONTAIN Peer Review meeting.² Our previous request of formalizing these test problems would probably satisfy the benchmarking of this radiative heat transfer model.

D.8.2.5. Identified Deficiencies and Options for Model Improvements

The one area of uncertainty is the interaction of the dispersed fuel debris and its radiative properties with nominal considerations for radiative energy transfer within the compartment and its structures. The corium fuel debris would come out as a cloud of hot particles, and the interaction of these particles and the surrounding atmosphere is complex enough to make this mode of heat transfer highly uncertain; e.g., radiative self-shielding could reduce this form of energy transfer to a cloud surface phenomena. The CONTAIN manual should expand its discussion of the limitations of the simple radiation model used under these conditions with airborne fuel debris, and perhaps indicate the importance of this portion of the energy transfer process. What is given within CONTAIN for the analyst is completely consistent with the other models, but more user guidance or some parametric effects should be discussed or calculations provided.

D.8.2.6. Importance of Model to Prediction of Dominant Phenomena

This heat transfer phenomena is important particularly for high pressure melt ejection and combustion events, where the heat loss to heat structure surfaces is primarily affected by this energy transfer mechanism. The model used in CONTAIN is reasonable, although more guidance under the highly transient DCH conditions would be useful for the analyst.

D.8.2.7. Technical Adequacy of Model and Documentation

The radiation heat transfer model is considered to be consistent with and representative of the current state of knowledge. The Committee feels it is a first-order model with well-understood knowledge of the underlying physics. The models used in CONTAIN are felt to be validated. The major recommendation for this section is that the manual description of the use of radiation parameters given the presence of corium fuel debris needs to be further refined to give the analyst more guidance and the uncertainties associated with its use. Once this is done, the technical adequacy of this model is classified as Category 1.

D.8.3. Convection Heat Transfer (Free and Forced)

D.8.3.1. Model Description and Pedigree

The transfer of energy from the gas atmosphere to the heat structures due to temperature differences is driven by convection and is described in Sec. 10.1 of Ref. D.8-1. The CONTAIN logic distinguishes between free and forced convection by calculating the average control volume velocity (or it is input by the analyst as a parameter) and then computing the heat transfer coefficient by either free or forced correlations. The larger coefficient is then used in the computations for heat loss from the gas atmosphere.

² See Footnote 1.

For the free convection correlation, CONTAIN uses the standard Nusselt correlation where there is no inherent system length scale required and for forced convection uses the standard Nusselt correlation for a flat plate. The average control volume velocity is estimated by an arithmetic average of the inlet and outlet velocities to the compartment control volume, where the inlet and outlet velocities are computed from the known mass flows and the density of the gas mixture. This calculated value can be superseded by user input of some specific constant velocity that the analyst specifies.

D.8.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The convective heat transfer model used in CONTAIN is standard for control volume modeling of fluid systems. The Committee sees no inconsistencies or flaws in its use within the CONTAIN modeling structure. One exception is that the Grashof number should be defined based on density difference, not the temperature difference. However, the largest uncertainty revolves around the appropriate value one should use for the forced convective velocity and the associated characteristic length within a compartment control volume. The procedure to use some arithmetic average of the junction flow velocities is expected and is one of the few choices analysts have at their disposal. Nevertheless, it can be quite unsatisfying under particular circumstances, and the CONTAIN development staff should consider providing expanded user guidance, including a general modeling strategy and examples.

D.8.3.3. Results of Model Sensitivity Studies

There were no specific sensitivities presented in the CONTAIN manual.

D.8.3.4. Results of Benchmarking/Validation Studies

Once again the validation and benchmark calculations do not appear in the CONTAIN manual but are part of the integral standardized test problems previously mentioned.³ Because the heat transfer relations used in this model are quite standard, it does not seem reasonable to consider separate validation studies. Rather, a more formal presentation of these test problems is most appropriate.

D.8.3.5. Identified Deficiencies and Options for Model Improvements

We would recommend that the SNL staff consider further guidelines for the analyst who is to use CONTAIN on how to approach the decision of free versus forced convection treatment of the heat transfer (and mass transfer), with some considerations of the effect of entry or exit velocities to the velocity in the compartment control volume and the associated characteristic length. This recommendation is open ended since the Committee is not sure what is the proper approach, but simply that current discussions seem too sparse, and any additional guidance would be helpful.

D.8.3.6. Importance of Model to Prediction of Dominant Phenomena

This model is the secondary means of energy transport from the gas atmosphere to the heat structure surface for most accident situations.

³ See Footnote 1.

D.8.3.7. Technical Adequacy of Model and Documentation

The convective heat transfer model is state of the-art and accurately reflects the proper knowledge of physics within a first-order model that is consistent with the rest of the system model. Better guidelines need to be added to the manual to help the analyst in handling the use of a forced velocity and the characteristic length scale in the compartment control volume for convective coefficients. Given this improvement, the technical adequacy of this model is classified as Category 1.

D.8.4. Mass Transfer

D.8.4.1. Model Description and Pedigree

The mass transfer model employed in CONTAIN is described in Sec. 10.2 of Ref. D.8-1). Mass transfer of water vapor, to and from heat structure surfaces due to condensation and evaporation, is driven by the concentration differences (exhibited by pressure differences) at these surfaces. For example, if a condensate film layer exists on the heat structure surface below the dew point temperature (local saturation at the total pressure), the partial pressure of the noncondensable gas (air and/or hydrogen) at this interface in the boundary layer will be higher than the bulk mixture value. This condition occurs because the noncondensable gas is carried with the vapor toward the interface where it can accumulate. The increase in the partial pressure of the noncondensable gas produces a driving force for diffusion of the noncondensable gas away from the surface. This diffusion opposes the diffusive motion of the water vapor towards the surface. Although the total pressure of the system remains constant, the water vapor partial pressure is lower at this surface interface within the boundary layer than in the bulk mixture and condensation occurs. If the surface temperature of the heat structure is above the point of local saturation, then the partial pressure gradient is reversed and we have evaporation from the surface.

To model this condensation phenomenon, the CONTAIN mass transfer model utilizes the Reynold's analogy between momentum transfer and heat transfer and applies it to mass transfer processes. By this analogy one only needs some empirical information for the local (or average) friction coefficient for momentum transfer on the structure surface and the effect of molecular (or turbulent) diffusivities of mass to momentum to estimate the mass transfer coefficient. Once this mass transfer coefficient is estimated, one can compute the mass flux of water vapor condensing on the surface of a structure and the energy carried along with it. To model the evaporation process, one need only determine that the surface temperature is above the local saturation value and any excess heat applied to the water on the structure wall would result in evaporation of a proportional amount of this condensate film.

The second resistance to condensation is the condensate film itself, due to the conduction of heat across the film. Outside the containment, a film can develop by water added directly to the outer steel shell of the containment as an evaporative cooling aid. In either case, CONTAIN has developed a film tracking model to determine the inventory of water on the heat structures available for evaporation or as a barrier for condensation. Two different models are available. First, the analyst can specify a critical film thickness. If the condensate or added water film is below this value, the film simply accumulates by condensation or diminishes by evaporation without motion. If it is calculated to go above this limit, then excess condensate is instantaneously diverted to the associated water pools for each compartment. The alternative approach is to use a more mechanistic film tracking model, which assumes that the film flows in a laminar or turbulent flow regime down the

structure surface, and the CONTAIN model tracks the thickness on these structures to determine the associated conduction resistance similar to a Nusselt condensate laminar film analysis.

D.8.4.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The models for mass transfer are considered to be adequate for the level of detail in the CONTAIN system model. There were two deficiencies identified in this review. First, the definition of the Grashof number should be based on the gas mixture density difference rather than the temperature difference. Second, the film tracking model methodology is not easily understood in the CONTAIN manual write-up. The methodology is really embodied in Equations 10.21 - 27 (Ref. D.8-1) and we feel the exposition of the model can be improved. We are aware that the use of a laminar or turbulent film model is correlation based for high film flowrates, but we feel it is consistent with the level of detail of the rest of the model.

D.8.4.3. Results of Model Sensitivity Studies

There were no specific sensitivities presented in the CONTAIN manual.

D.8.4.4. Results of Benchmarking/Validation Studies

These models for condensation and evaporation are known to be useful estimates for the rate of mass transfer at the heat structure interface. However, the Committee feels that comparison to benchmark data is still warranted, especially when the flow is in a mixed convection or natural convection regime. This comment is consistent with those of the previous two sections because mass transfer also was considered in these "standardized test problems" for the CONTAIN development. One important point to make is that the CONTAIN staff has specifically compared the CONTAIN mass transfer model to more recent data from the Massachusetts Institute of Technology and the University of California, Berkeley, for the modeling of the SBWR systems. Continued comparisons are considered important with other recent benchmark data for the AP600 or other more fundamental data to validate the model. In fact, the staff may consider adding to the "standardized test problems" from these more well-defined experiments. Such data for this regime is hard to determine, thus we recommend that the SNL staff continue to have its comparison to data be made available by the NRC and by the vendors for advanced reactor containment design.

D.8.4.5. Identified Deficiencies and Options for Model Improvements

The model and documentation deficiencies have been detailed above. The second-order high mass transfer correction terms must be included. Also the film tracking model methodology should be better explained in the CONTAIN manual to provide guidance to the analyst.

D.8.4.6. Importance of Model to Prediction of Dominant Phenomena

This model is the primary energy transfer mechanism from the gas atmosphere to heat structure surfaces for all containment conditions.

D.8.4.7. Technical Adequacy of Model and Documentation

The mass transfer model reflects the current state of knowledge for condensation and evaporation processes off of heat structures and is consistent with the other CONTAIN models. The physics of the process is considered to be understood and the model is of first order. Validation is possible if the SNL staff focuses on new available benchmark data, particularly in the mixed convection regime. The improvements needed seem to be in the redefinition of the Grashof number and in the better exposition of the film tracking model. If these improvements are implemented, then the technical adequacy of this model is classified as Category 1.

D.8.5. Thermodynamics

D.8.5.1. Model Description and Pedigree

The thermodynamics modeling approach used in CONTAIN is described in Sec. 4.1 of the CONTAIN manual (Ref. D.8-1). The modeling philosophy used in CONTAIN is similar to many other reactor containment system models, in that the containment compartments are considered to be divided into control volumes within which mass and energy for the homogeneous gas mixture are balanced. The gas mixture has one mixture temperature, pressure, and composition within the control volume, all which determine its thermodynamic state. The auxiliary equations of state for each material are then averaged to form the mixture values for mass (density) and energy (internal). These relations have been discussed in Sec. D.1 of this review. There are separate mass and energy balances for the fuel debris that may be ejected into the atmosphere due to a high-pressure melt ejection. Also separate mass and energy balances are used to keep track of water pools; see Sec. D.2.2 of this review. The complete formulation for these balance equations are given in Tables 4.2 - 4.4 in Ref. D.8-1.

D.8.5.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The model used for the thermodynamics of the containment compartments is state of the art and seems quite reasonable. The Committee does not see any deficiencies or needs for improvement given the basic modeling philosophy. We do caution the analyst not to use the CONTAIN model inappropriately. Because it is a control volume (lumped) formulation, one must be careful not to overinterpret the results and to consider other analytical or computational models if more detailed flows, or spatially refined temperatures or pressures, are required for analysis. Because the control volume approach is utilized with a one-dimensional momentum equation, it is fundamentally limited to large volumes or compartments of the containment. Too large of a subdivision of the containment gas volumes would not improve accuracy for this type of model. The manual does indicate this and the Committee feels the proper cautions have been identified.

D.8.5.3. Results of Model Sensitivity Studies

There were no sensitivities noted in the CONTAIN manual, although Sec. 4 does give good user guidance on the selection of control volumes.

D.8.5.4. Results of Benchmarking/Validation Studies

The standardized test problems do not directly benchmark the thermodynamics model. There are test problems that check the overall mass, energy, and momentum transport for

simplified containment situations and these are shown to be satisfactory. The comparison to experiments both integral and separate effects indicate reasonable behavior.

D.8.5.5. Identified Deficiencies and Options for Model Improvements

There were no deficiencies noted for this model.

D.8.5.6. Importance of Model to Prediction of Dominant Phenomena

Given that this model serves as the backbone of the code structure its importance cannot be overstated.

D.8.5.7. Technical Adequacy of Model and Documentation

The CONTAIN thermodynamic model represents the current state of knowledge for control volume formulations of containment analyses. The physics at this level of sophistication is well understood and validated based on past information. The technical adequacy of this model is classified as Category 1.

REFERENCES

- D.8-1. "CONTAIN 1.2 Code Manual: A Computer Code for Severe Accident Analysis," Sandia National Laboratories report SAND94-2358, in preparation.
- D.8-2. K. E. Washington and D. E. Carroll, "Assessment of Models for Steam Release from Concrete and Implications for Modeling Corium Behavior in Reactor Cavities," Sandia National Laboratories report SAND88-2329c for the Sixteenth Water Reactor Safety Information Meeting, Gaithersburg, MD, October 24-27, 1988.

D.9. Boiling Water Reactor

D.9.1. Suppression Pool Model

D.9.1.1. Model Description and Pedigree

Suppression Pool Flow Model

Once the liquid level reaches the vent elevation, the vent is assumed to be open/clear, and the gas flow through the vent path is then initiated. The gases vented through the pool are assumed to thermally equilibrate with the pool liquid and saturate to 99% relative humidity at the pool surface. The gas flow rate is calculated based on an orifice flow equation with a discharge coefficient of unity.

The effect of multiple vents is simulated by assuming that the effective vent area increases linearly with pressure difference, beginning at the gas pressure difference sufficient to support the liquid level:

for $\Delta P \geq \Delta P_{\min}$,

$$A_{\text{eff}} = \frac{(\Delta P - \Delta P_{\min})}{(\Delta P_{\max} - \Delta P_{\min})} A_v$$

and A_{eff} is set to zero for $\Delta P \leq \Delta P_{\min}$. Here, $\Delta P_{\min}$ is the minimum pressure difference for vent opening, $\Delta P_{\max}$ is the sum of $\Delta P_{\min}$ and a user-specified pressure range for area to go from zero to maximum, ΔP_d , taking into account the flow direction.

The code documentation does not state that the above correction is only relevant to a multi-vent system. In addition, user guidance is not provided for these pressure estimates.

Suppression Pool Energy Equation

Before initiation of vent flow actuation, the pool energy transfer process is governed by the CONTAIN "implicit boiling model" described in Sec. 4.3 of Ref. D.9-1. The App. K referenced on page 4-36 was unavailable for review. The steps involved in derivation of the equations for this model should be provided in the revised code documentation.

Following vent flow actuation, the energy transfer from the vented stream to the pool water includes the effects of vapor condensation and thermal equilibration of non-condensibles, pool flashing, and bubble re-saturation to 99% relative humidity. The model does not include potential effects of thermal stratification. This could be important for ALWRs with passive containments.

The mass and energy transfer at the pool/atmosphere interface uses standard models for simultaneous heat and mass transfer (see also the peer review comments related to the atmosphere/pool thermodynamic and intercell flow models).

D.9.1.2 Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

In general, the pressure suppression pool models are physically reasonable and a recent code benchmarking exercise (Ref. D.9-2) of CONTAIN applications to selected DBA cases showed the capabilities and limitations of these models in predicting the dominant phenomena. However, it should be noted that essentially no experimental benchmarking of the CONTAIN suppression pool thermal-hydraulics models are currently available.

D.9.1.3. Results of Model Sensitivity Studies

A number of sensitivity calculations have been performed with CONTAIN for several BWR DBA scenarios and compared to existing results using the CONTEMPT computer code (Ref. D.9-2). Differences in the pool energy transfer models between CONTAIN and CONTEMPT impact the wetwell behavior; however, validity of the CONTAIN calculated results is difficult to confirm in the absence of any experimental benchmarking studies.

D.9.1.4. Results of Benchmarking/Validation Studies

Experimental benchmarking of the suppression pool models has not been performed.

D.9.1.5. Identified Deficiencies and Options for Model Improvements

In general, the suppression pool flow models appears to represent most of the dominant processes for BWR application. The pool energy transfer model description should be expanded to show the analytic steps in deriving various equations of the model. The model does not include potential effects of thermal stratification. The potential influence of pool stratification should be evaluated and if found to be significant, it should be included in the model. In addition, the model requires experimental validation.

D.9.1.6. Importance of Model to Prediction of Dominant Phenomena

This is one of the most important models for application to design-basis and severe-accident conditions in BWRs. This model has a direct bearing on the prediction of containment pressure and temperature loads in BWRs and perhaps even advanced PWRs that include an in-containment water storage tank, through which the power operated relief valves could discharge. These models could also indirectly impact the fission product retention effectiveness of the pressure suppression pool during severe accidents.

The energy transfer processes to water pools (steam condensation) in presence of noncondensibles remains experimentally deficient.

D.9.1.7. Technical Adequacy of Model and Documentation

In general, the pressure suppression pool model appears to adequately represent the general trends of major processes under thermal-hydraulics conditions of interest to BWRs. However, the following inadequacies should be noted:

- The code documentation should be improved and additional user guidelines provided.
- The effect of pool stratification is not included, and the pool energy transfer model needs experimental validation.

The technical adequacy of this model is classified as Category 1.

D.9.2. Vent Clearing Model

D.9.2.1. Model Description and Pedigree

The CONTAIN vent clearing model is based on the steady state Bernoulli's equation of the form:

$$(P_w - P_d) + \rho_l g(H_w - H_d) + \rho_l (v_w^2 - v_d^2) + \Delta P_L = 0.0$$

$$\Delta P_L = \frac{1}{2} \rho_l (K_w v_w^2 + K_d v_d^2)$$

$$\beta v_d = v_w,$$

where β is the ratio of vent area, A_v , to the wetwell pool surface area, A_{wp} ; K_d is the user-specified loss coefficient; K is the sudden expansion loss coefficient for drywell to wetwell flow $[(1/\beta - 1)^2]$; P is the pressure; H is the elevation; v is the velocity; and ρ is the density. The subscripts d, w, and l refer to the drywell, the wetwell, and the liquid, respectively.

The velocity v_d is related to vent liquid level displacement and solved analytically to obtain the displacement. The model also allows for the effect of overflow as well as flow direction (drywell to wetwell and vice-versa).

This formulation neglects the inertial effects of liquid within the vent, and the multiple horizontal vents (that exist in BWRs with MARK-III containments) are lumped into a single equivalent vent.

D.9.2.2 Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The vent clearing model is physically reasonable, even though some limitations are noted and discussed in later subsections.

D.9.2.3. Results of Model Sensitivity Studies

A number of sensitivity calculations have been performed with CONTAIN for several DBA scenarios and compared to existing results using the CONTEMPT computer code (Ref. D.9-2). These BWR calculations show that the CONTAIN predicted peak containment pressure (early phase of DBAs) can be made to agree to the CONTEMPT results by using (1) a similar vent loss coefficient and (2) an artificial adjustment in the vent elevation for the CONTAIN single/lumped vent model. However, the late phase containment pressure behavior could not be adequately simulated by CONTAIN. Some improvement in the CONTAIN calculated results were noted when ΔP_d was varied. It was

concluded in Ref. D.9-2 that the multiple vent clearing behavior is difficult to predict using the CONTAIN single/lumped vent model.

D.9.2.4. Results of Benchmarking/Validation Studies

No results are given.

D.9.2.5. Identified Deficiencies and Options for Model Improvements

In general, the vent clearing model appears to represent most of the dominant processes for BWR application. However, several deficiencies were noted and are listed below.

The vent clearing model neglects the inertia effects of the liquid; however, a limited comparison of CONTAIN calculated vent clearing behavior with the CONTEMPT code predictions (note that the vent clearing model in CONTEMPT is very detailed and includes the inertia effects of the liquid) showed that the effect of fluid inertia is not significant, so the CONTAIN approximation appears justified.

The single/lumped vent model currently available in CONTAIN is not adequate for mechanistic prediction of multiple vent clearing behavior. This issue is important for both DBAs and severe accidents (i.e., vent clearing plays a key role in loads following high-pressure melt ejection in BWRs). Incorporation of additional vent paths is analytically straightforward; however, implementation into the CONTAIN program architecture is difficult to assess.

D.9.2.6. Importance of Model to Prediction of Dominant Phenomena

This is one of the most important models for application to design basis and severe accident conditions in BWRs. This model has a direct bearing on the prediction of containment pressure and temperature loads in BWRs and perhaps even, Advanced PWRs that include an in-containment water storage tank, through which the PORVs could discharge. These models could also indirectly impact the fission product retention effectiveness of the pressure suppression pool during severe accidents.

The knowledge of physics is excellent for vent flow dynamics.

D.9.2.7. Technical Adequacy of Model and Documentation

In general, the vent clearing model appears to adequately represent the general trends of major processes under thermal-hydraulics conditions of interest to BWRs; however, the single/lumped vent model is not adequate for mechanistic prediction of vent clearing behavior in multi-vent system pressure suppression pools.

The technical adequacy of this model is classified as Category 4.

D.9.3 Suppression Pool Scrubbing Model

D.9.3.1. Model Description and Pedigree

The CONTAIN code has two model options for aerosol retention in suppression pools. The SCRUB model, which was developed for the VANESA code, is based on

Fuchs' treatment of sedimentation, impaction, and diffusion in spherical bubbles. The user may specify the initial bubble diameter, which is defaulted to 1.0 cm. The scrubbing efficiency is sensitive to the input parameter VROVR, the ratio of the gas circulation velocity to bubble rise velocity. Bubble expansion is calculated as a bubble rises in a pool but vapor evolution effects are neglected.

The SPARC model includes some but not all of the model features of the 1985 version of SPARC. This model extends Fuchs' model to consider elliptical bubbles. It accounts for bubble growth and the deposition limiting effects of vapor evolution during bubble rise. The CONTAIN version does not include some important features in the 1985 version of SPARC or that have been included in more recent versions of SPARC (Ref. D.9-3) such as vapor evolution in rising bubbles, aerosol growth by condensation, the effects of hygroscopicity on aerosol growth, expansion work of rising bubbles, hydrodynamic description of bubble swarms, and bubble breakup models.

Neither model includes the analysis of vapor iodine retention in suppression pools.

D.9.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The SPARC model is capable of representing some of the principal phenomenological aspects of suppression pool retention of aerosols but does not currently include some important mechanisms that can have a significant impact on analysis results.

D.9.3.3. Results of Model Sensitivity Studies

Example BWR cases have been performed with CONTAIN that have exercised the suppression pool model, but no sensitivity studies have been reported for the models as implemented.

D.9.3.4. Results of Benchmarking/Validation Studies

Some validation studies have been performed for the NRC for later versions of SPARC. The accuracy of the currently implemented version can be expected to be very approximate. There has been no effort to validate the model within the CONTAIN development program.

D.9.3.5. Identified Deficiencies and Options for Model Improvements

A number of improvements in later versions of SPARC could be incorporated into CONTAIN:

- Bubble swarm
- Bubble breakup
- Condensation growth
- Expansion work effect on bubble saturation
- Effect of hygroscopicity.

In addition, an elemental iodine removal model is needed to be able to analyze the fate of iodine in containment.

D.9.3.6. Importance of Model to Prediction of Dominant Phenomena

Suppression pool removal of radionuclides has a dominant impact on the analysis of severe accidents in LWRs. The accurate modeling of the dependence of decontamination factor on aerosol size is critical. Simple estimates of decontamination factors can be in error by orders of magnitude.

D.9.3.7. Technical Adequacy of Model and Documentation

Although the models appear to satisfy the requirements for a first-order mechanistic treatment, subsequent improvements in the SPARC code indicate that the existing treatment is inadequate. The documentation of the suppression pool models is also minimal. Because the physics are understood and the model is inadequate, the model is classified as Category 4.

REFERENCES

- D.9-1. "CONTAIN 1.2 Code Manual: A Computer Code for Severe Accident Analysis," Sandia National Laboratories report SAND94-2358, in preparation.
- D.9-2. K. Almenas, F. J. Munno, N. Ennaciri, and H. Esmaili, "Recomputation of Selected CONTEMPT Code Design Basis Containment Transients Using the CONTAIN Code," Energy Research, Inc. report ERI/NRC 93-209, August 1993.
- D.9-3. P. C. Owczarski and K. W. Burk, "SPARC-90: A Code for Calculating Fission Product Capture in Suppression Pools," Pacific Northwest Laboratory report NUREG/CR-5765, October 1991.

D.10. Engineered Safety Features

D.10.1. Fan-Cooler Model

D.10.1.1. Model Description and Pedigree

The fan-cooler model has a thermal-hydraulic model and an aerosol removal model. The MARCH fan-cooler model is not recommended. The more mechanistic fan-cooler model includes a condensation mass heat transfer coefficient and a convective heat transfer coefficient. The Nusselt number, which is used to determine the heat and mass transfer coefficients for flow over horizontal tubes, is based on a correlation for tube banks without fins.

Aerosol deposition in the fan cooler is calculated based on the condensation rate. The only mechanism modeled is diffusiophoresis. Aerosols travel with the condensate to sump volumes.

D.10.1.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The mechanistic fan-cooler model must be used with care. Input data must be provided to the model using plant data. In addition, the model should be tested or possibly tuned against steady-state plant performance data.

The aerosol model treats the dominant deposition mechanism. Although approximate, the aerosol removal treatment is consistent with the accuracy of the thermal-hydraulic model.

D.10.1.3. Results of Model Sensitivity Studies

Generic sensitivity studies would be of limited value. The accuracy of the fan-cooler model will depend on the fan cooler design being modeled.

D.10.1.4. Results of Benchmarking/Validation Studies

Benchmarking of this model must be made on a plant-by-plant basis.

D.10.1.5. Identified Deficiencies and Options for Model Improvements

The model does not account for tube banks with fins. Filters, which are often used with fan coolers, are not modeled. In addition, the removal of elemental iodine is not modeled.

D.10.1.6. Importance of Model to Prediction of Dominant Phenomena

The details of fan-cooler equipment designs are often not available to the analyst and fan cooler performance is benchmarked against steady-state data. It is, therefore, necessary to have a parametric capability in the model. A very accurate prediction of fan-cooler heat removal is typically not very important to the results of the analysis, however. Fan coolers can be effective in preventing overpressurization of containment and in

reducing the airborne concentration of aerosols. However, dominant accident sequences are most often associated with conditions under which fan coolers are not effective.

D.10.1.7. Technical Adequacy of Model and Documentation

The fan cooler physics are understood and the model is first order. The fan-cooler model may be more applicable to some fan-cooler designs than others but is assessed to be adequate. The documentation of the model within the manual is sufficient. The technical adequacy of this model is classified as Category 1.

D.10.2. Ice-Condenser Model

D.10.2.1. Model Description and Pedigree

The ice-condenser model involves a thermal-hydraulic model and an aerosol removal model. The thermal-hydraulic model is quite simple. Heat transfer by convection is calculated from flowing gases to a column of ice. Both turbulent natural convection and forced convection are considered. As the ice melts, the length of the column decreases and reduces the heat transfer area. The condensate, aerosols, and associated fission products flow to a receiver volume. The outlet temperature of this effluent is an input parameter to the code.

The heat balance for the ice and melted water account for heating of the ice to its melting point, melting at constant temperature, and heatup of the melted ice water as it exits the ice bed. Radiative heat transfer is included for DCH conditions.

The effective velocity used for the forced-convection heat transfer correlations is based on the calculated inlet velocity and the assumption that the flow undergoes an isentropic expansion. Most of the input parameters for the model involve design data but some require "discretion" on the part of the user.

The aerosol decontamination model treats settling, impaction/interception, Brownian diffusion, diffusiophoresis, and thermophoresis. The model is based on the ICEDF model developed by Owczarski and others (Ref. D.10-1).

D.10.2.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The thermal-hydraulic model is a very simple approximation of the very complex processes in an ice condenser. Successful use of the model would require benchmarking against Pacific Northwest Laboratories (PNL) experiments for comparable conditions.

The aerosol removal mechanisms modeled are the appropriate mechanisms for ice-condenser deposition. Prediction of aerosol deposition depends on accurate prediction of the thermal-hydraulic conditions as well as the aerosol mechanisms, however.

D.10.2.3. Results of Model Sensitivity Studies

No sensitivity studies have been performed within the CONTAIN formulation.

D.10.2.4. Results of Benchmarking/Validation Studies

Some comparison calculations have been performed with the PNL experimental data (Ref. D.10-2). The results were reported to be in qualitative agreement with experiment.

D.10.2.5. Identified Deficiencies and Options for Model Improvements

Preferential channeling through a localized region of the icebed could result in a substantial decrease in heat transfer and aerosol removal. The development of a more detailed model would be a significant undertaking, however.

D.10.2.6. Importance of Model to Prediction of Dominant Phenomena

The icebed affects the pressure and temperature of the containment atmosphere and the extent of aerosol removal. In scenarios in which the icebed is effective, containment pressurization is typically limited and retention of aerosol is high.

D.10.2.7. Technical Adequacy of Model and Documentation

Although the thermal-hydraulic and fission product modeling of the ice condenser goes beyond a typical zeroeth-order model, the thermal-hydraulic conditions within an icebed are very complex. Knowledge of the physics of icebed behavior is incomplete (questionable) and the model is assessed to be zeroeth order. The technical adequacy of this model is classified as Category 2.

D.10.3. Containment Sprays

D.10.3.1. Model Description and Pedigree

CONTAIN has models for spray drop settling velocity, heat transfer to the drop, aerosol removal, and fission product gas (or vapors, I_2 , and CH_3I , or any gas/vapor species) removal. The aerosol removal models were discussed in Sec. D.5. The models for drop settling velocity, water vapor condensation/evaporation from the drop, heat transfer to the drop, and fission product removal are presented here in a table format. Note that for sprays, convection/diffusion is effective for removal of fission product gases/vapors. The sprays could also lead to an increased fogging in the containment.

D.10.3.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The models are reasonable except that no allowance is made for the direct cooling of structures by the impingement of spray drops.

D.10.3.3. Results of Model Sensitivity Studies

CONTAIN sensitivity studies Ref. D.10-3 have shown that that the calculated (e.g., iodine removal, etc.) results are strongly dependent on the values chosen for the model parameters, although the sprays are invariably quite effective in removing the fission products.

D.10.3.4. Results of Benchmarking/Validation Studies

The use of the models, appears to give a fair simulation of fission product/aerosol removal. Good data on controlled experiments on fission products/mixed aerosols are sparse (most data date back to the 1970s) and results of CONTAIN validation against experiments are not available. Comparison of CONTAIN calculations with a NUPEC hydrogen distribution experiment including sprays (ISP-35) has shown that direct cooling of structures by impingement of spray drops is an important effect that is not modeled in the code (Ref. D.1-4).

Model for drop settling velocity

Process	Model (Expression)	Pedigree (Reference)
drop settling velocity	<p>The spray drops are assumed to fall at a constant terminal velocity:</p> $v_t = \frac{v_{\text{air-steam}}}{d_{\text{drop}}} B^2$ <p>where B is a complicated factor:</p> $B = \frac{q_u - 9.06}{2}$ <p>where q_u is a numerical factor:</p> $q_u = \sqrt{82.0836 + 9.06 \sqrt{X_{\text{numl}} / D_{\text{enl}}}}$ <p>and X_{numl} is the "intermediate factor" calculated from $64\rho_l\rho_g d_{\text{drop}}^3 g$, and D_{enl} is $72\mu_{\text{gas}}^2$</p>	not given.

D.10.3.5. Identified Deficiencies and Options for Model Improvements

The models are rather simple, especially with respect to drop descriptions and the chemistry. The models can be improved if desired, following some of the developments of Ref. D.10-5. Cooling of structures by impingement of spray drops is an important effect not modeled in the code.

D.10.3.6. Importance of Model to Prediction of Dominant Phenomena

Use of correct models is important to source term calculations.

D.10.3.7. Technical Adequacy of Model and Documentation

The models used are simple to implement and appear to capture the dominant effects.

The documentation needs to be improved; the derivation of formulas should be explained in clearer mathematics and physics. The model needs to be modified to allow a fraction of the spray drops to be added to the water film on specified structures.

The technical adequacy of this model is classified as Category 1.

Models for mass (water vapor) and heat transport between a drop and the containment environment

Process	Model (Expression)	Pedigree (Reference)
Water vapor condensation /evaporation from drop	Because a drop is assumed to remain at a constant size, it is not clear if the water vapor transport is accounted in determination of drop size. It is, however, taken in to account in determining heat transfer (see below). This indicates some inconsistency in modelling.	
Heat transfer to drop	<p> $q = q_{conv} + q_{cond}; q_{conv} = h_c(T_{gas} - T_{drop}); q_{cond} = j_m h_{vl}$ where, $h_c = \frac{k_{gas(mix/bulk)}}{d_{drop}} N_{Nu};$ $j_m = K_g M_v (P_{v,gas(mix/bulk)} - P_{v,sat(drop)})$ and, $K_g = \frac{P D_v}{R T d_{drop}} \left(\frac{1}{P_{v,gas} - P_{v,sat}} \ln \frac{P - P_{v,gas}}{P - P_{v,sat}} \right) N_{Sh}$ </p> <p>The Nusselt and the Sherwood Numbers are taken as</p> $N_{Nu} = (2 + 0.6 N_{Re,drop}^{1/2} N_{Pr,gas}^{1/3})$ $N_{Sh} = (2 + 0.6 N_{Re,drop}^{1/2} N_{Sc,v}^{1/3})$ <p>The nomenclature is either obvious, or follows from the manual.</p>	Is based on standard formula for convection-diffusion and convection-conduction to spheres.

Models for and fission product (gas/vapor) removal

Process	Model (Expression)	Pedigree (Reference)
Fission product removal (I ₂ or CH ₃ I)	$\frac{dm_1(t)}{dt} = -m_1(t)N_D IC_{final};$ <p>where,</p> <p>$m_1(t)$ = the total Iodine mass in the atmosphere at time t,</p> <p>N_D = the number of drops that fall through the atmosphere per sec, and</p> $IC(t) = \frac{m_{I,drop}(t)}{m_1(t)}; \text{ with}$ $IC_{final} = \frac{m_{I,drop}(t)}{m_1(t)} \Big _{t=\text{at the completion of the fall}}$ <p>where $m_{I,drop}(t)$ is the Iodine content of a drop at time t.</p> <p>Thus, in a time Δt_c the ratio of Iodine removed from the atmosphere, to that remaining in the atmosphere is:</p> $\Rightarrow F_1(t_c) = \frac{\Delta m_1}{m_1} = 1 - \exp(-N_D IC_{final} \Delta t_c);$ <p>IC_{final} is determined from the sequential equations:</p> $IC_{i+1} = \frac{IC_i + S_i(PC_i)\Delta t / V_{atmosphere}}{1 + S_i\Delta t / V_{drop}};$ <p>where, IC_i is the value of IC at a given fall increment i,</p> <p>PC is the Iodine partition coefficient (default 5000),</p> <p>V indicates respective volumes, and S_i is the volumetric Iodine absorption (by the drop, m³ / s) rate:</p> $S_i = \pi d_{drop}^2 \frac{1}{PC_i \frac{1}{k_{gl}} + \frac{1}{k_{el}}}$ <p>where $k_{g(l)l}$ are the mass transfer coefficient (m / s), or the deposition velocity, for Iodine in the gas / liquid phase.</p> <p>These are determined from the relations:</p> $k_{gl} = \frac{D_{lg}}{d_{drop}} N_{sh}; \quad k_{el} = \frac{6.9757 D_{ll}}{d_{drop}}$	<p>the model is based on simple mass balance, and convection-diffusion considerations (I stands for I₂). The derivation of the equation for IC, however, needs to be clarified.</p>

D.10.4. Passive Containment Cooling System

D.10.4.1. Model Description and Pedigree

Representation of the PCCS in an ALWR involves the application of the basic models in CONTAIN rather than the use of unique models. The PCCS for the SBWR and AP600 are completely different systems and are modeled quite differently. Both can be used for DBA as well as severe-accident analyses. The elements of the SBWR PCCS are:

- steam supply line
- vertical shell-and-tube single-pass heat exchanger
- condensate flow line
- noncondensible gas vent line

The difficult modeling aspect of the SBWR PCCS is the treatment of the film of condensed steam. A mass and momentum balance is performed for laminar film flow. An energy balance is performed at the liquid-film interface employing a heat mass transfer analogy (Dittus-Boelter Equation). Shear forces and suction are excluded from the model.

The AP600 PCCS involves heat transfer through the steel containment shell to water draining down the external surface of the containment and to air flowing by natural convection in an annular region between the containment and the shield building. The difficult modeling aspects of the AP600 PCCS are the treatment of the external water film and the condensing heat transfer at the inner wall surface. The distribution of water on the external surface is treated parametrically, rather than mechanistically. Evaporation of the liquid film is based on mass transfer coefficients in the duct.

The modeling of the interior of the containment includes mass transfer coefficients, steam stratification and submerged concrete heat sinks. CONTAIN is also capable of modeling dry or long term performance of the PCCS. In this case, radiative and convective heat transfer are modeled in the duct.

D.10.4.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The PCCS representation for both ALWR designs involves the use of basic CONTAIN thermal-hydraulic and aerosol transport and deposition models. These models are expected to be adequate to reasonably predict the physical phenomena associated with these systems, within the constraints of the control volume approach and approximate treatment of three-dimensional flow behavior. Benchmarking of the treatment of the PCCS (e.g., manner in which the systems are nodalized) against experimental data is not complete.

D.10.4.3. Results of Model Sensitivity Studies

A sensitivity study has been performed for the AP600 PCCS to assess the importance of key parameters (Ref. D.10-6). The study concluded that during wet operation there is very little pressure sensitivity to modeling assumptions regarding heat transfer within containment or in the duct. For dry operation, pressure sensitivity was

found for radiation modeling in the duct, convective heat transfer in the duct, and air flow resistance.

D.10.4.4. Results of Benchmarking/Validation Studies

Benchmarking of the SBWR PCCS modeling approach has been performed against UCB data with excellent results (Ref. D.10-7).

Benchmarking of the AP600 PCCS modeling approach has been performed against Westinghouse experimental data (Ref. D.10-8). Results are in reasonable agreement.

D.10.4.5. Identified Deficiencies and Options for Model Improvements

Both models are at an early stage of testing and validation.

D.10.4.6. Importance of Model to Prediction of Dominant Phenomena

Both models appear capable of predicting dominant phenomena with reasonable accuracy.

D.10.4.7. Technical Adequacy of Model and Documentation

The physics of the PWR phenomena are understood but the BWR physics are considered questionable. Both models are first order. Both models satisfy the adequacy requirements established for the CONTAIN code. Neither model has been documented in the draft manual provided to the Peer Review Committee. The technical adequacy of this model is classified as Category 2.

D.10.5. Vapor Fission Product Transport

The limited models in CONTAIN for vapor fission product transport were not evaluated because of the changes in the NRC's severe-accident code strategy (see App. E). The TRENDS models that were being considered for incorporation into CONTAIN are discussed in Sec. 5.2 of this report.

D.10.6. Fission Product Characterization

D.10.6.1. Model Description and Pedigree

The analysis of fission product behavior in CONTAIN includes the treatment of decay chains, decay heating, host exchanges, transport, generation during core-concrete interactions and removal by ESFs. The approach used for the treatment of fission products involves the identification of fission product hosts (repositories). A host can be gas, an aerosol, structures, or a lower cell layer or pool. If the host is gas, the fission product is transported between containment volumes with the gas flow. As discussed in Sec. D.5, a variety of transport and removal mechanisms are treated for the aerosol transport of fission products.

D.10.6.2. Applicability/Physical Reasonableness of Model to Prediction of Dominant Phenomena

The fission product decay chains and decay heat associated with radionuclide decay are well known in comparison with most severe-accident phenomena. The fission product host approach is quite general and a rational approach to tracking fission product species.

D.10.6.3. Results of Model Sensitivity Studies

No sensitivity studies related to fission product characterization were presented to the Committee.

D.10.6.4. Results of Benchmarking/Validation Studies

The choice of approach to characterizing fission product behavior affects the structure of the computer code. Benchmarking studies are not necessary to establish the validity of the approach. The fission product decay chains have been well established.

D.10.6.5. Identified Deficiencies and Options for Model Improvements

None.

D.10.6.6. Importance of Model to Prediction of Dominant Phenomena

The model is of moderate importance to source term behavior but has low importance to containment loads.

D.10.6.7. Technical Adequacy of Model and Documentation

The host approach to fission product characterization is adequately described in the documentation. Fission product decay chain coefficients are well known. The model is assessed to be adequate.

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- D.10-2. N. Russell and D. Williams, "Comparison of CONTAIN Code Simulations to Experimental Ice Condenser Test Data," Sandia National Laboratories report SAND89-3096C, presented at the Second International Conference on Containment Design and Operation, Toronto, Canada, October 1990.
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- D.10-4. R. O. Mahoney, "AEA Participation in CSNI ISP35 - A Blind Hydrogen Distribution Test," AEA document AEA RS 5609, Commercial in Confidence, 1994.

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- D.10-6. J. Tills, K. K. Murata, and K. E. Washington, "AP600 Design Basis and Severe Accident Scoping Calculations with the CONTAIN Code," 20th Water Reactor Safety Information Meeting, Bethesda, MD, October 21-23, 1992.
- D.10-7. J. Tills, "SBWR Models and Assessment," Presentation at CONTAIN Peer Review Meeting No. 3, January 19, 1994.
- D.10-8. J. Tills, "AP600 Plant Analysis," Presentation at CONTAIN Peer Review Meeting No. 3, January 19, 1994.

APPENDIX E

Revised Severe-Accident Code Strategy

While the CONTAIN Peer Review was in progress, the NRC issued a draft "Revised Severe-Accident Code Strategy" that incorporated revised design objectives and targeted applications for the CONTAIN code. The remainder of this appendix is the information package released by the NRC to both national and international institutions having interest in the NRC's severe-accident strategy. The information package includes: (1) a cover letter providing the background and rationale for developing a revised severe-accident code strategy, a description of strategy options, and identification of the preferred option, (2) an attachment describing the "Severe-Accident Code Strategy Review Rationale," (3) revised design objectives, targeted applications, and success criteria for the MELCOR code, (4) revised design objectives, targeted applications, and success criteria for the CONTAIN code, and (5) revised design objectives, targeted applications, and success criteria for the SCDAP/RELAP5 code.

The information package was issued for review and comment. Members of the CONTAIN Peer Review Committee were requested to review and comment on the revised severe accident code strategy. The Committee members performed the requested review and provided comments as requested.¹

The information package containing the draft revised severe-accident code strategy was issued after the Committee had completed its bottom-up review and while it was approaching completion of its top-down review. Because the revised strategy had been issued for review and comment, the Committee did not repeat its review using the revised CONTAIN design objectives, targeted applications, and success criteria. Subsequently, it became clear from discussions with NRC and SNL staff that the NRC had adopted and was implementing the revised severe-accident code strategy. Given this reality, the Committee carefully considered the revised strategy and associated revised CONTAIN design objectives and targeted applications when assigning priorities to its recommendations (see Sec. 6). For example, a low priority was assigned to correction of code deficiencies for code features that no longer are an essential element of the revised CONTAIN design objectives. One such example is that correction of deficiencies related to fission product models was assigned a low priority because the NRC will expend future effort and resources in maintaining this capability only for the MELCOR code.

¹ B. E. Boyack, "Committee Comments on Revised Severe Accident Code Strategy," Los Alamos National Laboratory Group TSA-12 letter TSA-12-94-56 to F. Eltawila dated February 14, 1994.

UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

Dr. Nestor R. Ortiz
Nuclear Energy Technology
Organization 6400
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185

JAN 14 1994

Dear Dr. Ortiz: *Nestor*

As we reflect on our operational experiences with the NRC severe accident codes, it has become increasingly evident to us that we need to modify our overall severe accident code strategy and realign the objectives for each code so they better match today's needs. Also, recent reviews have frequently touched on the similarities between some of the codes and have questioned our adherence to the so-called two-tier code strategy (see Attachment 1). However, we are not too concerned with comments regarding some code appearing to embody characteristics called for in another tier. What does concern us is whether there is unnecessary duplication of code capability between the various codes and whether the code is adequate for its intended applications. The purpose of this letter is to request your input as we reexamine our strategy and the objectives and targeted applications for the severe accident codes.

Since we are involved in the above process, we believe your input will be very important to us. Also, to be most useful, the NRC needs to address any modifications to the development efforts at the various involved code development laboratories very soon so as to minimize any inefficient efforts in FY94 activities. Thus, your response to this request would be appreciated by February 11, 1994.

The framework for our code development efforts is described in the Severe Accident Research Program Plan Update (SARP) NUREG-1365, Rev. 1. Key words from which are provided in Attachment 2. The principal focus of this current discussion is on the three system level codes: SCDAP/RELAP5, MELCOR and CONTAIN. Considering that we are reviewing our code strategy, we have taken a fresh look at each code's Objectives and Targeted Applications and have revised them to clearly identify the basis or rationale for each code's existence and plans as we see them today. They can be found in Attachments 3, 4, and 5. As a part of this review of code strategy we are asking for comments on these sets of objectives from the NRC code users' in NRR and in RES/DSIR.

A major motivation for the review of our code strategy has been that the MELCOR, CONTAIN and SCDAP/RELAP5 codes all have fission product handling capability, but only the MELCOR code is designated as the source term code. Further, only the MELCOR code can model the generation of radionuclides during an accident and produce the resulting fission products without the need to run other codes to develop part of the information.

We have reviewed the objectives of our other more detailed severe accident codes as well. These are VICTORIA, COMMIX and IFCI. Generally, these codes have been developed to perform specific functions that require detailed modeling, as stated in NUREG-1365. These codes are also used to benchmark the system level codes.

Since we are reviewing our overall code strategy, we have examined several options which are listed here in order of preference, indicating the competing ideas that we have considered.

1. "Consolidate fission products modeling." This option would involve improving the fission product capabilities in MELCOR, as necessary to adequately calculate the source term, including putting the better modeling from CONTAIN into MELCOR as appropriate and if cost effective. This option would also eliminate the fission product release and transport models from the SCDAP/RELAP5 code. The CONTAIN code capabilities would be primarily limited to thermal-hydraulic analyses, particularly for severe accident containment load calculations and for ALWR DBA calculations. Similarly, SCDAP/RELAP5 capability would focus on evaluation of in-vessel core damage progression and accident management. As will be discussed later, the CONTAIN code will be eventually archived, once the work on ALWR certifications is complete.

This is our preferred approach.

2. "Modify CONTAIN." This option envisions replacing the existing CONTAIN code framework with the analogous framework from MELCOR (i.e., the containment part of MELCOR). It would also involve stripping away all the existing thermal-hydraulic models from the CONTAIN code which are not currently in MELCOR and adding them "back into" the new containment code framework. This would correct the long standing problems associated with the less structured approach in building CONTAIN software vs. the better software approach in MELCOR using the modularized, "package" subroutine architecture which is often considered superior to CONTAIN. SCDAP/RELAP5 would be treated as in Option 1.

This option would require extensive reconstruction of a new CONTAIN-type code from MELCOR which would result in unnecessary duplications. This could be very inefficient and expensive without any apparent benefit, and hence it has been rejected.

3. "Archive CCNTAIN." This option envisions the completion of NRC support for CONTAIN code development and would focus all source term and containment modeling improvements on the MELCOR code. This acknowledges that MELCOR can be effectively used to model and

calculate containments for severe accidents as it currently exists and can be upgraded as has been planned for CONTAIN. For containment analyses MELCOR can simply be run without activating the COR Package and the RCS system (a major portion of the MELCOR running time is associated with the in-vessel calculations). SCDAP/RELAP5 would be treated as in Option 1, and more detailed in-vessel fission product analyses could be performed with VICTORIA taking boundary conditions, etc., from a SCDAP/RELAP5 calculation.

As an outcome of Option 1 we would eventually cease developmental activities for CONTAIN when we have completed ALWR evaluations. Coupled with the RELAP code, the CONTAIN code is currently the code of choice for detailed evaluation of ALWR containment effects primarily because it has received more validation with containment test data than MELCOR. Therefore, in order not to interrupt the ALWR activities, this option will be put on hold until the ALWRs efforts are completed.

4. Merge all three codes. This option envisions (a) creating a modular code with the best and most detailed models from all three (MELCOR, CONTAIN, and SCDAP/RELAP5) existing system-level codes (assuming continued CPU running time improvements will be made by the industry during the period this work would be ongoing), and (b) having the ability for the code user to choose to run only the portions or modules of the whole code (e.g., containment or in-vessel melt-progression) which are needed at the time. This option reflects some recent interests in running RELAP5 and CONTAIN, linked computationally for design basis accidents for ALWRs.

As in Option 2, this would require extensive reconstruction of the MELCOR code. Although cost/benefit favors a single code approach for integrated systems analysis of severe accidents, the current state-of-knowledge will make it difficult to accomplish this goal. We believe that more than one analytical approach will be needed in the near future to analyze experiments and develop the models needed for an integrated systems code. However, we should revisit this option in 2-3 years.

5. "Stay the course." This option means that after review there would be little if any change to our directions for the codes; i.e., continue to implement fission product tracking into the MELCOR and CONTAIN system level codes and continue to evaluate the need for this in SCDAP/RELAP5.

Since we have determined that our code strategy needs to be revised, we eliminate this "stay the course" option.

At this point, we believe Option 1 is the best approach. As stated earlier, we have started implementing this strategy and put on hold developmental improvement of the fission product capabilities in CONTAIN and SCDAP/RELAP5. We anticipate a period of study of the individual and comparative code attributes and the currently proposed improvements needed for each code.

We need to undertake this effort on a fairly expeditious basis because activities are already well underway in defining the code development plans for FY1994, although we do not foresee any major changes to the current FY1994 plans. We would be glad to discuss this with you; if you wish, please call Dr. F. Eltawila at 492-3525. Again, your reply by February 11, 1994, would be much appreciated.

Brian W. Sheron, Director
Division of Systems Research
Office of Nuclear Regulatory Research

Attachments:

- 1) Two-tier code layout
- 2) Severe Accident Code Strategy Review Rationale
- 3) MELCOR objectives and targeted applications
- 4) CONTAIN objectives and targeted applications
- 5) SCDAP/RELAP5 objectives and targeted applications

cc: S. Thompson, SNL
J. Kelly SNL
K. Washington, SNL

Tier 1: INTEGRATED CODES

MELCOR (2nd Generation)

Tier 2: DETAILED MECHANISTIC CODES

COMMIX

DEBRIS

VICTORIA

CORCON (MOD3)

HMS BURN

SCDAP/RELAP5 (MOD)3

CONTAIN

MACCS

Thermal Hydraulics	Core Melt	FP Release from fuel	FP Transport in HCS	Pressure Vessel Failure	Core-Concrete Interaction	Release from Fuel Debris	FP Transport in Containment	Containment Load	Containment Performance	Off Site Consequences
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PROGRESSION OF ACCIDENT PHENOMENA

Figure 2.4.1 NRC Severe Accident Codes

ATTACHMENT 2

Severe Accident Code Strategy Review Rationale

As we reflect on our operational experiences with the NRC severe accident codes, it has become increasingly evident to us that we need to modify our overall severe accident code strategy and realign the objectives for each code so they better match today's needs. Also, recent reviews have frequently touched on the similarities between some of the codes and have questioned our adherence to the so-called two-tier code strategy. We are not so concerned about whether some code appears to embody characteristics called for in another tier, but we are concerned about whether there is unnecessary duplication of code capability between the various codes and whether the code is adequate for its intended applications.

It appears that there is indeed some unnecessary duplication in our code development. For example, a CONTAIN code reviewer noted "there appears to be a large degree of similarity in terms of modeling of physical/chemical phenomena between CONTAIN and MELCOR. The MELCOR thermal-hydraulics and heat transfer models are comparable and at times more sophisticated than those of CONTAIN." Another example of similarity appears in our plan to improve the fission product capabilities in both CONTAIN (e.g., addition of TRENDS models) and in MELCOR. In examining this issue of similarity between MELCOR and CONTAIN, we have considered the original basis for including fission product modelling in CONTAIN. First, since CONTAIN is a containment code, it was logical to include fission product modelling. Moreover, since CONTAIN was intended as the more mechanistic of the two codes, logically CONTAIN would include more mechanistic models of fission product transport and deposition. Secondly, it is our belief that CONTAIN was selected for performing fission product calculations in containment supporting NUREG-1150 because during that time frame MELCOR was not sufficiently robust for performing a multitude of calculations. More recently, as a result of our efforts to improve MELCOR, code performance has been sufficiently enhanced so that MELCOR analysis has been used to support work on the source term update.

Since MELCOR calculates both the generation and release of radionuclides as well as transport and deposition both within the RCS and the containment, it is not necessary to run another code first to determine source term results from MELCOR. However, for CONTAIN to be used for fission product transport and deposition calculations, the code must first have input on fission product releases from the RCS supplied from other analyses using MELCOR or VICTORIA. It is our conclusion that since larger uncertainties in fission product tracking are tolerable in comparison with the better accuracy required for thermal hydraulic analyses, it is worthwhile to reconsider the above mentioned need for more detailed or more mechanistic modelling of fission product transport and removal processes with the CONTAIN code. In this regard, any needed radionuclide improvements should be incorporated into the MELCOR code.

Similarly, the use of SCDAP/RELAP5 for detailed tracking of in-vessel fission product release and transport has been undergoing evaluation at the laboratories, and previous plans to improve fission product handling capability as recommended by the SCDAP/RELAP5 Peer Review Committee have been

postponed. This decision is based on the fact that VICTORIA can perform any necessary detailed in-vessel fission product calculations with input in initial, boundary and thermal hydraulic conditions from SCDAP/RELAP5. It is our opinion that fission product effects on core melt progression and natural circulation are negligible. Therefore, our current position is that no fission product modeling capability should be incorporated in SCDAP/RELAP5. Again, in this case, the MELCOR code could handle the release and transport of radionuclides throughout the accident.

It is recognized that some important chemical reactions that affect the deposition and revaporization of radionuclides are not modeled by the MELCOR code at this time. But, simple models for these effects which capture the most important effects during accident sequences, as determined by the VICTORIA code, may be incorporated into MELCOR.

The framework for our code development efforts is described in the Severe Accident Research Program Plan Update (SARP) NUREG-1365, Rev. 1. Key words from this report are repeated as follows:

The development of severe accident phenomenological models and computer codes continues to have a role in achieving the objectives of the severe accident research program. The codes now under NRC's sponsorship and support are SCDAP/RELAP5, MELCOR, and CONTAIN. In addition, several other codes such as VICTORIA, COMMIX, and IFCI are being developed and maintained to perform specific functions that require detailed modeling. These codes will be used to benchmark the system level codes discussed earlier. Also, the core concrete interaction code, i.e., CORCON, will be incorporated into the CONTAIN and MELCOR codes. The relationship of these codes to various severe accident progression phenomena is shown in [Attachment 1]. Additional discussion on the status of each of these codes is provided below.

The principal focus of this current discussion is on the three system level codes: SCDAP/RELAP5, MELCOR and CONTAIN. For perspective, the objectives of each of these three codes, as taken from the latest Severe Accident Research Plan (NUREG-1365, Rev. 1, p. 30 et. seq.), are provided below, each followed by either updated, more detailed objectives or a comment based on our current needs:

- a) "The objective of the SCDAP/RELAP5 program is to develop an analytical tool that will provide the NRC with the capability to perform detailed analyses of in-vessel core melt progression phenomena during various severe accident conditions and scenarios." To embody the understanding of severe accident behavior from initial core uncover through reactor vessel failure, the code is designed to model the coupled interactions that occur between the RCS, the core, and the fission products during a severe accident.

In addition to the above, except for the last sentence regarding fission products interactions, the objectives for SCDAP/RELAP5 are to: develop and maintain the capability to independently assess severe accident scenarios and

to develop in-depth understanding of severe accident behavior and its consequences; and evaluate the effect of different accident management strategies to gain more quantitative understanding of core damage progression during the various stages of severe accidents which could enable us to better anticipate the plant response to severe accidents.

- b) The current program for the MELCOR code, which is designed to model the entire spectrum of severe accident phenomena including the reactor coolant system and containment thermal-hydraulic response, core heating, degradation and relocation and fission product release and transport for both BWR's and PWR's, is intended to produce "a second-generation integrated severe accident code that should (1) appropriately model phenomena essential to the understanding of severe core damage accidents, (2) provide predictions of the progression and consequences of severe core damage accidents, (3) permit estimates of the uncertainties associated with such predictions, and (4) have a structure that facilitates the incorporation of new or alternative phenomenological models based on the ongoing experimental research program." Also, it is intended to "provide a code that includes major phenomenological developments from severe accident research in adequate detail to address the phenomenology and has a practical running time for severe accident analyses."

Focusing the above paragraph, a more current and concise objective for the MELCOR code is to develop and maintain a fast running severe accident code for probabilistic risk assessment applications and to independently gain quantitative understanding of the overall probabilities of core damage, containment failure and fission product releases.

- c) "The CONTAIN code is a detailed mechanistic code for the integrated analysis of containment phenomena. It has the capability to predict the physical, chemical, and radiological conditions inside a nuclear reactor containment as well as fission product releases to the environment in the event of containment failure. It models intercell flow, hydrogen and carbon monoxide combustion, heat and mass transfer (radiation, convection, conduction), aerosol behavior, fission product behavior (decay heating, transport), engineered safety systems (sprays, fan coolers, ice condensers), BWR-specific systems (suppression pools and safety relief valve discharge), core-concrete interaction, and simple treatment of direct containment heating.

A primary objective of the current research program is to develop and validate models related to the ALWR performance for both design basis accidents and severe accidents. [We anticipate completing the implementation of most of these models during FY94, therefore, we do not anticipate any interruption of these efforts.] Other activities include

updating the code with improvements in modeling already developed under other programs.

A more succinct current statement of objectives for this code is as follows: The CONTAIN code is intended as a thermal hydraulic computer code for the integrated analysis of containment phenomena. It should have the capability of predicting pressure and temperature conditions inside a variety of containment types. The code should be useful for analyzing design basis accidents as well as postulated severe accident scenarios.

A more detailed set of "Objectives and Targeted Applications" for each of these codes is given in Attachments 3, 4, and 5. The format was initially developed for use by the code peer reviewers. But now, considering that we are reviewing our code strategy, we have taken a fresh look at these Objectives and Targeted Applications and have revised them to clearly identify the basis or rationale for each code's existence and plans as we see them today.

In short, the MELCOR, CONTAIN and SCDAP/RELAP5 codes all have fission product handling capability, but only the MELCOR code is designated as the source term code, and only the MELCOR code can model the generation of radionuclides during an accident and produce the resulting fission products without the need to run other codes to develop part of the information.

However, since the adoption of the new source term (Ref: NUREG-1465), which embodies substantially more understanding of fission product behavior than in the original TID 14844 source term, the analyses of source terms may not be such a pressing problem either by the applicants or by the NRC. Nevertheless, MELCOR is still the basic analytical tool which NRC uses to perform independent checks, including sensitivity studies of vendors' proposed severe-accident-related design features for ALWR's and for modifications to existing containments. This can be particularly useful when industry makes claims based on MAAP analyses of fission product releases to containment. In that regard it is our intent to keep MELCOR consistent with the state-of-the-art for source term analyses and make appropriate modifications or improvements to the code as necessary. It would appear then, that there should be no further need to improve fission product capabilities in CONTAIN or in SCDAP/RELAP5. For those situations where CONTAIN has capability to treat radionuclides better than MELCOR, those models will be incorporated into MELCOR when practical and cost effective. Earlier, it had been intended to incorporate models from the TRENDS code into CONTAIN to provide mechanistic modeling of iodine chemistry and other fission product physical and chemical processes. Incorporation of this TRENDS package would have further advanced the overall capability in CONTAIN to predict fission product release constituents and fission product spatial heating effects. But, as noted above, we have put this on hold. Similarly, it had been intended to improve the fission products release and transport models in the SCDAP/RELAP5 MOD3 to provide up-to-date modeling. But, as noted above, we have also put this on hold.

We have reviewed the objectives of our other more detailed severe accident codes as well. These are VICTORIA, COMMIX and IFCI. Generally, these codes have been developed to perform specific functions that require detailed

modeling, as stated in NUREG-1365. These codes are also used to benchmark the system level codes. The objectives of these codes, as currently modified from NUREG-1365 are as follows:

The objective of the VICTORIA code is to predict both the release of fission products from degrading reactor fuel and the transport of these fission products through the reactor coolant systems during severe accident conditions. The objectives of current efforts to complete the code include coupling of vapor and aerosol species mass rates to provide the source term rates for neighboring domains, modification of the chemistry solver to include a frozen chemistry model, minor revisions to the decay heat model, and improvements to revaporization of fission products to include non ideal solutions.

The objective of the COMMIX code is to perform steady state/transient, single-phase/multicomponent three dimensional analysis of fluid flow systems with heat and mass transfer. It should have the capability to characterize containment gaseous stratification and bulk circulation patterns. Principally, the code should be useful for analyzing hydrogen mixing and transport. Moreover, in the AP600 containment performance review in which reliance on natural circulation is used for removal of decay heat through the containment shell, COMMIX calculations will complement the traditional control volume (i.e., CONTAIN) predictions.

The objective of the Integrated Fuel-Coolant Interaction (IFCI) code is to analyze the effect of molten fuel materials when they come into contact with water. Such fuel-coolant interactions (FCIs) can occur for a variety of in-vessel and ex-vessel conditions including: reflood of a partially molten core, melt pouring into the lower plenum, and melt pouring out of the vessel lower head into a water-filled reactor cavity under low or high pressure. In these situations non-explosive or explosive FCIs may occur. Both modes of FCIs can be analyzed by IFCI, but both the mode and resulting energetics of FCIs depend on the complex interaction of various thermal, physical, and chemical processes including: coarse mixing, particle fragmentation, and heat transfer.

In summary, we have proposed an in-depth review of the system-level codes and the formulation of an improved strategy for completion of all the severe accident codes. Several options we have considered are discussed below.

OPTIONS:

1. "Consolidate fission products modeling." This option would involve improving the fission product capabilities in MELCOR, as necessary to adequately calculate the source term, including putting the better modeling from CONTAIN into MELCOR as appropriate and if cost effective. This option would also eliminate the fission product release and transport models from the SCDAP/RELAP5 code. The CONTAIN code capabilities would be primarily limited to thermal-hydraulic analyses, particularly for severe accident containment load calculations and for ALWR DBA calculations. Similarly, SCDAP/RELAP5 capability would focus on

evaluation of in-vessel core damage progression and accident management. As will be discussed later, the CONTAIN Code will be eventually archived, once the work on ALWR certifications is complete.

This is our preferred approach.

2. "Modify CONTAIN." This option envisions replacing the existing CONTAIN code framework with the analogous framework from MELCOR (i.e., the containment part of MELCOR). It would also involve stripping away all the existing thermal-hydraulic models from the CONTAIN code which are not currently in MELCOR and adding them "back into" the new containment code framework. This would correct the long standing problems associated with the less structured approach in building CONTAIN software vs. the better software approach in MELCOR using the modularized, "package" subroutine architecture which is often considered superior to CONTAIN. SCDAP/RELAP5 would be treated as in Option 1.

This option would require extensive reconstruction of a new CONTAIN-type code from MELCOR which would result in unnecessary duplications. This could be very inefficient and expensive without any apparent benefit, and hence it has been rejected.

3. "Archive CONTAIN." This option envisions the completion of NRC support for CONTAIN code development and would focus all source term and containment modeling improvements on the MELCOR code. This acknowledges that MELCOR can be effectively used to model and calculate containments for severe accidents as it currently exists and can be upgraded as has been planned for CONTAIN. For containment analyses MELCOR can simply be run without activating the COR Package and the RCS system (a major portion of the MELCOR running time is associated with the in-vessel calculations). SCDAP/RELAP5 would be treated as in Option 1, and more detailed in-vessel fission product analyses could be performed with VICTORIA taking boundary conditions, etc., from a SCDAP/RELAP5 calculation.

As an outcome of Option 1 we would eventually cease developmental activities for CONTAIN when we have completed ALWR evaluations. Coupled with the RELAP code, the CONTAIN code is currently the code of choice for detailed evaluation of ALWR containment effects primarily because it has received more validation with containment test data than MELCOR. Therefore, in order not to interrupt the ALWR activities, this option will be put on hold until the ALWRs efforts are completed.

4. Merge all three codes. This option envisions (a) creating a modular code with the best and most detailed models from all three (MELCOR, CONTAIN, and SCDAP/RELAP5) existing system-level codes (assuming continued CPU running time improvements will be made by the industry during the period this work would be ongoing), and

(b) having the ability for the code user to choose to run only the portions or modules of the whole code (e.g., containment or in-vessel melt-progression) which are needed at the time. This option reflects some recent interests in running RELAP5 and CONTAIN, linked computationally for design basis accidents for ALWRs.

As in Option 2, this would require extensive reconstruction of the MELCOR code. Although cost/benefit favors a single code approach for integrated systems analysis of severe accidents, the current state-of-knowledge will make it difficult to accomplish this goal. We believe that more than one analytical approach will be needed in the near future to analyze experiments and develop the models needed for an integrated systems code. However, we should revisit this option in 2-3 years.

5. "Stay the course." This option means that after review there would be little if any change to our directions for the codes; i.e., continue to implement fission product tracking into the MELCOR and CONTAIN system level codes and continue to evaluate the need for this in SCDAP/RELAP5.

Since we have determined that our code strategy needs to be revised, we eliminate this "stay the course" option.

At this point, we believe Option 1 is the best approach. As stated earlier, we have started implementing this strategy and put on hold developmental improvement of the fission product capabilities in CONTAIN and SCDAP/RELAP5. We anticipate a period of study of the individual and comparative code attributes and the currently proposed improvements needed for each code.

ATTACHMENT 3

MELCOR CODE

Design Objectives

1. MELCOR should be capable of modeling of key severe accident phenomena for a variety of initiating events in nuclear power plants. The phenomena include core degradation, relocation, and vessel failure; reactor coolant system and containment thermal-hydraulic response; and fission product release and transport in both BWRs and PWRs.
2. Models incorporated in MELCOR should be able to address the key accident phenomena in adequate detail from the risk assessment perspectives, but permit a practical running time for accident sequence analysis including sensitivity studies.
3. MELCOR should provide reasonable predictions of the progression and consequences of severe accidents and permit estimates of uncertainties associated with such predictions.
4. MELCOR should be portable, maintainable, and have a structure that facilitates incorporation of new or alternative phenomenological models.
5. MELCOR should permit extrapolation of the results of simulation of small-scale separate effects and integral experiments to full-scale plant cases.

Targeted Applications

1. Accident sequence analysis in light water reactor plants under severe accident conditions to predict thermal-hydraulic and radiological conditions inside the reactor vessel, in the primary system, and in the containment.
2. Source term calculations to provide necessary inputs to probabilistic risk assessment (PRA) studies of BWRs and PWRs and to provide an independent audit capability.

Success Criteria

1. MELCOR predictions of phenomenological events should be in qualitative agreement with the current understanding of the physics of such events based either on the results of certain well-defined and controlled experiments or on analytical results derived from first principles.
2. Uncertainties in key parameters describing a phenomenon as calculated by MELCOR should not exceed the uncertainties in experimentally measured or analytically derived values of these parameters.

3. MELCOR phenomenological models should be parametric to the practical extent possible so that uncertainties in the phenomena can be adequately represented through parametric variation and sensitivity analysis. Simple mechanistic models may be incorporated into MELCOR so long as such actions do not result in an undue run time penalty.
4. MELCOR code architecture should be sufficiently modular to permit easy incorporation of new phenomenological models. Interfaces between various packages within MELCOR should be sufficiently robust.
5. MELCOR should be a relatively fast-running and machine-independent code. For most accident sequence analysis, the warp factor (ratio of simulation time versus run time) for MELCOR should be much larger than that for other mechanistic codes, i.e., MELCOR should run faster than other mechanistic codes for the same input problem. As for machine-independent criterion, MELCOR outputs from different machines should ideally differ only in terms of round-offs. Machine errors should not be exponential and unbounded.
6. The maintenance of MELCOR should follow accepted quality assurance standards for configuration control, testing, and documentation.

ATTACHMENT 4

CONTAIN CODE

Design Objectives

1. The CONTAIN code is intended as a thermal hydraulic computer code for the integrated analysis of containment phenomena. It should have capability of predicting pressure and temperature conditions inside a variety of containment types.
2. The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected design basis accidents. It should permit estimates of the uncertainties of containment loads predictions without requiring modifications to the code.
3. Models incorporated in CONTAIN should be able to address key containment accident phenomena in adequate detail from the risk assessment perspectives.
4. CONTAIN should permit relatively straightforward extrapolation of the results of simulation of small-scale separate effects and integral experiments to full-scale plant cases.
5. CONTAIN should be portable, maintainable, and have a structure that facilitates incorporation of new or alternative phenomenological models.

Targeted Applications

1. Containment response analysis in light water reactor plants under severe accident conditions and certain design basis events to predict thermal-hydraulic conditions inside containment.
2. As a code developmental tool for evaluating selected containment issue resolutions, and to analyze phenomena so that simpler models can be justified for incorporation into the MELCOR code.

Success Criteria

1. CONTAIN predictions of phenomenological events should be in qualitative agreement with the current understanding of the physics of such events based either on the results of certain well-defined and controlled experiments or on analytical results derived from first principles.
2. Uncertainties in key parameters describing a phenomenon as calculated by CONTAIN should not exceed the uncertainties in experimentally measured or analytically derived values of these parameters.

3. CONTAIN phenomenological models should where feasible be mechanistic in nature and capture the dominate processes to the practical extent possible. Otherwise, parametric models are acceptable and uncertainties in the phenomena can be adequately represented through parametric variations and sensitivity analysis.
4. The code should be transportable for mainframe and workstation computing machines. The maintenance of the code should follow accepted Quality Assurance standards for configuration control, testing, and documentation.

ATTACHMENT 5

SCDAP/RELAP5 CODE

Design Objectives

1. Modeling detail shall be capable of representing key and important phenomena of severe accident experiments relevant to anticipated plant accidents and transients, and the TMI-2 accident.
2. The code should provide best estimate predictions of the in-vessel melt progression phenomena during the course of a severe accident. It should permit estimates of the uncertainties of severe core damage predictions without requiring modifications to the code.
3. The code should be applicable for severe core damaged studies under various accident sequences for both pressurized water reactors (PWR) and boiling water reactors (BWR).
4. The code should have minimum user-input parameters (i.e., only when data are lacking for deriving mechanistic models.) and should be robust, portable, and fast running.

Targeted Applications

1. Experimental analysis and support for in-vessel severe accident experimental programs such as CORA, PBF, LOFT, NRU FLHT, ex-reactor experiments.
2. Selected plant analyses in light water reactors including advanced light water reactors (PWRs and BWRs) under various severe accident conditions; this is to analyze in-vessel melt progression phenomena including lower head failure mode and provide initial and boundary conditions for the calculation of containment loadings.
3. Selected detailed analysis for specific technical issues -- influence of water addition, natural circulation during a station blackout accident, hydrogen generation upon reflood, depressurization strategy to mitigate direct containment heating, and accident management evaluations.
4. MELCOR benchmarking and assessment.

III. Success Criteria

1. SCDAP/RELAP5 predictions of in-vessel core melt progression phenomena should be quantitatively comparable to the integral and/or separate-effects experimental results.
2. Expected modeling uncertainties of key parameters as calculated by SCDAP/RELAP5 should be within uncertainties in integral severe accident experiments and TMI-2 accident results.
3. The code should not abort prematurely due to user input errors or numerical nonconvergence but should exit with sufficient diagnosis messages for users.
4. Numerical precision should be compatible with modeling precision. Spatial convergence should be compatible with modeling scale. Time step control should be automatic.
5. The code should be transportable for mainframe and workstation computing machines.
6. The maintenance of the code should follow accepted Quality Assurance standards for configuration control, testing, and documentation.

APPENDIX F

CONTAIN User Survey

CONTAIN users are asked to provide important information in support of an independent peer review of the CONTAIN code that will start in May 1993. The CONTAIN peer review will focus on the LWR applications of the code. This survey requests information related to the technical adequacy of the code. There are four sections. The first section explores code technical adequacy issues related to the CONTAIN code "design objectives" that have been set forth by the NRC. The second section investigates code technical adequacy in relation to the NRC-specified "targeted applications" specified by the NRC. The third section asks for a ranking of "level of completeness" of the code with respect to design objectives and a listing of CONTAIN-related reports or papers generated by your organization. The fourth section is a single sheet asking for user-related information. You are encouraged to add additional sheets as needed to provide space for comments that exceed the space provided.

Please do not be discouraged by the length of this survey. Try to concentrate on and give detailed answers to those areas with which you have the most experience. By doing so, you will be providing information that will influence future code-related activities. Be as specific as possible. We want you to provide as many answers as you can. We do recognize, however, that there may be questions that you are unable to address. Also, please identify the code version to which each of your answers applies (many users have experience with several versions of the code).

Responses to surveys frequently focus on deficiencies and do not comment on praiseworthy aspects. Such a focus leaves an unwarranted negative impression of a product. Therefore, we strongly encourage you to provide positive, as well as negative, comments in this survey.

Your timely response is important since the CONTAIN Peer Review Committee will soon begin its activities. We hope that you will avail yourself of this opportunity to provide input to the CONTAIN Peer Review Committee, the NRC, and to the CONTAIN code development staff. Thank you for your participation.

I. CONTAIN Code-Design Objectives

1. Modeling detail shall be capable of representing key and important phenomena of severe accident experiments, and anticipated plant accidents and transients.

Question: What experience can you relate that shows that the user can adequately model PWR and BWR containment systems, operator actions, and experimental facilities with the code? In addition, please provide any insights you may have regarding the containments of advanced reactor designs.

- a. Expected modeling uncertainties should be comparable to uncertainties in integral severe-accident experiments.

Question: Are the uncertainties in important parameters calculated by the code less than or equal to measured values? (For example, if the uncertainties in the measured temperatures and associated boundary conditions are +/-20%, would you expect to find that the associated code-computed values are also within +/-20%?) Please provide examples of your findings.

b. User-defined parameters, other than those needed to define experiments or plant unique features, should be eliminated but only where an experimental or other credible basis exists to define those parameters (e.g., user guidance documentation is required)

Question: What user-defined parameters, other than those noted, have you encountered that should be eliminated from the code input?

2. The code should provide reasonable predictions of containment transient response and consequences during the course of severe accidents and selected DBAs. It should permit estimates of the uncertainties of containment loads and fission product release predictions without requiring modifications to the code.

Question: What do your analyses show regarding the code's capability to predict major trends for dominant phenomena based on assessment against integral facility data? How well does the code predict values of important parameters associated with dominant phenomena within measurement uncertainty when assessed against integral facility data? Did you employ a "frozen" released version of the code without any code modifications made during the period of assessment?

3. The code should be applicable for containment transient studies under various accident sequences for PWRs, BWRs, and ALWRs.

Questions: What experience can you relate that demonstrates that the code can predict containment loads resulting from risk-dominant accident sequences identified by probabilistic risk assessment studies for both PWRs and BWRs? In addition, please provide any insights you may have regarding containments for the ALWR designs. Are physical models, as well as component models, adequate to accurately predict dominant phenomena? How would you compare the level of detail of the CONTAIN code models compared to level of detail of the code models found in the MELCOR code? If you have made any studies using both CONTAIN and MELCOR for the same problem, how did the results compare?

4. The code should be robust, portable, and fast running.

Question: Although run time is certainly machine dependent, what have you found regarding the "reasonableness" of the code run time? How has this affected your ability to perform sensitivity and/or uncertainty analyses for the phenomena/conditions the code is designed to model? What is the fraction of the code runtime compared to the time required to perform an entire analysis? Please give as many examples as possible.

Question: How effective are the code-user guidelines and other lessons-learned information in the code manual? How useful is documentation in setting up a plant model (input deck) to accurately represent a full-scale LWR plant and successfully perform plant calculations?

a. The code should not abort prematurely because of user-input errors or numerical nonconvergence, but should exit with sufficient diagnostic messages for users.

Question: What has your experience been in this area? Did you encounter problems where the code did not converge? If so, please describe. Does the code output give you sufficient detail to determine where most of the computation time

was spent (what model, subroutine, limiting parameter, or control volume, for example)? Overall, how would you characterize the code's "user friendliness"? Give examples, if possible.

b. Numerical precision should be comparable with modeling precision. Spatial convergence should be comparable with the modeling scale.

Question: What has your experience been with the CONTAIN numerical precision and spatial convergence (nodding sensitivities)?

c. The code should be transportable for mainframe and workstation computing machines.

Question: How transportable is the code? Please give examples from your implementation experience, if possible.

5. The maintenance of the code should follow accepted QA standards for configuration control, testing, and documentation.

a. All code changes should be controlled and verified by redundant means.

Question: What are your comments on this design objective? Please specify whether you believe the standards currently being applied are sufficient.

b. Testing standards and benchmarks should be defined for all versions released for production applications.

Question: Do you have any comments on this design objective? Please describe further the level of testing you believe to be appropriate and whether the standards currently being applied are acceptable.

c. Documentation should define the theoretical basis, experimental database, limits of applicability, quantification of uncertainties, user guidance, and testing or assessment results of the code.

Question: What strengths and weaknesses do the code documents have in these areas?

II. CONTAIN-Targeted Applications

1. Experimental analysis and support for containment-related severe-accident experimental programs such as HDR, LACE, NTS, and SURTSEY. In addition, please provide any insights you may have regarding experimental programs for the ALWR designs.

Question: What has your experience been in applying the code for any of these facilities? Do you believe the code provides reasonable predictions of dominant containment phenomena ("reasonable" here means that compared to experimental data, the calculated results will be within the experimental uncertainty bands)?

2. LWR plant analysis to predict the physical, chemical, and radiological conditions inside containment, and fission product releases as a result of predicted containment failure.

Question: What has your experience been in applying the code to analyze LWRs, and do you believe the code can provide reasonable predictions of associated dominant phenomena or the ability to perform sensitivity studies? Also, what assessments have you performed against experimental data that demonstrates the code's capability to predict containment phenomena?

3. Selected detailed analysis for specific technical issues such as hydrogen combustion and migration, build-up of noncondensable gases, direct containment heating, and accident management evaluations.

Question: What has been your experience in applying the code to detailed analyses of these specific technical issues and predicting the associated dominant phenomena? What related assessments have you performed against experimental results in these areas?

4. MELCOR benchmarking and assessment.

Note: The NRC is pursuing a two-tier development strategy for its severe-accident codes. One tier contains detailed, mechanistic codes incorporating the evolving knowledge regarding severe-accident processes. CONTAIN and SCDAP/RELAP5 are examples of codes in this tier; these codes focus on selected portions of severe-accident sequences. Once the detailed models are developed and tested, simplified models that capture key phenomenological features but are faster running can be incorporated into an integrated, full-sequence integral analysis code. The fast-running, full-scenario integral code occupies the other tier in the two-tier strategy. MELCOR is the NRC-developed code for this tier. Accordingly, the CONTAIN Peer Review Committee wishes to know the extent to which CONTAIN has been compared to MELCOR, either directly or through assessments using the same data.

Question: What benchmarks and assessments of the MELCOR code containment-related behavior have you performed with CONTAIN (at least for integral experiments)? What were your results? How would you characterize the use of CONTAIN to benchmark the MELCOR code?

5. ALWR design-basis and severe-accident evaluation.

Question: What evaluations of hypothetical ALWR design-basis and severe accidents have you performed with the code? Did you obtain a reasonable prediction of the dominant phenomena? What were your results, in summary?

III. Ranking of Code "Level of Completeness" and Listing of Papers and Reports

1. You have made separate replies to questions related to whether the code satisfies its design objectives and targeted applications. A ranking (list) of code objectives and targeted applications would provide your overall appraisal of the completeness of the code.

Question: What is your ranking of the code's level of completeness with regard to satisfying code objectives and code-targeted applications? Please list the items that you addressed in I and II with "most complete" first and "least complete" last. For example:

Example Ranking :

-
- II-4. MELCOR Benchmarking *(most complete)*
I-3. Applicability for PWRs, BWRs, and ALWRs

(all the rest that one responds to...)

- I-5b. Numerical precision, ... *(least complete)*

(Note: this is only a fictitious example to demonstrate format for ranking.)

2. The CONTAIN Peer Review Committee wants to ensure that it considers all applicable light water reactor documentation. Please provide a list of the papers and reports generated by your organization that contain information that would assist the Committee in performing the peer review. We ask that you provide a complete listing of all applicable documentation. If some of the reports contain proprietary information and are, therefore, not available to the Committee, we still request that you provide the citation under the proprietary category. Please identify the language in which the report is written (e.g., English, German, Spanish, etc.)

Papers

Reports (Unrestricted)

Reports (Those Containing Proprietary Information)

IV. User Information Request

Date Survey Completed:

Name:

Organization:

Address

Telephone:

Fax/e-mail:

Computer(s) Used to Run Code:

Computer Operating System(s):

Version of Code Used:

Latest version of Code Implemented at Your Site:

Identify Any Significant Local Modifications or Model Additions:

Additional Comments:

Level of CONTAIN User Experience in Your Organization: Check one

☐ High

☐ Medium

☐ Low