

Title: **IN-FACILITY TRANSPORT CODE REVIEW**

Author(s): **James W. Spore, TSA-10  
Brent E. Boyack, TSA-10  
William R. Bohl, TSA-10  
R. Gasser, SNL  
L. Hamm, Westinghouse Savannah Co.  
J. Saunders, Battelle Columbus Laboratory**

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**IN-FACILITY TRANSPORT CODE REVIEW**  
**In-Facility Transport Working Group**

by

**J. W. Spore, Chair**  
**B. E. Boyack**  
**W. R. Bohl**  
**Los Alamos National Laboratory**

**R. Gasser**  
**Sandia National Laboratory**

**L. Hamm**  
**Westinghouse Savannah Company**

**J. Saunders**  
**Battelle Columbus Laboratory**

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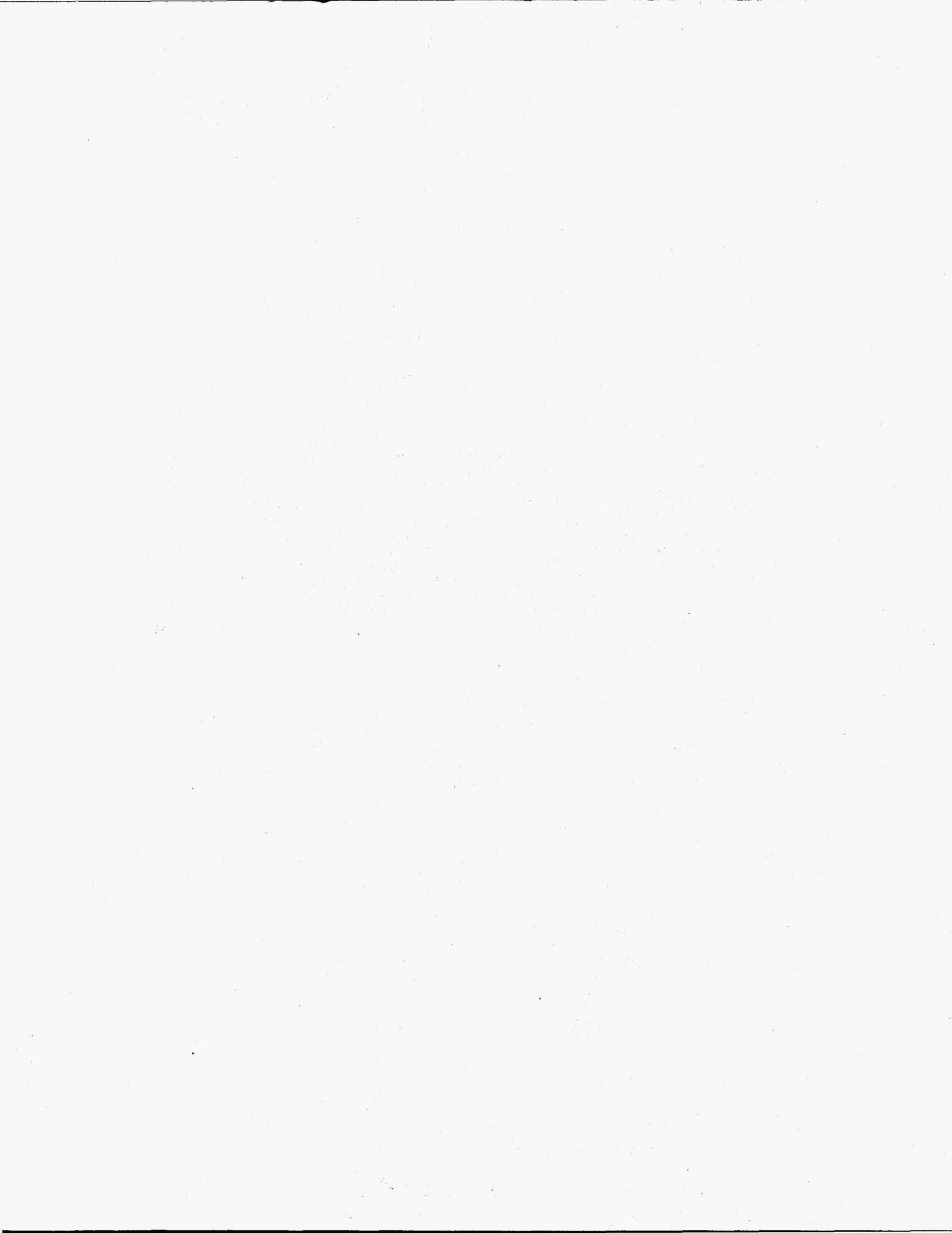
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# IN-FACILITY TRANSPORT CODE REVIEW

## In-Facility Transport Working Group

by

J. W. Spore, Chair,\* Brent E. Boyack,\* William R. Bohl,\* R. Gasser,\*\*  
L. Hamm,† and J. Saunders††

### ABSTRACT

The following computer codes were reviewed by the In-Facility Transport Working Group for application to the in-facility transport of radioactive aerosols, flammable gases, and/or toxic gases: (1) CONTAIN, (2) FIRAC, (3) GASFLOW, (4) KBERT, and (5) MELCOR. Based on the review criteria as described in this report and the versions of each code available at the time of the review, MELCOR is the best code for the analysis of in-facility transport when multidimensional effects are not significant. When multidimensional effects are significant, GASFLOW should be used.

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### 1.0. BACKGROUND

In-facility transport is the model/method used to link the source release with the release to the environment/atmosphere or to link the source release to an onsite worker dose/consequence model/calculation (or, in the case of flammable gas transport, with an ignition source). The output of the in-facility transport analysis is the input to the atmospheric dispersion analysis, the dose/consequence model for the onsite worker, or, in the case of flammable gas transport, a combustion model. The release could be a toxic gas, flammable gas, or radioactive aerosol. The in-facility transport modeling effort is an attempt through conservative but reasonable models and methods to address mechanisms that would reduce the source concentration between the source location and either the release to the atmosphere or contact with an in-facility worker, or contact with an ignition source. Uncertainties in the actual source term may tend to dominate safety analysis; however, in-facility transport modeling may help to mitigate the impact of source-term uncertainties by reducing the concentration of the final release to the environment or exposure to the in-facility worker.

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\* Los Alamos National Laboratory

\*\* Sandia National Laboratories

† Westinghouse Savannah Company

†† Batelle Columbus Laboratory



The goal of the In-Facility Transport Working Group was to produce an evaluation (review) against specified criteria of the models, methods, documentation, and other relevant characteristics in available in-facility transport codes. This evaluation was performed in accordance with guidance from the Executive Committee of the Accident Phenomenology and Consequence Analysis Methodology Assessment Program.

## **2.0. DEPARTMENT OF ENERGY (DOE) ORDERS AND STANDARDS**

DOE-STD-3009<sup>1</sup> requires that the accident analysis of a safety analysis report (SAR) meet evaluation guidelines regarding doses from radioactive materials and exposure to toxic chemicals. Although there are no evaluation guidelines for flammable gases, the transport of these gases within a facility is important from the perspective of influencing transport and producing dispersible radioactive or toxic materials. In addition, many DOE facilities have technical safety requirements (TSRs) that state that flammable gases cannot accumulate in a facility above a specified fraction of the lower flammability limit (LFL) (i.e., typically 25% of the LFL). A flammable gas transport/mixing analysis may be required to ensure that any normal or abnormal operations do not exceed this type of TSR.

In addition, the functional classification process, including safety classification of structures, systems, and components (SSCs) as defined in Refs. 2 and 3, may require safety analysis relative to onsite workers to determine the safety significance of SSCs. Although there are no evaluation guidelines described for onsite workers in Ref. 3, the functional classification process may require a determination of the onsite worker dose because of the release of radioactive material within a facility. For these types of analyses, in-facility transport will be part of the safety analysis for onsite workers.

## **3.0. COMPUTER CODES TO BE REVIEWED**

The criteria for choosing codes to be reviewed for in-facility transport were:

- models to address in-facility transport phenomena,
- nonproprietary code,
- sufficient documentation available to allow for code review,
- codes developed to the point where they could be or had been used in safety analysis, and
- assessment and application results available.

The following codes were chosen for review:

- CONTAIN,
- FIRAC,

- GASFLOW,
- KBERT, and
- MELCOR.

#### 4.0. ACCIDENT SCENARIOS AND REVIEW CRITERIA

Based on the accident scenarios presented in Appendix A, one or both of the two broad modeling activities listed below are involved with in-facility transport.

- Mixing—modeling of a hazardous gas (i.e., toxic, flammable, and/or radioactive) as it transports from its release location through a facility
- Aerosol transport—modeling of a radioactive aerosol as it transports from its release location through a facility.

Variations on these two broad modeling activities are the impact of (1) no ventilation vs ventilation, (2) the hazardous gas lighter/heavier than air, and (3) aerosols with particle-size distributions, etc. The mitigation aspect of the in-facility transport modeling effort is the reduction in concentration as the hazardous gas/aerosol mixes with air/ambient gas within the facility and the facility barriers that tend to contain the release.

In general, it would appear that the standard operating procedure for analysis of aerosol transport within DOE facilities is to use "accepted" multipliers for various barriers, such as a factor of 0.001 for an initial high-efficiency particulate air (HEPA) filter and 0.002 for any subsequent HEPA filter.

The analysis performed for Accident Scenario 3.0., Appendix A, addressed the question of aerosol transport without an operative building ventilation system because of questions reviewers raised on the applicability of asserted "conservative" multipliers for this situation. Significant uncertainty exists in accident scenarios and source terms that produce an aerosol; therefore, demands of excessive sophistication for aerosol transport calculations are unwarranted.

From the calculations performed and the feedback received, adequate aerosol transport modeling would be accomplished by addressing questions such as:

- Where the convective gas currents go?
- Where and when does deposition occur?
- What agglomeration occurs either with larger particulate, such as soot, or with liquid drops, such as water?

As noted elsewhere, the sophistication of any analysis depends on the accident scenario and the accuracy required. Convective flows must be specified by the user for KBERT. FIRAC, MELCOR, and CONTAIN calculate flows between control

volumes, whereas GASFLOW has field variables allowing detailed compressible multidimensional calculations. Other computational fluid dynamics (CFD) programs, commercially available but beyond the scope of the working group's review, provide even more precise following of flow fields using body-fitted coordinates (FLOW3D) or finite element techniques (FIDAP).

The first approach to deposition is to ignore it. A better approximation is to include the most straightforward mechanism, settling by gravity, as performed in KBERT and FIRAC. However, experience suggests more sophistication is desirable when analyzing an accident scenario where evaluation guidelines may be approached if deposition is neglected. For such cases, ignoring any mechanism of "sticky" particle removal needs arguments and justification. Deposition can occur from diffusion, convective air currents and turbulent diffusion leading to impaction, thermophoresis, diffusiophoresis, and external forces (such as settling by gravity). Of these, it is believed that deposition from pure diffusion of aerosols can be neglected because particle diffusion coefficients are much smaller than molecular diffusion coefficients. Some treatment of the remaining four mechanisms should be examined where detailed aerosol transport calculations are believed to be necessary.

In a fire, it has been suggested that much of the radioactive components will be combined with the unburned particulate, or soot, which is more likely to be removed by deposition. Activation of water sprays also will remove aerosols. The source term should include some combined particles; however, respirable radioactive aerosols will collide with more than gas molecules, and some type of multicomponent capability with agglomeration seems to be required. Collisions and agglomeration will occur whenever a relative velocity exists; the most commonly treated mechanisms for obtaining a relative velocity are Brownian motion, gravitational settling, and turbulence. A relevant summary of aerosol deposition mechanisms is given by Heames and Brockmann.<sup>4</sup>

Comments on other possible aerosol transport code requirements are:

- Entrainment—Entrainment is important for such phenomena as dust explosions and the treatment of thick powder beds. However, it also may be argued that entrainment is part of the source term. Actual resuspension of deposited aerosols during transport calculations is likely to be less than the uncertainty in the deposition rate.
- Chemistry—Chemistry is difficult to represent. A rough ability to formulate mass exchanges between components, and produce energy, is desirable. The multicomponent treatment suggested above will require multiple gas species. However, real chemistry possibly should be argued as being part of the source term; aerosol transport would represent the consequences of chemical reactions. Consequently, allowance for mass and energy sources appears necessary.

- Particle-size distribution—To the extent that differently sized particles are believed necessary for a given transport simulation, the need might be satisfied by allowing different particle “components” to be defined and allowing agglomeration between components. Perhaps a mean particle size with equations representing effects from an assumed distribution would be sufficient. Aerosol production, or deagglomeration, is seen as part of the source term at this time.
- Ventilation system and filters—A limited ability to represent a ventilation system is desirable. However, if the ventilation system operation both determines the aerosol transport and requires a detailed representation with multiple ducts, filters, fans, dampers, and other volumes, it is likely that a control volume approach should be used with a more approximate treatment of aerosol transport.
- Heat transfer and condensation—These are required both for gas transport and aerosol deposition from thermophoresis and diffusiophoresis. Radiation, particularly from luminous flames, seems desirable and will change the flow field. However, inclusion is complex, and the influence on ultimate aerosol release or personnel dose is speculative.

Other considerations are:

- Apparently, some form of differential velocity calculation may be desirable. Lagrangian aerosol trajectory calculations may be the most straightforward approach for the treatment of deposition and agglomeration. One example of this approach would be an extension of formalism in the SOLA-DM code<sup>5</sup> with appropriate constitutive terms.
- Any attempt to provide a comprehensive list of requirements seems to have at least two difficulties. First, it is difficult to separate out a pure aerosol transport problem; there is a tendency to include features of fires, explosions, and spills that would be more appropriate for an integrated accident analysis code. Second, it is easy to add so many requirements that any code meeting them contains the excessive sophistication referred to above; such a complex code does not exist now because there may not be resources for its construction, it may be impractical to run, and it likely will imply a calculational precision that does not exist.
- Although aerosol science has been studied for many years, it is only relatively recently that the desire has arisen for some detailed aerosol transport calculations to satisfy some DOE requests for higher fidelity in-facility accident analyses. A meaningful Working Group recommendation to use one existing code for all DOE in-facility transport analysis is not possible. In situations where detailed calculations are required, some focused research appears to be desirable and perhaps could be funded.

Based on the accident scenarios in Appendix A, the system modeling capabilities required for in-facility transport have been developed.

In-facility transport system physical and geometric modeling capabilities are:

- Ventilation system components—ducts, manifolds, dampers, blowers, filters, and dryers,
- Room/tanks/glove boxes—control volume or three-dimensional (3D) CFD model, and
- The capability to interconnect multirooms/tanks/glove boxes with the ventilation system to have a complete model of the facility.

In-facility transport phenomena modeling capabilities are:

- Fluid convective transport, including the effects of
  - multiple species;
  - multiple dimensions;
  - variable densities and temperatures;
  - gravity, structure friction, and other forces;
  - turbulence and diffusion;
  - mass and energy sources from evaporation, and condensation;
  - pyrolysis and combustion; and
  - compressible flow.
- Particle transport, including the effects of
  - drag,
  - deposition from gravity and other mechanisms,
  - entrainment and resuspension, and
  - agglomeration.
- Heat transport, including the effects of
  - conduction,
  - convection, and
  - radiation.
- Other effects of chemistry.

The importance of each modeling capability depends on the accident scenario and the accuracy required. For example, if all source-term hazardous material is released directly into the environment and the result still is easily within the safety envelope for the facility, then the in-facility transport and the effect of barriers to contain the release are of little importance. An in-facility transport analysis still may be required

for this facility; however, a bounding/conservative lumped-parameter analysis without attention to detailed mechanistic calculations would be appropriate. As the results of instantaneous and complete release approach the safety envelope for the facility, more detailed mechanistic but still conservative in-facility transport modeling activities will be employed. In addition, detailed mechanistic calculations also may be performed to verify the conservatism in the lumped-parameter analysis.

Based on the available DOE Orders, the accident scenarios reviewed in Appendix A, and the discussion above concerning modeling requirements the Code Review Criteria given in Appendix B, were developed by the In-Facility Working Group. The Code Review Criteria given in Appendix B identify general criteria that are of importance for any computer code to be used for safety analysis, followed by specific criteria for in-facility transport.

## 5.0. CODE REVIEW

CONTAIN,<sup>6</sup> FIRAC,<sup>7</sup> GASFLOW,<sup>8</sup> KBERT,<sup>9</sup> AND MELCOR<sup>10</sup> were reviewed according to the criteria in Appendix B, and the results are given in Appendices C, D, E, F, and G. In comparing CONTAIN and MELCOR, the Working Group decided that MELCOR was superior to CONTAIN for in-facility transport applications because MELCOR includes the typical ventilation system models that would be required. Ventilation systems models can be developed via input for CONTAIN; however, CONTAIN has no advantages over MELCOR in terms of modeling in-facility transport phenomena. KBERT cannot calculate flows through the ventilation system and therefore was not applied to the standard test problem described in Ref. 11. The two-lumped parameter or control volume codes that were applied to the test problem given in Ref. 11 were FIRAC and MELCOR. FIRAC failed the operability criteria because it was not able to complete the test problem and did not provide the user with sufficient information on how to correct the input to obtain a completed calculation. In addition, FIRAC calculated flow resistances that were found to give unreasonable results. Input of manually calculated flow resistances gave reasonable results, but the calculation still failed.

CONTAIN, GASFLOW, KBERT, and MELCOR can be used to model in-facility transport safety analyses that involve the two broad areas of mixing/transport of a hazardous gas and/or aerosol transport of a hazardous material. However, GASFLOW is the only code reviewed that includes the capability to perform detailed multidimensional calculations; therefore, GASFLOW is recommended for safety analysis in which the consequence is approaching the safety goal or criteria and for benchmark analysis to estimate the amount of conservatism assumed to exist in the lumped parameter or control volume approach. Application of FIRAC to the standard problem given in Ref. 11 has been found to be incapable of completing the transient and therefore is not recommended for safety analysis. CONTAIN, FIRAC, and MELCOR are very similar in terms of the capability of modeling the in-facility transport in terms of a control volume or lumped-parameter approach. Of the codes

reviewed, CONTAIN AND MELCOR both have a detailed mechanistic model for the transport/deposition/agglomeration of aerosols (both codes use the MAEROS<sup>12</sup> models for aerosol). CONTAIN does not have the complete list of ventilation system models available; therefore, it is recommended that MELCOR be used for in-facility transport calculations that require detailed aerosol modeling with agglomeration as an important phenomena.

It is anticipated that in most accident analysis that involve in-facility transport that the aerosol models within the GASFLOW code should be adequate. Ignoring agglomeration is usually conservative because agglomeration tends to increase particle size, and small particles of respirable size (<10 mm) are most significant for dose/consequence analysis. In some cases, underestimating the deposition may be nonconservative (e.g., considering re-entry into a contaminated room).

KBERT has the limitation that all ventilation flow rates must be known and provided as input. This implies that the accident scenario must not involve a significant change from the normal operating conditions of the facility, or ventilation flow rates must be obtained from another computer code. However, KBERT has the advantage of including the Mishima database for source terms for a variety of accident scenarios, and provides as output the dose/consequence for in-facility workers under assumed worker behavior. CONTAIN, GASFLOW, and MELCOR must have source terms provided as input. CONTAIN, FIRAC, GASFLOW, and MELCOR output must be used as input to provide dose/consequence for in-facility workers.

## 6.0. RECOMMENDATIONS FOR APPLICATIONS

Currently, there do not appear to be any advantages of CONTAIN over MELCOR for analysis of in-facility transport problems. Therefore, the Working Group recommends that MELCOR be used for applications in which agglomeration of aerosols is an important phenomenon (e.g., aerosols that involve sticky particles). In addition, the aerosol models in MELCOR have been assessed and validated against experimental data and can provide a benchmark for aerosol models in GASFLOW that do not include agglomeration. If multidimensional effects are important, then of the five computer codes reviewed, GASFLOW is the only code with this capability. Multidimensional effects will be important in assessing aerosol and/or hazardous gas concentration profiles within a room or several rooms (e.g., to answer the question of how much aerosol can escape from a room while a door is open vs closed). In addition, multidimensional analysis may be required to determine LFLs as opposed to room/compartment average flammability limits.

KBERT should be used for analysis to support functional classification of safety-class structures, equipment, etc. For accident scenarios that involve no significant upset to the ventilation system, KBERT can be used with normal operating ventilation flow rates. For accident scenarios involving ventilation system upsets, fires, explosions, loss of ventilation systems, changes in damper settings, etc., ventilation

system flow rates must be calculated with another computer code and provided to KBERT as input. KBERT was intended for assessing onsite worker safety issues; however, it can provide the output that would be required as input for an atmospheric dispersion code.

Our recommendations are summarized as follows.

<b>CODE</b>	<b>Recommendation for applications</b>
CONTAIN	None
FIRAC	None
GASFLOW	A benchmark tool and when multidimensional effects are important
KBERT	For in-facility worker safety analysis, where the time-dependent ventilation flow rates are known or can be supplied via another computer code
MELCOR	When multidimensional effects are not important

#### **7.0. RECOMMENDATIONS FOR DEVELOPMENT, MAINTENANCE, AND BENCHMARKS**

1. CONTAIN—There are no recommendations.
2. FIRAC—If FIRAC is to be used in the future, documentation needs to be brought up to date with the current released computer code. The code needs to be modified to eliminate the nonconservative result and to fix the code bug identified in Ref. 11.
3. GASFLOW—Documentation needs to be brought up to date with the current released computer code. Two areas of improvement for GASFLOW should be considered (i.e., user convenience and improved modeling capability). In the user convenience area, source-term modeling capability should be added to address fires involving solids and liquids. In the improved modeling area, the GASFLOW framework would benefit by adding capability to model aerosol agglomeration, further consideration of aerosol deposition, and additional comparisons of calculated aerosol behavior to experimental data.
4. KBERT—This code is currently lacking in the area of benchmarks and example applications. KBERT should be benchmarked against other computer codes and/or experimental data. The lumped parameter flow solutions from MELCOR or CONTAIN should be incorporated into KBERT to eliminate the need to know the time-dependent ventilation system flow rates.



5. MELCOR—Development of a graphical user interface (GUI) for I/O would save substantial amount of time for a user to prepare input and understand output.

## 8.0. REFERENCES

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## APPENDIX A

### ACCIDENT SCENARIOS INVOLVING IN-FACILITY TRANSPORT

#### 1.0. WASTE TANK GAS RELEASE/BURN OF FLAMMABLE GAS

A tank in a waste tank farm releases a mixture of flammable gases (typically fuels such as hydrogen, ammonia, methane, and carbon monoxide, and oxidizers such as nitrous oxide). During a gas release, the ventilation system may or may not be operative. The accident scenario is that at some time during a gas release event (GRE), an ignition source is present in the system. The resulting flammable gas burn may or may not fail the HEPA filters in the ventilation system. During the burn, flow will be out of both the normal inlets and outlet to the waste tank. Radioactive particles from the waste surface will be entrained into the dome space during the burn, and some portion of those particles will be transported out of the waste tank and ventilation system into the atmosphere. Parameters of interest are as follows.

- Gas is released as a flammable mixture of gases (i.e., fuel and oxidizer both exist in the release gas). For how long following a GRE does a flammable mixture of gases exist?
- Will there be a flammable mixture of gases in the ventilation system ductwork? Will a flammable mixture of gases transport into another tank in the tank farm?
- Do the HEPA filters fail during a GRE?
- Is the resulting pressure rise during a GRE sufficient to reverse the flow in the waste tank inlets?
- Given a burn following or during a GRE, will the HEPA filters fail?
- How much radioactive material is entrained during a burn?
- How much radioactive material eventually leaves the waste tank and reaches the atmosphere?
- How much radioactive material is released from the stack, and how much is released at or near the ground from the waste tank inlet?
- What is the waste surface temperature during burn (i.e., does waste burn)? The radioactive material source term is significantly larger when the waste burns, and it lasts longer.

The component/system modeling capabilities required to model the waste tank farm are:

- Gas dome space model—control volume or 3D CFD capability
- Ventilation system model—ducts, dampers, filters, and blowers
- Interconnected ventilation system—capability to connect multi-3D blocks/room components into interconnected ventilation system

Important phenomena during normal operation are:

- Convective gas flow patterns—This implies the capability to model turbulence, buoyancy driven flows, and heat transfer from the waste surface and to waste tank walls.
- Flow through the ventilation system—This implies the capability to model flow resistance or flow losses associated with ducts, filters, and dampers, and flow developed via blowers.

Important phenomena during GREs are:

- Multi-species transport—This implies the capability to model the diffusion and convective transport of different species of gases. This is important for obtaining concentration distributions during the GRE.
- Convective gas flow patterns—This implies the capability to model turbulence, buoyancy-driven flows, and heat transfer from the waste surface and to waste tank walls.
- Flow through the ventilation system—This implies the capability to model flow resistance or flow losses associated with ducts, filters, and dampers and flow developed via blowers.

Important phenomena during burn are:

- Compressible flow—During the burn, significant pressure, temperature, and density changes occur within the gas dome space. Propagation of the pressure change into the ventilation system determines whether the HEPA filters fail.
- Convective gas flow patterns—This implies turbulence modeling.
- Flow through the ventilation system—This implies the capability to model transient flow resistance or flow losses associated with ducts, filters, and dampers and the transient behavior of blowers.
- Aerosol transport—These include entrainment, deposition, re-entrainment, agglomeration, gravitational settling, and turbulence.

- Chemistry—An energy source from the burn itself must be included, either by direct solution of the combustion rate equations based on the species concentrations present or via a global burn model.
- Heat transfer—Radiation, convection, and conduction will be important in determining the waste surface temperature. If the waste surface is heated to the point where combustion of the waste is possible, then the radioactive source term is increased significantly for this accident scenario.

## 2.0. BENZENE MIXING IN THE IN-TANK PRECIPITATION (ITP) TANK

Benzene is produced at different stages of the waste processing in the ITP tank. The rate of benzene production varies, depending on the stage of the processing. The wash cycle results in the largest benzene production rate. Under normal operations, nitrogen is injected into the ITP tank in an attempt to ensure that the benzene in the gas dome space does not mix with an oxidizer; however, air leaks into the ITP tank during normal operations. The accident scenario assumes that the nitrogen purge system fails during the wash cycle stage of the waste processing and that it will take three days to install a portable backup exhauster. The objective of the analysis of this accident scenario is to demonstrate that there will or will not be an accumulation of sufficient benzene within the ITP such that a resulting burn would cause significant structural damage. However, there also are questions about normal operation associated with the mixing of the nitrogen purge, benzene, and air coming in because of leakage. This in-facility transport scenario does not include the transport of radioactive material that would be released given a benzene burn, but rather includes the mixing of a flammable gas (i.e., benzene) with air and nitrogen within the facility.

Additional factors that affect the ITP tank model are:

- A support column in the center of the ITP tank—The gas dome space appears as a doughnut
- Cooling coils in the ITP tank—The ITP tank contains rows and rows of cooling coils that represent heat sinks in the gas dome space, and that introduce obstacles in the gas dome space flow field
- Nitrogen injection—Nitrogen injection into the gas dome space via a high-velocity jet (choked flow in the nozzle) from a nozzle pointed at an angle into the gas dome space

Parameters of interest are:

- During normal operations, how much air leaks into the ITP tank?

- During normal operations, can pockets of low mixing occur? Can a pocket of flammable gas develop during normal operation?
- With ventilation system failure, will natural circulation flow rates be sufficient to mix the benzene?
- With ventilation system failure, how much benzene will there be in a flammable configuration after three days?

Component/system modeling capabilities required to model waste tank farm are:

- ITP tank geometry of a cylindrical tank with a support column in the middle
- Cooling coils both as a heat sink and as an obstacle to flow
- Leakage path capability

Important phenomena during normal operation are:

- Multispecies transport/diffusion—The transport/diffusion of benzene (heavier than air) and hydrogen (lighter than air) from the waste surface into gas dome space is important to the calculation of the flammable gas concentration as a function of time and space.
- Convective gas flow patterns—Modeling of turbulence, buoyancy-driven flows, and impact of heat sinks/sources on flow patterns all are important to the modeling of convective gas flow patterns.
- Turbulent and buoyant jet behavior—The effect of the nitrogen jet into the gas dome space is determined by the behavior of a turbulent jet of nitrogen into the gas dome space. The nitrogen coming into the gas dome space may be a different temperature than the ambient atmosphere in the gas dome space; therefore, buoyancy forces may affect the jet spreading. In addition, the interaction of the nitrogen jet with the cooling coils and the support column also will affect the flow patterns during normal operation.
- Condensation of benzene/water on the cooling coils—A condensation of benzene and water on these coils may provide a mechanism to increase the concentration of benzene near the waste surface level.

Important phenomena during ventilation system failure are:

- Multi-species transport/diffusion—The transport/diffusion of benzene (heavier than air) and hydrogen (lighter than air) from the waste surface

into gas dome space is important to the calculation of the flammable gas concentration as a function of time and space.

- Convective gas flow patterns—Modeling of turbulence, buoyancy-driven flows, and the impact of heat sinks/sources on flow patterns all are important to the modeling of convective gas flow patterns.
- Condensation of benzene/water on the cooling coils—Condensation of benzene and water on these coils may provide a mechanism to increase the concentration of benzene near the waste surface level.

### 3.0. AEROSOL TRANSPORT IN BOUNDING FIRE ACCIDENT IN PF-4

This accident scenario involves a fire outside a glovebox that breaches the glovebox in a multiroom facility. The basic elements of the localized fire scenario are that a short circuit starts an electrical fire, which then involves oil from a pump or a rupture of a hydraulic line under the glovebox. The laboratory room is unattended, and the initiating fire is allowed to spread and ignite the bottom of a polymethyl methacrylate (PMMA) slab [the plastic material used to shield workers against neutrons emitted from the ( $\alpha,n$ ) reactions occurring inside the glovebox]. The fire suppression system is not available and does not put out the fire; the PMMA burning surface grows upward exponentially and fails the gloves, thus breaching the glovebox. The nonsafety class ventilation system cannot be assumed to function. The source term is finely powdered  $^{238}\text{Pu}$  in oxide form. The attenuation of the source term released into the environment depends on transport of the aerosol within the building and on the openings present (external doors, building leakages, ventilation inlet, exhaust, and bleed-off paths).

Parameters of interest are:

- How much radioactivity material can escape, even if all doors remain closed?
- What is the escape of radioactivity as a function of time during which external doors remain open from an egress of people from the remainder of the building?

Component/system modeling capabilities required to model in-facility transport in the PF-4 facility are:

- Modeling multirooms with multiboundary conditions, and
- Modeling the ventilation system.

Important phenomena are:

- Aerosol transport—Entrainment, deposition, re-entrainment, agglomeration, gravitational settling, and turbulence.
- Radiation heat transport—PMMA burns with a luminous flame; therefore, it is important to ascertain whether the fire spreads to other PMMA-shielded gloveboxes or ignites additional combustibles or the gypsum ceiling wallboard.
- Convective gas flow patterns—Modeling of turbulence, buoyancy-driven flows, impact of heat sinks/sources on flow patterns, and multidimensional flow are all important to the modeling of convective gas flow patterns.
- Chemistry—The energy source from the burn itself must be included either by direct solution of the combustion rate equations based on the species concentrations present or via a global burn model.

#### **4.0. OXIDATION OF TRITIUM IN A FIRE IN THE REPLACEMENT TRITIUM FACILITY (RTF)**

An important factor in determining the consequences of a tritium release is whether the tritium is released as a gas or as a liquid (tritium oxide). For accident scenarios in which tritium storage containment has failed during a cable tray fire (i.e., design basis earthquake), it is important to determine the amount of tritium that will be oxidized by the fire. With the ventilation system off and as the cable trays burn, convective flow patterns will be established within the fire room. In addition, the fire room will be at a slightly higher pressure than the rest of the ventilation system; therefore, flow will tend to go back out the ventilation system inlets and outlets for the fire room. If no source of oxygen is available (i.e., no oxygen leakage into the room from the doors), the fire eventually will become oxygen starved, and burning of the cable trays will stop. While the cable trays are burning, tritium that has been injected into the room because of a failure of tritium containment will be swept by the fire and oxidized. However, some of the tritium also will exit the fire room through the ventilation inlets and outlets before it has been oxidized. In addition, some of the tritium will be in the convective flow patterns in the fire room and will neither exit the room nor flow past the cable tray fire.

Parameters of interest are:

- What is the effect of ventilation system failure or nonfailure?
- What is the effect of changing the elevation of the diffuser inlets?



The component/system modeling capabilities required to simulate tritium oxidation in a room in the RTF are:

- To model a room with multiboundary conditions, and
- To model the ventilation system.

Important phenomena are:

- Convective gas flow patterns—Modeling of turbulence, buoyancy-driven flows, impact of heat sinks/sources on flow patterns, and multidimensional flow are all important to the modeling of convective gas flow patterns.
- Chemistry—The energy source from the burn itself must be included either by direct solution of the combustion rate equations based on the species concentrations present or by a global burn model.
- Multispecies transport/diffusion—The transport/diffusion of tritium (lighter than air) from its release location into the room and toward the cable trays is important in determining the fraction of oxidized tritium released.

## APPENDIX B

### CODE REVIEW CRITERIA

#### 1.0. GENERAL CRITERIA

0. Code name
1. Sponsor/developing organization
2. Current custodian/phone/fax/internet
3. Genealogy
4. Abstract
5. Input summary
6. Output summary
7. Evaluation of computer model vs DOE requirements
8. Can graded approach philosophy be addressed with this code (i.e., can level of modeling detail be changed)?
9. Applicability and modeling assumptions
10. Data and input parameter and boundary condition requirements
11. User friendly
12. Typical execution time
13. Machine/operating system requirements
14. Validation
15. Q/A
16. - software development plan and requirements
17. - validation reference
18. - benchmark reference
19. - users manual
20. - error handling/reporting
21. Life-cycle status
22. Applications
23. Statistical aspects of in-facility transport
24. Overall strengths, limitations, and weaknesses
25. Operability—the capability to complete a typical calculation and if code failure occurs, the capability to give the user adequate information to determine why the code failed, and what must be done to complete the calculation.

#### 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct		
Damper/valve		
Blower/fan		
Filter		
Manifold		

### 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped parameter		
Multi-D hydro		
Representation of non-orthogonal shapes		
Finite elements		
Form-fitted coordinates		

### 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic		
k-ε		

### 5.0. DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular		
Turbulent		

### 6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available		
Can new species be added easily?		

### 7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model		
Settling model		
Deposition model		
Entrainment model		
Re-entrainment model		
Agglomeration model		

### 8.0. CHEMISTRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas		
Combustion model liquids		
Combustion model solids		

**9.0. BUOYANCY DRIVEN FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and composition (species)		

**10.0. COMPRESSIBLE FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure		

**11.0. HEAT TRANSFER**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction		
Convection		
Radiation		

**12.0. DETERMINATION OF INITIAL CONDITION**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-accident steady-state capability		

**13.0. GEOMETRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can the geometry, especially leakage paths, change during the calculation		
— as specified by the user		
— by built-in code models		

**14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Specified mainly by user input		
Specified mainly by internal models		
Specified mainly by user-written subroutines		
Specified mainly by input files calculated from other codes		

**APPENDIX C  
CODE REVIEW CRITERIA—CONTAIN**

**1.0. GENERAL CRITERIA**

- |    |                                       |  |
|----|---------------------------------------|--|
| 0. | Code Name—                            | CONTAIN 1.2  |
| 1. | Sponsor/developing organization—      | US NRC   |
| 2. | Current custodian/phone/fax/internet— | Richard Griffith<br>Org. 6421<br>MS-0739<br>P. O. Box 5800<br>Sandia National Lab<br>Albuquerque, NM<br>87185-0739<br>Ph. (505) 844-8232 |
- 
3. Genealogy—CONTAIN 1.2 was developed from CONTAIN 1.1 and was developed by Sandia National Laboratories (SNL) for the United States Nuclear Regulatory Commission (NRC) for best-estimate, mechanistic containment analysis for severe accidents in nuclear reactors. Version 1.2 was released in August 1995.
  4. Abstract—The CONTAIN 1.2 computer code is an integrated analysis tool used for predicting the physical, chemical, and radiological conditions inside a containment building following the release of radioactive material from the primary system in a severe reactor accident. It also can predict the source term to the environment. CONTAIN 1.2 is a highly flexible and modular code that can run problems that are either quite simple or highly complex.
  5. Input Summary—Input is via free-field, key word-driven format. Physical models are activated only by the presence of associated key words in the input stream and are otherwise inactive. Most models allow the user to specify individual physical parameters; however, default values are available to the user.
  6. Output Summary—Two basic types of time-dependent output written to the main output file are long edits and short edits. The presence or absence of much of the long-edit output is controlled by output keywords. In addition, the user can include user-implemented output writes. The user may access either global or cell level variables through the user-implemented output writes. In addition, plot files are written that may be postprocessed by the POSTCON and HISPLOTT computer programs or another user-provided post-processor program.

7. Evaluation of computer model vs DOE requirements—To evaluate dose/consequence, the output from CONTAIN can be used as input to the MACCS computer code. In terms of TSRs that are related to flammable gas concentrations, CONTAIN results can be used directly. For calculations involving worker safety, the results of the CONTAIN calculation must be input into another model or computer code to determine the dose/consequence.
8. Can graded approach philosophy be addressed with this code (i.e., can level of modeling detail be changed)—CONTAIN can perform lumped parameter/control volume type analysis, but is limited in terms of providing detailed multidimensional modeling of a room or gas dome space. The number of control volumes can be increased and linked together to simulate a two-dimensional (2D) or 3D grid; however, for the low flows expected during most in-facility transport calculations, the lack of the momentum flux terms and viscous shear terms make this approach inadvisable.
9. Applicability and modeling assumptions—Applicable to any facility (i.e., buildings, tanks, single rooms, etc.) with and without ventilation systems. Applicable to multispecies gas mixing/transport problems as well as aerosol transport problems. Major assumptions in CONTAIN:
  - Each control volume gas space is well mixed, except CONTAIN, which includes lower/upper cell models that allow for accumulation of liquid water in the lower cell while the upper cell is gas. The upper cell gas volume is assumed to be well mixed.
  - Each gas species has the same velocity in the flow path connections.
  - Noncondensable gases are assumed to be ideal.
  - Turbulence and species diffusion within a control volume are not modeled, except in the aerosol model and condensation/evaporation on surfaces.
10. Data and input parameter and boundary condition requirements—
  - Default gas properties are available for the following gas species:

H <sub>2</sub>	Hydrogen
O <sub>2</sub>	Oxygen
CO <sub>2</sub>	Carbon Dioxide

CO	Carbon Monoxide
N <sub>2</sub>	Nitrogen
CH <sub>4</sub>	Methane
He	Helium
Ar	Argon
D <sub>2</sub>	Deuterium
FeV	Iron vapor
PuO <sub>2</sub> V	Plutonium oxide vapor
PuV	Plutonium vapor
NaV	Sodium vapor
UV	Uranium vapor
H <sub>2</sub> OV	Water vapor

- Ventilation system components do not appear to be available for blowers/fans and filters. The effect of cooling fans can be modeled with CONTAIN, and the DP version of CONTAIN developed for Savannah River applications includes a filter capability; however, it is not available in the released version.
  - Boundary condition volumes appear to be represented by large control volumes with an initial temperature, pressure, and composition.
11. User-friendly—With the limited capability to model blowers/fans and filters, it will be difficult to use CONTAIN to simulate a typical hazardous material release within a typical DOE facility.
  12. Typical execution time—The ratio of real time to run time can vary from 0.5 to 100, depending on the nodalization.
  13. Machine/operating system requirements—CONTAIN is supported on the following platforms: CRAY and UNIX workstations (i.e., SUN, HP, IBM, and DEC).
  14. Validation
    - K. D. Bergeron and J. L. Tills, "Results of Blind Predictions of HDR Steam Blowdown Experiments Using the CONTAIN Code," SAND83-1368C, presented at the 1983 ANS Winter Meeting, San Francisco, California, October 30–November 4, 1983.
    - P. Vater, R. Dersch, R. Brandt, G. Luthardt, and W. Rudolph, "Aerosol Behaviour Calculations Performed with the CONTAIN Code in Comparison to PARDISEKO Calculations

and to Experiments," *Journal of Aerosol Science* 18, No. 6, 935-8, (December 1987).

- F. Beonio-Brocchieri, E. Caglioti, A. Markovina, and R. Ricchena, "Performance of an Integrated Thermohydraulics and Aerosol Behaviour Code (CONTAIN) in a Benchmark on LACE LA-4 Simulating Late Containment Failure," International Conference on Nuclear Power Performance and Safety, Vienna, Austria (September 1987).
- K. Muramatsu and K. Soda, "Analysis of Hydrogen Burn in the Three Mile Island Unit 2 Accident with the Contain 1.1 Computer Code," *Nuclear Technology* 87, No. 4, 907-11 (December 1989).
- H. van Rij, "Hydrogen Burn Assessment with the CONTAIN Code," Netherlands Energy Research Foundation, The Netherlands, presented at the Third Workshop on Integrity of Containments for Nuclear Power Plants, Washington, DC, published as Sandia National Laboratories report SAND85-2771C (May 1986).
- P. N. Smith, and G. Roberts, "Application of the CONTAIN Code to the Analysis of Large-Scale Aerosol Experiments," CEC/NEA Workshop on Water-Cooled Reactor Aerosol Code Evaluation and Uncertainty Assessment, Brussels, Belgium (September 1987).

15. Q/A

- Software Development Plan & Requirements—"Quality Assurance Procedures for the CONTAIN Severe Reactor Accident Computer Code," Sandia National Laboratories report SAND90-011, NUREC/CR-5518 (January 1991).
- Validation Reference—B. E. Boyack et. al., "CONTAIN Independent Peer Review," Los Alamos National Laboratory report LA-12866 (January 1995).
- Benchmark Reference—J. Dienstbier, "CUBE 1000: Benchmarking of CONTAIN, JERICO and MELCOR Codes Against Simple Thermal Hydraulic Problems," Nuclear Research Institute Rez, plc. document UJV Z 13-T (August 1994).
- User's Manual—
  - K. K. Murata et. al., "User's Manual for Contain 1.1: A Computer Code for Severe Nuclear Reactor Accident



Containment Analysis," Sandia National Laboratories report SAND87-2309 (November 1989).

- "CONTAIN 1.2 Code Manual: A Computer Code for Severe Accident Analysis," Sandia National Laboratories draft report for review (April 1993).
  - Error Handling/Reporting—Yes
16. Life-Cycle Status—Several versions released, maintenance continues. The NRC has released a position paper stating that CONTAIN will not be developed further.
  17. Applications—
    - D. E. Carroll et. al. "Integrated Analysis of Core Debris Interactions and Their Effects on Containment Integrity Using the CONTAIN Computer Code," *Nuclear Engineering and Design* 104 (1987).
    - D. C. Williams et. al., "Containment Loads due to Direct Containment Heating and Associated Hydrogen Behavior: Analysis and Calculations with the CONTAIN Code," NUREG/CR-4896 (1987).
    - D. C. Williams and D. L. Y. Louie, "CONTAIN Analyses of Direct Containment Heating Events in the Slurry Plant," ANS/ENS International Meeting, Washington, DC (1988).
    - K. D. Bergeron and D. C. Williams, "CONTAIN Calculations of Containment Loading of Dry PWRs," SAND84-1233J, *Nuclear Engineering and Design* 90, 153 (1985).
    - Many more applications.
  18. Statistical aspects of in-facility transport—Sensitivity calculations can be performed by varying input parameters.
  19. Overall strengths, limitations, and weaknesses—

Strengths are:

    - The code is fast running because of the control volume approach.
    - There is no limit to the number of flow path connections to a single control volume.

- Spray models are available if sprays are important to the analysis.
- Two-phase flow can be modeled if multiphase flow is important to the analysis.
- The code is versatile.
- The aerosol model is based on MAEROS model, which is a detailed mechanistic model.
- The code is well assessed.

Limitations are:

- There is limited diffusion and turbulence modeling within a control volume.
- Multidimensional flow within a room cannot be simulated easily or accurately.

Weaknesses are:

- There is no multi-D capability.
- Disk overhead is associated with multiphase flow and reactor models. All subroutines appear to be loaded independently of whether or not models are activated.
- Limited fan/blower or filter models are available.
- Momentum balance ignores spatial acceleration term.

20. Operability—because of the similarity of CONTAIN and MELCOR for these types of applications, CONTAIN was not accessed in this area.

## 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct	Yes	Flow loss due only to user input flow loss factors. No wall drag is included. Flow assumed to be 1D
Damper/Valve	Yes	Flow assumed to be 1D
Blower/Fan	Yes	Flow specified as a function of time
Filter	No	

Manifold Yes

### 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped Parameter	Yes	
Multi-D Hydro	Yes	Very limited and not practical
Representation of non-orthogonal shapes	No	
Finite elements	No	
Form-fitted coordinates	No	

### 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic	Yes	Only for aerosols and for evaporation/condensation on surfaces
k-ε	No	

### 5.0. SPECIES DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular	Yes	Only for aerosols and for evaporation/condensation on surfaces
Turbulent	Yes	Only for aerosols and for evaporation/condensation on surfaces

### 6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available	Yes	15 species available
Can new species be added easily?	Yes	

### 7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model	Yes	
Settling model	Yes	
Deposition model	Yes	

Entrainment model	No
Re-entrainment model	No
Agglomeration model	Yes

**8.0. CHEMISTRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas	Yes	Hydrogen and carbon monoxide
Combustion model liquids	No	
Combustion model solids	No	

**9.0. BUOYANCY DRIVEN FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and composition (species)	Yes	Not buoyancy driven flows in a single control flow/room, but from one control volume/room to the next

**10.0. COMPRESSIBLE FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure	Yes	

**11.0. HEAT TRANSFER**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction	Yes	1D, planar, cylindrical, and spherical
Convection	Yes	
Radiation	Yes	

**12.0. DETERMINATION OF INITIAL CONDITION**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-accident steady-state capability	Yes	User specified

### 13.0. GEOMETRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can geometry, especially leakage paths, change during the calculation:		
— As specified by the user	Yes	
— By built-in code models	Yes	Based on pressure differences

### 14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Must be specified mainly by user input	Yes	
Specified mainly by internal models	Yes	Only hydrogen and carbon monoxide
Specified mainly by user written subroutines		
Specified mainly by input files calculated from other codes		

## APPENDIX D

### CODE REVIEW CRITERIA—FIRAC

#### 1.0. GENERAL CRITERIA

0. Code Name—  
FIRAC  
FIRAC/CFAST  
FIRAC/PC  
FIRAC/FIRIN
1. Sponsor/developing organization— USNRC/DOE-EH
2. Current custodian/phone/fax/internet—William S. Gregory  
M/S K575  
Los Alamos National Lab  
Los Alamos, NM 87545  
Ph. (505) 667-1120  
bgregory@lanl.gov
3. Genealogy—FIRAC is one of a family of codes designed to provide improved safety analysis methods for the nuclear industry. Its predecessors include:
  - TVENT (a code to analyze tornado-induced gas dynamics,
  - TORAC (a code to analyze tornado-induced gas dynamics and material transport),
  - EXPAC ( a code to analyze explosion-induced gas dynamics and material transport), and
  - FIRAC-PC (FIRAC running on an IBM PC) and FIRAC2 versions of FIRAC have been recently released.
4. Abstract—FIRAC is designed to estimate radioactive and nonradioactive source terms and predict fire-induced flows and thermal and material transport within the facilities. Particular focus is on transport through the ventilation system of these facilities. FIRAC includes a fire compartment module based on the FIRIN computer code, which was developed at Pacific Northwest Laboratory. The FIRIN module calculates fuel mass loss rates and energy generation rates within the fire compartment. It can also calculate the generation rate and size distribution of radioactive particles that become airborne as a result of a fire in a nuclear facility. More recently, a second fire module (based on the CFAST computer code) was added to FIRAC. CFAST was

developed by the National Institute of Standards and Technology to model fire growth and smoke transport in multicompartment structures. The new combined code is called FIRAC2. The FIRIN and CFAST modules can be bypassed, and arbitrary gas/particulate release, energy, mass functions of time can be specified. In addition, temperature and pressure functions can be specified.

5. Input Summary—A FIRAC2 preprocessor runs on IBM PC and compatible computers with EGA or VGA graphics capability. The input to the preprocessor is via data windows.
6. Output Summary—Both printer and graphics output files are generated by FIRAC. A post-processor program called POST can be used to display the FIRAC plot files.
7. Evaluation of computer model vs DOE requirements—In terms of dose/consequence, the output from FIRAC must be used as input into another model/computer-code to determine onsite/offsite dose/consequence. In terms of TSRs that are related to flammable gas concentrations, FIRAC results can be used directly. For calculations involving worker safety, the results of the FIRAC calculation must be input into another model or computer code to determine the dose/consequence.
8. Can a graded-approach philosophy be addressed with this code (i.e., can level of modeling detail be changed)?—FIRAC can perform lumped parameter/control volume-type analysis but is limited in terms of providing detailed multidimensional modeling of a room or gas dome space.
9. Applicability and modeling assumptions—Applicable to any facility (i.e., buildings, tanks, multiple rooms, etc.) with and without ventilation systems. Applicable to multispecies gas mixing/transport problems, as well as aerosol transport problems. Major assumptions in FIRAC:
  - Each control volume gas space is well mixed, except in the fire model where there is a hot layer and cold layer.
  - Each gas species has the same velocity in the flow path connections.
  - Noncondensable gases are assumed to be ideal.
  - Turbulence and species diffusion within a control volume are not modeled, except in the aerosol model, which includes turbulence modeling.

10. Data and input parameter and boundary condition requirements are:
  - Up to five gas species can be included in each calculation.
  - Input is available to describe ventilation system components such as blower, dampers, and filters.
  - Time-dependent user-specified boundary conditions for pressure, temperature, mass fractions, and velocities can be specified.
11. User-friendly—Input is via a GUI. Input error checking is performed.
12. Typical execution time—Depends on problem size and duration of the transient. Usually a matter of seconds or minutes.
13. Machine/operating system requirements—IBM PC, SUN, and CRAY
14. Validation:
  - W. S. Gregory et. al., "Fires in Large Scale Ventilation Systems," *Nuclear Engineering design* **125**, 403–410 (1991).
  - S. Claybrook, Numerical Applications Inc., "Comparisons of FIRIN Predictions to 1986 LLNL Enclosure Fire Tests 9 and 10" personal communications, June 1992.
  - N. J. Alvares et. al., "Force Ventilation Enclosure Fires," *Combustion Science and Technology* **39**, 55–81 (1984).
  - "Numerical Approaches to Combustion Modeling," *Nuclear Systems, Progress in Astronautics and Aeronautics*, AIAA, **135**, Chap. 24 (1984).
15. Q/A
  - Software Development Plan & Requirements—none.
  - Validation Reference—B. D. Nichols et. al., "Fire-Accident Analysis Code (FIRAC) Verification," 19th DOE/NRC Nuclear Air Cleaning Conference, Los Alamos National Laboratory document LA-UR-86-2860 (1986).
  - Benchmark Reference—W. S. Gregory et. al., "FIRAC Code Predictions of Kerosene Pool Fire Tests," unpublished Los Alamos National Laboratory report, May 23, 1989.



- User's Manual:

- S. W. Claybrook, "FIRAC/CFAST Preprocessor: User's Manual," Numerical Applications, Inc. document NAI9411-01 (July 1994).
- B. D. Nichols et. al., "FIRAC User's Manual: A Computer Code to Simulate Fire Accidents in Nuclear Facilities," Los Alamos National Laboratory manual LA-10678-M (April 1986).
- William S. Gregory et. al., "FIRAC-PC Users Manual," Los Alamos National Laboratory draft report (May 1992).

- Error Handling/Reporting—Yes, needs improvement.

16. Life-Cycle Status—Several versions released and documented, continued maintenance and development.

17. Applications are:

T. L. Allison, "Fire Load Verification for RTF Room 9, 15, 17, EPD-SR-92-1159," Westinghouse Savannah River Co. (November 1992).

18. Statistical aspects of in-facility transport—No

19. Overall strengths, limitations, and weaknesses:

Strengths are:

- Fast running,
- User-friendly user interface,
- Includes source term models for fires, and
- No limit on the number of flow paths, except that the FIRIN fire compartment is limited to no more than three connections.

Limitations are:

- Diffusion and turbulence within a control volume is not modeled.
- Multidimensional flow within a room cannot be easily or accurately simulated.

Weaknesses are:

- Momentum balance ignores spatial acceleration term,
  - PC version may be slow running on relatively large problems, and
  - Multigas species are not included in the EOS.
20. Operability—FIRAC does not appear to have a high degree of operability. Users indicated that the code can fail without any meaningful error message and regularly fails. Users reported that interaction with the original code developers is typically required to complete calculations.

## 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct	Yes	
Damper/Valve	Yes	
Blower/Fan	Yes	
Filter	Yes	
Manifold	Yes	

## 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped Parameter	Yes	
Multi-D Hydro	No	
Representation of non-orthogonal shapes	No	
Finite elements	No	
Form-fitted coordinates	No	

## 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic	No	
k- $\epsilon$	No	

## 5.0. DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular	No	
Turbulent	No	

## 6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available	No	
Can new species be added easily?	No	

## 7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model	No	
Settling model	Yes	
Deposition model	Yes	
Entrainment model	Yes	
Re-entrainment model	No	
Agglomeration model	No	

## 8.0. CHEMISTRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas	Yes	
Combustion model liquids	Yes	
Combustion model solids	Yes	

## 9.0. BUOYANCY DRIVEN FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and composition (species)	Yes	Only a function of temperature and not species.

## 10.0. COMPRESSIBLE FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure	Yes	

## 11.0. HEAT TRANSFER

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction	Yes	
Convection	Yes	

Radiation Yes

**12.0. DETERMINATION OF INITIAL CONDITION**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-accident steady-state capability	Yes	

**13.0. GEOMETRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can geometry, especially leakage paths, change during the calculation	Yes	
— As specified by the user	Yes	
— By built-in code models	No	

**14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Must be specified mainly by user input	Yes	Used for spills, explosions, etc.
Specified mainly by internal models	Yes	FIRIN and CFAST available as modules to FIRAC when fires are modeled
Specified mainly by user-written subroutines	No	
Specified mainly by input files		
calculated from other codes	No	

## APPENDIX E

### CODE REVIEW CRITERIA—GASFLOW

#### 1.0. GENERAL CRITERIA

0. Code Name— GASFLOW 2.0
1. Sponsor/developing organization— LANL/DOE/NRC
2. Current custodian/phone/fax/internet— Kin Lam  
M/S K575  
Los Alamos National Lab  
Los Alamos, NM 87545  
Ph. (505) 665-3362  
Fax (505) 665-0879  
klam@lanl.gov
3. Genealogy—GASFLOW 2.0 is the same as the GASFLOW 1.1 code version, except one-dimensional (1D) ventilation system models and multiblock capability have been added to the GASFLOW 2.0 code version. GASFLOW 1.1 was based on the HMS series of codes originally developed by the NRC for the investigation of hydrogen in containments. The GASFLOW series of codes has been funded by DOE-DP, DOE-EM, and the NRC.
4. Abstract—GASFLOW 2.0 can model geometrically complex containments, buildings, and ventilation systems with multiple compartments and internal structures. It can calculate gas and aerosol behavior of low-speed buoyancy-driven flows, diffusion-dominated flows, and turbulent flows during deflagrations. The code can model condensation in the bulk fluid regions; heat transfer to wall and internal structures by convection, radiation, and condensation; chemical kinetics of combustion of hydrogen or hydrocarbons; fluid turbulence; and the transport, deposition and entrainment of discrete particles. Heat conduction within walls and structure is 1D.
5. Input Summary—Input is via namelist parameters that describe the geometry, identify gas component species, boundary conditions, heat structures, interconnections between 3D blocks and 1D ventilation system components, initial conditions, and models to be used.
6. Output Summary—Output is a form of printed output as well as graphical output. The graphical output can be displayed with the graphics package included with GF2. In addition, selected information

is written to the terminal and message files. Input is echoed to the TAPE16 file.

7. Evaluation of computer model vs DOE requirements—In terms of dose/consequence, the output from GF2 must be used as input into another model/computer-code to determine onsite/offsite dose/consequence. In terms of TSRs that are related to flammable gas concentrations, GF2 results can be used directly. For calculations involving worker safety, the results of the GASFLOW calculation must be input into another model or computer code to determine the dose/consequence.
8. Can the graded approach philosophy be addressed with this code (i.e., can the level of modeling detail be changed)?—Level of detail of modeling with GASFLOW can be increased or decreased, depending on the number of nodes, number of aerosol particle sizes/classes, and models selected.
9. Applicability and modeling assumptions—Applicable to any facility (i.e., buildings, tanks, single rooms) with and without ventilation systems. Applicable to multi-species gas mixing/transport problems, as well as aerosol transport problems. Major assumptions in GF2:
  - Each cell is well mixed.
  - Each gas species has the same velocity at cell boundaries.
  - Agglomeration is currently ignored in the aerosol model.
  - Diffusion of species is based on mixture diffusion equations.
  - Gases is assumed to behave as ideal gas.
  - Choking is currently not considered in the ventilation system components.
10. Data and input parameter and boundary condition requirements:
  - Gas properties are available as fits for the following gas species:

C	—	Carbon particles
CO	—	Carbon Monoxide
CO <sub>2</sub>	—	Carbon Dioxide
H <sub>2</sub>	—	Hydrogen
H <sub>2</sub> O	—	Water vapor

N <sub>2</sub>	—	Nitrogen
N <sub>2</sub> O	—	Nitrous Oxide
O <sub>2</sub>	—	Oxygen
Air		
Ar	—	Argon
He	—	Helium
NH <sub>3</sub>	—	Ammonia
CH <sub>4</sub>	—	Methane
OH	—	Hydroxyl
H	—	Hydrogen
HO <sub>2</sub>	—	Hydroperoxyl
NO	—	Nitric Oxide
O	—	Oxygen
NH	—	Imidogen
HNO	—	Nitroxyl Hydride
H <sub>2</sub> O <sub>2</sub>	—	Amidogen
LG	—	Light Gas
CH <sub>6</sub>	—	Benzene

- Depending on the models selected, additional model inputs are required. For example:
  - Algebraic turbulence model needs mixing length input.
  - Kappa-epsilon turbulence model needs k-ε turbulence parameters.
  - Blower model needs vendor information on performance characteristics.
- Time-dependent user-specified boundary conditions for pressure, temperature, mass fractions, and velocities can be specified.

11. User friendly—

- Input error checking attempts to find all input errors before the code stops.
- 3D blocks can be built with only a few inputs.
- Cylindrical and rectangular geometries are available.
- Building of 1D duct network is based on easily specified 3D coordinate space.

12. Typical execution time—This depends on the machine, detail of the model, and the length of the transient. Runtimes on the CRAY vary

from a few seconds to a few hours. Typical runtimes for Hanford waste tank burps and burns are several hours on an SGI workstation. Typical runtime for long multiday transients for a large passively ventilated tank farm are several days on a SUN SPARC 10 workstation. TA-55 analysis took ~1 h on the CRAY, which implies 4-5 h on an SGI workstation.

13. Machine/operating system requirements—GF2.0 is currently running on CRAY (UNICOS), SGI (UNIX), and SUN (UNIX) workstations. GF2.0 requires a FORTRAN 77 compiler. Memory requirements depend on the problem size.
14. Validation—Previous versions (i.e., HMS and GASFLOW 1.0 have Assessment Manuals). GF2.0 has been applied to previous assessments to verify that GF2.0 is giving the same results as previous versions.
15. Q/A
  - Software development plan and requirements.
  - Validation Reference—J. R. Travis, K. L. Lam, T. L. Wilson, "GASFLOW: A Three-Dimensional Finite-Volume Fluid-Dynamics Code for Calculating the Transport, Mixing, and Combustion of Flammable Gases in Geometrically Complex Domains, Vol. 3 Assessment Manual," Los Alamos National Laboratory report LA-UR-94-2270 (July 11, 1994).
  - Benchmark Reference—J. R. Travis, K. L. Lam, T. L. Wilson, "GASFLOW: A Three-Dimensional Finite-Volume Fluid-Dynamics Code for Calculating the Transport, Mixing, and Combustion of Flammable Gases in Geometrically Complex Domains, Vol. 3 Assessment Manual," Los Alamos National Laboratory report LA-UR-94-2270 (July 11, 1994).
  - User's Manual—J. R. Travis, K. L. Lam, T. L. Wilson, "GASFLOW: A Three-Dimensional Finite-Volume Fluid-Dynamics Code for Calculating the Transport, Mixing, and Combustion of Flammable Gases in Geometrically Complex Domains, Vol. 2 User's Manual," Los Alamos National Laboratory report LA-UR-94-2270 (July 11, 1994).
  - Error Handling/Reporting - Yes
16. Life-Cycle Status—Currently at end of development stage and is soon to be released with documentation.
17. Applications are:
  - Hanford Waste Tank Ventilation Studies—Single-shell tanks (SSTs) with passive ventilation systems



- Hanford Waste Tank Ventilation Studies—Double-shell tanks (DSTs) with active ventilation systems
- Burp and burn calculations for Hanford Waste Tanks, both DST and SST
- Replace Tritium Facility tritium mixing and combustion
- TA-55 Fire Bounding Fire
- Benzene mixing problem
- Bureau of Mines combustion data for H<sub>2</sub>-N<sub>2</sub>O-air mixtures
- (h) Savannah River K Reactor
  - AP600
  - Hydrogen Rule for Large Dry Containments
  - NRC Containment Loads Working Group Standard Problems

18. Statistical aspects of in-facility transport—input parameters can be varied to investigate sensitivity of results. Aerosol model includes statistical treatment of particles.

19. Overall strengths, limitations, and weaknesses:

Strengths are:

- Full governing equations solutions (i.e., no assumptions about incompressible flow)
- Multidimensional flow, multispecies diffusion, and chemistry models
- The availability of several turbulence models
- Multiblock can be interconnected by 1D ductwork models (it has the capability to model in detail selected rooms in a building, with coarser models in the other rooms in a building)
- The availability of a Lagrangian aerosol model
- A complete ventilation system modeling capability

Limitations are:

- For ventilation system modeling, only six connections are allowed per cell. However, multicells can be used to model a single manifold.
- No solids or liquids combustion model are available. Energy and mass source for solids and/or liquids burning must be provided as input.

Weaknesses are:

- There is no agglomeration model; however, this should be conservative because agglomeration would in general increase particle sizes and would tend to reduce the respirable fraction because of agglomerated particles that become too big to be respirable and because of settling.
  - Currently, no internal code model for user-friendly representation of log-normal particle-size distribution.
20. Operability—adequate for GASFLOW 2.0. New user not familiar with GASFLOW 2.0 was able to put together two simple test problems and obtain results within three days after a few hours of instruction from the GASFLOW code developers. Within the time available, a third test problem input was prepared, but the calculation was not completed. This exercise identified several areas where additional input error checking needed to be added to GASFLOW.

## 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct	Yes	Flow assumed to be 1D
Damper/Valve	Yes	Flow assumed to be 1D
Blower/Fan	Yes	Vendor information on performance characteristics.
Filter	Yes	Information on flow loss required
Manifold	Yes	Limited to six connections per cell; however, manifold model can contain multicells, which implies six more connections per added cell

### 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped Parameter	Yes	Can be used by coarsely noding an effective lumped parameter or control volume approach
Multi-D Hydro	Yes	
Representation of non-orthogonal shapes	Yes	Requires blocking of cells in coordinate system to obtain desired geometry
orthogonal		
desired		
Finite elements	No	
Form-fitted coordinates		

### 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic	Yes	
k-ε	Yes	

### 5.0. DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular	Yes	Uses mixture diffusion coefficients for multi-component diffusion
Turbulent	Yes	

### 6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available.	Yes	Available species number 23.
Can new species be added easily?	Yes	Requires a run with the CHEMKIN code and a fitting code to obtain the fit coefficients. However, this has been automated.

### 7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model	Yes	
Settling model	Yes	

Deposition model	Yes
Entrainment model	Yes
Re-entrainment model	Yes
Agglomeration model	No

#### 8.0. CHEMISTRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas	Yes	Currently limited to hydrogen, methane, carbon monoxide, ammonia, with air, oxygen, or nitrous oxide
Combustion model liquids	No	
Combustion model solids	No	

#### 9.0. BUOYANCY DRIVEN FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and composition (species).	Yes	Species must be available in the property fits table.

#### 10.0. COMPRESSIBLE FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure	Yes	Species must be available in the property fits table.

#### 11.0. HEAT TRANSFER

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction	Yes	1D
Convection	Yes	Based on Reynolds analogue
Radiation	No	Has been added to special versions of GF2

#### 12.0. DETERMINATION OF INITIAL CONDITION

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-accident steady-state capability	Yes	Requires a transient run with constant boundary conditions

### 13.0. GEOMETRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can geometry, especially leakage paths, change during the calculation		
— As specified by the user	Yes	Time-dependent tables
— By built-in code models	No	Has been added to special versions of GF2

### 14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Must be specified mainly by user input	Yes	
Specified mainly by internal models	Yes	Only for gas burns
Specified mainly by user written subroutines	No	
Specified mainly by input files calculated from other codes	No	

## APPENDIX F

### CODE REVIEW CRITERIA—KBERT

#### 1.0. GENERAL CRITERIA

0. Code Name— KBERT
1. Sponsor/developing organization— DOE
2. Current custodian/phone/fax/internet— K. E. Washington  
MS 0722  
Org. 6913  
Sandia National Laboratories  
Albuquerque, NM 87185-  
0722
3. Genealogy—KBERT was developed specifically for DOE for the analysis of Worker Safety Risks.
4. Abstract—The possibility of worker exposure to radioactive materials during accidents at nuclear facilities is a principal concern of the DOE. The KBERT software has been developed at SNL under DOE support to address this issue by assisting in the estimation of risks posed by accidents at chemical and nuclear facilities. The current prototype version of KBERT focuses on calculation of doses and consequences to in-facility workers resulting from accidental releases of radioactivity.
5. Input Summary—Input is via dialog boxes for rooms, HVAC plenums, structures, flowpaths, HVAC ducts, filters, workers, etc.
6. Output Summary—Output is via dialog boxes for rooms, workers, facility, etc. Includes a graphical screen view of the facility.
7. Evaluation of computer model vs DOE requirements—KBERT directly provides information on the dose consequence for workers, which can be used to determine functional classification for structures, safety equipment, etc. In addition, KBERT can provide source terms for input into atmospheric dispersion models. Also, KBERT provides distributions, releases to the environment, radiation levels in rooms, etc. The capability to track hazardous gases has not been added to the KBERT code.
8. Can graded approach philosophy be addressed with this code (i.e., can the level of modeling detail be changed)?—Multidimensional analysis is difficult to obtain with the current version of KBERT.

9. Applicability and modeling assumptions—Applicable to any facility, but flow rates for flow paths must be specified.
10. Data and input parameter and boundary condition requirements.
11. User-friendly—Yes, input and output is via a GUI.
12. Typical execution time—KBERT is currently very fast, but it does not solve for the flow field.
13. Machine/operating system requirements are:
  - IBM-compatible PC with an 80386 processor or higher, although a 486 or higher is highly recommended,
  - Microsoft Windows 3.1 or higher,
  - VGA graphics display (SVGA recommended),
  - A mouse or compatible pointing device, and
  - A hard disk with at least 10MB of free space.
14. Validation—Uses extensively validated Mishima release database.
15. Q/A
  - Software Development Plan & Requirements
  - Validation Reference
  - Benchmark Reference
  - User's Manual—D. S. Browitt et. al., "User's Guide for the KBERT 1.0 Code," SAND95-1324 (July 1995).
  - Error Handling/Reporting—On screen via a GUI
16. Life-Cycle Status—First version released in 1995.
17. Applications
18. Statistical aspects of in-facility transport—No.
19. Overall strengths, limitations, weaknesses.

Strengths are:

  - Fast running
  - Easy to use and give dose consequence directly

- Includes built-in Mishima database for sources
- Objective-oriented language used for development, which implies the resulting coding should be easy to add new models and/or capability

Limitations are:

- Only air available as a gas species
- Only radioactive releases considered

Weaknesses:

- All flow rates must be known for all times for the accident, but other codes can be used to supply flows.
- No turbulence and diffusion modeling within a control volume.

20. Operability—was not tested for this code.

## 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct	Yes	Flow rate specified
Damper/Valve		
Blower/Fan	No	
Filter	Yes	
Manifold	Yes	

## 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped Parameter	Yes	Flow rates specified
Multi-D Hydro	No	
Representation of non-orthogonal shapes	No	
Finite elements	No	
Form-fitted coordinates	No	

## 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic	No	
k-ε	No	



5.0. DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular	No	
Turbulent	No	

6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available.	Yes	1 species (air).
Can new species be added easily?	?	

7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model	Yes	Included in deposition model
Settling model	Yes	
Deposition model	Yes	
Entrainment model	No	
Re-entrainment model	No	
Agglomeration model	No	

8.0. CHEMISTRY

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas	No	
Combustion model liquids	No	
Combustion model solids	No	

9.0. BUOYANCY DRIVEN FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temp. and composition (species).	Yes	

10.0. COMPRESSIBLE FLOWS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure	No	

**11.0. HEAT TRANSFER**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction	No	
Convection	No	
Radiation	No	

**12.0. DETERMINATION OF INITIAL CONDITION**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-Accident steady-state capability	No	

**13.0. GEOMETRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can geometry, especially leakage paths, change during the calculation		
— As specified by the user	Yes	Leak paths can be changed during the calculation by way of time-dependent flow.
— By built-in code models	No	

**14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Must be mainly specified by user input	No	
Specified mainly by internal models	Yes	Mishima database.
Specified mainly by user written subroutines	No	
Specified mainly by input files calculated from other codes	Yes	Flows can be calculated and input from the CONTAM93 code.

**APPENDIX G  
CODE REVIEW CRITERIA—MELCOR**

**1.0. GENERAL CRITERIA**

0. Code Name— MELCOR 1.8.3
1. Sponsor/developing organization— NRC
2. Current custodian/phone/fax/internet— K. D. Bergeron  
Org. 6421  
MS-0739  
P. O. Box 5800  
Sandia National Lab  
Albuquerque, NM  
87185-0739  
Ph. (505) 844-2507
3. Genealogy—MELCOR has been developed by SNL for the NRC for the analysis of severe core damage accidents in a nuclear reactor system and containment building. MELCOR has been developed as the successor to the Source Term Code Package.
4. Abstract—MELCOR is a fully integrated, relatively fast-running code that models the progression of severe accidents in light-water nuclear power plants. An entire spectrum of severe accident phenomena is modeled in MELCOR. Characteristics of severe accident progression that can be treated with MELCOR include the thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings; core heatup and degradation; radionuclide release and transport; hydrogen production, transport, and combustion; core-concrete attack; heat structure response; and the impact of engineering safety features on thermal-hydraulic and radionuclide behavior.
5. Input Summary—Two input files are required to run MELCOR. The first input file is for the MELGEN program, which generates a restart file for the MELCOR code. The second input file is for the execution of the MELCOR code and is essentially timestep control information. Various models/modules are activated via the input [i.e., Control Function (CF) Package, Flow Path (FL) Package, Heat Structure (HS) Package, Noncondensable Gas (NCG) Package, Control Volume Hydrodynamics (CVH) Package, etc.]. Input is free format and requires an identifier field for each line of input.

6. Output Summary—Both MELGEN and MELCOR generate printed output. In addition, selected information is written also to the Diagnostic, Message, and Terminal Files. A plot file is also written, which can be read by the HISPLT program for postprocessing and will generate a graphics metafile containing plots requested by the HISPLT User Input File.
7. Evaluation of a computer model vs DOE requirements—To evaluate dose/consequence, the output from MELCOR can be used as input to the MACCS computer code. In terms of TSRs that are related to flammable gas concentrations, MELCOR results can be used directly. For calculations involving worker safety, the results of the MELCOR calculation must be input into another model or computer code to determine the dose/consequence.
8. Can graded approach philosophy be addressed with this code (i.e., can level of modeling detail be changed)?—MELCOR can perform lumped parameter/control volume type analysis but is limited in terms of providing detailed multidimensional modeling of a room or gas dome space. The number of control volumes can be increased and linked together to simulate a 2D or 3D grid; however, for the low flows expected during most in-facility transport calculations, the lack of the momentum flux terms and viscous shear terms make this approach inadvisable.
9. Applicability and modeling assumptions—Applicable to any facility (i.e., buildings, tanks, single rooms, etc.) with and without ventilation systems. Applicable to multispecies gas mixing/transport problems, as well as aerosol transport problems. Major assumptions in MELCOR:
  - Each control volume gas space is well mixed, except each cell does allow for a pool covered by a gas volume.
  - Each gas species has the same velocity in the flow path connections.
  - Noncondensable gases are assumed to be ideal.
  - Turbulence and species diffusion within a control volume are not modeled, except in the aerosol model and condensation/evaporation on surfaces.
10. Data and input parameter and boundary condition requirements:
  - Default gas properties are available for the following gas species:

H <sub>2</sub>	—	Hydrogen
O <sub>2</sub>	—	Oxygen
CO <sub>2</sub>	—	Carbon Dioxide
CO	—	Carbon Monoxide
N <sub>2</sub>	—	Nitrogen
CH <sub>4</sub>	—	Methane
He	—	Helium
Ar	—	Argon

- D<sub>2</sub>—deuterium ventilation system components can be built by user input for user-defined control functions and flow paths.
  - Time-dependent user-specified boundary conditions for pressure, temperature, and velocity can be specified.
11. User-friendly—
- MELGEN performs user input error checking before creation of the MELCOR restart file.
  - Interactive execution options allow the user to stop, continue, change timestep control, and change boundary conditions during the execution.
12. Typical execution time—Depends on machine, detail of the model, and the length of the transient. Runtimes on the CRAY vary from 0.1 s to on the order of 1 h. Runtimes for the Marviken-V Aerosol Transport Tests ATT varied from 3442 cpu(s) on a CRAY XMP-24, to 26,700 cpu(s) on a SUN Sparc2. Detailed code calculation of 24-h LaSalle Station Blackout calculation was 2 h on an HP. Simplified code calculation runtime for a 4-h sample problem transient was 15 min on an HP. The ratio of real time to runtime can vary from 0.5 to 100, depending on the nodalization.
13. Machine/operating system requirements—IBM, VAX/VMS, SUN, PC, CRAY, and MS-DOS PC versions are available. Memory requirement is 5 MB.
14. Validation—
- C. D. Leigh et. al., "MELCOR Validation Results," 14th Water Reactor Safety Information Meeting, Gaithersburg, Maryland, Sandia National Laboratories report SAND86-2128C (October 1986).

- C. D. Leigh et. al., "MELCOR Validation and Verification 1986 Papers," 14th Water Reactor Safety Information Meeting, Gaithersburg, Maryland, Sandia National Laboratory document SAND86-2689, NUREG/CR-4830 (October 1986).
- G. D. Wyss et. al., "MELCOR Adaptation and Validation for Modeling of N Reactor Core Phenomena," Proceedings of the International Topical Meeting on the Safety, Status and Future of Non-Commercial Reactors and Irradiation Facilities, Boise, Idaho, Sandia National Laboratory report SAND90-0115C (September 1990).
- M. I. Robertson, "Validation of Control Volume Thermal-Hydraulic Modeling," CSNI/CEC Workshop on Aerosol Behavior in the Containment, Fontenay-aux-Roses, France (November 1990).
- L. N. Kmetyk, "MELCOR 1.8.1 Assessment: LACE Aerosol Experiments LA4," Sandia National Laboratory report SAND91-1532 (September 1991).
- L. N. Kmetyk, "MELCOR 1.8.1 Assessment: ACRR Source Term Experiments ST-1/ST-2" (April 1992).
- L. N. Kmetyk, "MELCOR 1.8.1 Assessment: Marviken-V Aerosol Transport Tests ATT-2b/ATT-4," Sandia National Laboratories report SAND92-2243 (January 1993).
- L. N. Kmetyk, "MELCOR Assessment: Gedanken Problems Volume 1," Sandia National Laboratory report SAND92-0763 (January 1993.)
- Francisco J. Souto et. al., "MELCOR 1.8.2 Assessment: Aerosol Experiments ABCOVE AB5, AB6, AB7, and LACE LA2," Sandia National Laboratory report SAND94-2155 (October 1994).

15. Q/A

- Software development plan and requirements
- Validation Reference—C. D. Leigh et. al., "MELCOR Validation and Verification 1986 Papers," 14th Water Reactor Safety Information Meeting, Gaithersburg, Maryland, Sandia National Laboratory report SAND86-2689, NUREG/CR-4830 (October 1986).
- Benchmark Reference—C. D. Leigh et. al., "MELCOR Validation and Verification 1986 Papers," 14th Water Reactor Safety

Information Meeting, Gaithersburg, Maryland, Sandia National Laboratory report SAND86-2689, NUREG/CR-4830 (October 1986).

- User's Manual - R. M. Summers et. al., "MELCOR 1.8.0: A Computer Code for Severe Nuclear Reactor Accident Source Term and Risk Assessment Analyses," Sandia National Laboratory report SAND90-0364, NUREG/CR-5531 (January 1991).
- Error Handling/Reporting—Yes

16. Life-Cycle Status—Released to the public, maintenance; development is continuing.

17. Applications—

- S. E. Dingman et al., "Analysis of Peach Bottom Station Blackout with MELCOR," 14th Water Reactor Safety Information meeting, Gaithersburg, Maryland, Sandia National Laboratory report SAND86-2129C (October 1986).
- E. A. Boucheron et al., "MELCOR Analysis of the Three Mile Island Unit 2 Accident," *Nuclear Technology* 87, 1050 (December 1989).
- L. A. Miller et. al., "N Reactor Probabilistic Risk Assessment Supporting Calculations," Volume 1: Main Report, Sandia National Laboratory report SAND89-2101 (June 1990).
- S. E. Dingman, et. al., "MELCOR Analyses for Accident Progression Issues," Sandia National Laboratory report SAND89-0082, NUREG/CR-5331 (draft to be published).
- I. R. Madni, "MELCOR Simulation of the PBF Severe Fuel Damage Test 1-1," AICHE Symposium Series, Proceedings of the 26th National Heat Transfer Conference, Philadelphia, Pennsylvania (1989).

18. Statistical aspects of in-facility transport—Sensitivity coefficients are available to investigate sensitivity of results to uncertainty in selected coefficients and parameters in models.

19. Overall strengths, limitations, and weaknesses

Strengths are:

- Is fast running because of the control volume approach.

- There is no limit on the number of flow path connections to a single control volume.
- Spray models are available if sprays are important to the analysis.
- Two-phase flow can be modeled if multiphase flow is important to the analysis.
- Code is versatile.
- Aerosol model is based on MAEROS model, which is a detailed mechanistic model.

Limitations are:

- There is limited diffusion and turbulence modeling within a control volume.
- Multidimensional flow within a room cannot be easily or accurately simulated.

Weaknesses are:

- There is no multi-D capability.
  - Memory overhead is associated with multiphase flow and reactor models.
  - Ventilation system components must be built by user input (no specific component models exist).
  - Momentum balance ignores spatial acceleration term.
20. Operability—Knowledgeable user was able, within a week, to put together a moderately complicated test problem and obtain results. Oscillatory flow when fans were operating is still under investigation.

## 2.0. VENTILATION SYSTEM MODELS

<u>Ventilation components</u>	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Duct	Yes	Flow is assumed to be 1D.
Damper/Valve	Yes	Flow is assumed to be 1D.
Blower/Fan	Yes	Performance characteristics must be supplied via Control Function.



Filter	Yes
Manifold	Yes

### 3.0. ROOM/TANK/GLOVE BOX MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Lumped Parameter	Yes	Very limited and not practical
Multi-D Hydro	Yes	
Representation of non-orthogonal shapes	No	
Finite elements	No	
Form-fitted coordinates	No	

### 4.0. TURBULENCE MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Algebraic	Yes	Only for aerosols and for evaporation/condensation on surfaces
k-ε	No	

### 5.0. DIFFUSION MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Molecular	Yes	Only for aerosols and for evaporation/condensation on surfaces
Turbulent	Yes	Only for aerosols and for evaporation/condensation on surfaces

### 6.0. MULTI-SPECIES MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Number of species available	Yes	Nine species available
Can new species be added easily?	Yes	Requires temperature dependent fit for $C_v$ , requires molecular weight, etc.

### 7.0. AEROSOL MODELS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Drag model	Yes	
Settling model	Yes	
Deposition model	Yes	

Entrainment model	No
Re-entrainment model	No
Agglomeration model	Yes

**8.0. CHEMISTRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Combustion model gas	Yes	Hydrogen gas and carbon monoxide
Combustion model liquids	No	
Combustion model solids	No	

**9.0. BUOYANCY DRIVEN FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and composition (species)	Yes	No buoyancy-driven flows in a single control flow/room, but from one control volume/room to the next

**10.0. COMPRESSIBLE FLOWS**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Gas density function of temperature and pressure	Yes	

**11.0. HEAT TRANSFER**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Conduction	Yes	1D
Convection	Yes	
Radiation	Yes	

**12.0. DETERMINATION OF INITIAL CONDITION**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Pre-accident steady-state capability	Yes	Must run a null transient.

**13.0. GEOMETRY**

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Can geometry, especially leakage paths change during the calculation — As specified by		

the user	Yes	
— By built-in code models	Yes	Via user build functions/tables

14.0. CONNECTION TO THE ENERGY, MASS, AND RADIOACTIVE SOURCE TERMS

	<u>Yes/No</u>	<u>Limitations/Assumptions</u>
Must be mainly specified by user input	Yes	However, internal models mainly for reactor accidents
Specified mainly by internal models	Yes	However, internal models mainly for reactor accidents
Specified mainly by user written subroutines	No	
Specified mainly by input files calculated from other codes	No	

