SMART- IST: A Computer Program to Calculate Aerosol and Radionuclide Behaviour in CANDU Reactor Containments

S.R. Mulpuru and B.J. Corbett

Fuel & Fuel Channel Safety Branch
Atomic Energy of Canada Limited
Chalk River Laboratories
Chalk River, Ontario, K0J 1J0

ABSTRACT

The SMART-IST computer code models radionuclide behaviour in CANDU reactor containments during postulated accidents. It calculates nuclide concentrations in various parts of containment and releases of nuclides from containment to the atmosphere. The intended application of SMART-IST is safety and licensing analyses of public dose resulting from the releases of nuclides. SMART-IST has been developed and validated meeting the CSA N286.7 quality assurance standard, under the sponsorship of the Industry Standard Toolset (IST) partners consisting of AECL and Canadian nuclear utilities; OPG, Bruce Power, NB Power and Hydro-Québec. This paper presents an overview of the SMART-IST code including its theoretical framework and models, and also presents typical examples of code predictions.

1. INTRODUCTION

SMART (Simple Model for Aerosol Removal and Transport), the predecessor of SMART-IST was developed by AECL under the sponsorship of NB Power and Hydro-Québec. SMART was used in safety and licensing analyses of Canadian and off-shore single-unit CANDU stations that have been designed by AECL. A new code version, SMART-IST, was developed by AECL in the recent past, under the sponsorship of the IST (Industry Standard Toolset) partners (AECL, OPG, Bruce Power, NB Power and Hydro-Québec), incorporating a number of new models and code enhancements. The IST version was developed and validated according to AECL Software Quality Assurance procedures, meeting the CSA N286.7 Standard.

During a postulated accident in a CANDU reactor, radionuclides may be released from a break in the primary heat transport system and become airborne in the containment building. These nuclides can exist in the form of vapours and aerosols. A small fraction of these nuclides may be released to the outside atmosphere through escape paths, depending on the containment geometry and thermalhydraulic conditions. Analysis of public dose resulting from the nuclide releases is a part of the overall CANDU safety analysis. SMART-IST is designed to predict nuclide behaviour within containment considering various aspects such as releases of nuclides from the primary heat transport system, transport of nuclides among various rooms in containment, removal of nuclides from the containment atmosphere through various removal mechanisms, changes in nuclides resulting from radioactive decay and build-up, and releases of nuclides to the outside atmosphere through containment escape paths.

SMART-IST predictions are based on solving a system of differential equations derived from the mass conservation principle, describing the transport of aerosols and gases within a network of interconnected volumes. Containment thermalhydraulic information is required to solve these equations. SMART-IST obtains this information from the GOTHIC thermalhydraulic code [1] and provides the predicted results for public dose analysis.

SMART-IST models radioiodine in more detail than other nuclides using the IMOD-2 model developed at AECL [2]. IMOD-2 was incorporated into the overall mathematical framework of SMART-IST as a module modelling the chemical transformations between various iodine species and mass transfer of these species among gas, aqueous and adsorbed phases in containment.

This paper presents an overview of the SMART-IST code including its theoretical framework and models, and provides examples of typical predictions.

2. THEORETICAL FRAMEWORK AND MODELS

2.1 Geometry

The physical system modelled by SMART-IST is a CANDU reactor containment. The geometry model used to represent this system is a generalized network of inter-connected volumes with pathways for mass and energy transport within the system and between the system and its surroundings. The phenomena modelled within this network are associated with aerosol and nuclide transport including various sources and sinks for their mass and energy. The network may consist of components such as a containment compartment (room), a flow path connecting two compartments (link), a release path from containment to the outside atmosphere (hole), a break in the primary heat transport system providing a source of aerosols and nuclides, a dousing system providing a source of aerosols, an EFADS (Emergency Filtered Air Discharge System) that removes aerosols and nuclides, and walls and water pools within a compartment providing sources/sinks for nuclide and aerosol mass.

2.2 Nuclide and aerosol transport

SMART-IST models transport of two forms of nuclides; a) contained in and carried by aerosols and, b) existing in the gaseous form.

The following assumptions are made regarding aerosol and nuclide transport in containment:

- The transient thermalhydraulic properties within this network are available as input data for use in the calculation of nuclides and aerosol transport.
- Gaseous nuclides and aerosols in a room are perfectly mixed, with uniform nodal properties.
- Nuclide and aerosol processes within a room do not contribute to mass, momentum or energy exchange with the gas present in the room and, thus, do not feed the information back to the thermalhydraulic processes driving the transport of nuclides and aerosols.
- Airborne gaseous nuclides and aerosols are transported from one room to another by convection of the carrier gas through links.
- Gaseous nuclides and aerosols are transported from the free volume of a room to the external atmosphere by convection of the carrier gas through specified holes.
- Volumetric source or sink rates of nuclides and aerosols in a room are spatially uniform.

2.2.1 Transport of nuclides enveloped in aerosol

Mass balance is the law that governs aerosol transport in containment. Processes which can cause a change in the airborne aerosol mass and the nuclide mass contained in the aerosols in a room are:

1. coagulation,
2. link flows,
3. convective flow through holes to the external atmosphere,
4. removal due to aerosol deposition mechanisms,
5. EFADS sink, and
6. source from a break or other discharge into the room.

In order to formulate governing equations, in addition to the assumptions made in Section 2.2, it is further assumed that the aerosol mass is distributed over a finite number of discreet size ranges (classes). For convenience, aerosol volume instead of mass is considered in formulating the equations. The mass balance of nuclides contained in aerosols in a network of inter-connected rooms can be expressed by the following set of differential equations:

$$\frac{dX_{ijk}}{dt} = \text{B (Net addition due to aerosol coagulation) + C (Net addition due to link flows and escape path flows) + D (Various source and sink terms)} \quad (1)$$

where,

$$B = \frac{Q_{ij}}{VOL_i}\sum_{l=1}^{j-1}\frac{\beta_{jl}X_{ilk}}{v_1} - \frac{X_{ijk}}{VOL_i}\sum_{l=j+1}^{N}\frac{Q_{il}\,\beta_{jl}}{v_l}$$

$$- A_f\frac{X_{ilk}}{VOL_i}\beta_{ij}\frac{Q_{ij}}{v_j} + A_f\frac{X_{i(j-1)k}}{VOL_i}\beta_{j-1j-1}\frac{Q_{ij-1}}{v_{j-1}}$$

$$C = -\sum_m \frac{W_m X_{ijk}}{TM_i} + \sum_n \frac{W_n X_{Ijk}}{TM_i} - \frac{W_{Hi}X_{ijk}}{TM_i}$$

$$D = -\lambda_j X_{ijk} + S_{ijk} + \omega_{ijk} + N_{ijk} - E_{ijk}$$

Here, the subscripts i, j, and k represent node (room), size class and nuclide respectively, and the symbols represent:

X_{ijk} amount of nuclide k (moles) in aerosol volume Q_{ij} (m^3)

VOL_i node i volume (m^3)

A_f dimensionless constant used in partitioning aerosol volume between two classes after coagulation of two particles of same size

Tm_i total gas mass in node i (kg)

W_m flow rate in link m out of room i (kg/s)

W_n flow rate in link n into room i from donor room I (kg/s)

S_{ijk} break discharge source term (mol/s)

W_{hi} total flow rate through all holes connecting node i to the external atmosphere (kg/s)

β_{jl} coagulation kernel between class j and class l of aerosols (m^3/s)

v_j volume of aerosol particle j (m^3)

N_{ijk} source term due to iodine chemical transformation and mass transfer (mol/s)

E_{ijk} EFADS sink term (mol/s)

λ_j nuclide removal rate constant associated with aerosol deposition mechanisms (1/s)

ω_{ijk} net generation rate resulting from decay and build-up of nuclide k, in node i, and size class j (mol/s)

2.2.1.1 Aerosol sub-models

SMART-IST uses a number of aerosol sub-models to enable calculations of Equation 1. This section presents a brief description of these models.

2.2.1.1.1 Liquid aerosol source

When water discharges from a break in the primary heat transport system at a high pressure and temperature, it will break up into droplets of different sizes. Measurements of droplet sizes in such discharges were performed at AECL using a phase-Doppler anemometer [3]. These measurements show that the droplet sizes can be represented mathematically by log-normal distributions [3]. Based on these findings, SMART-IST assumes a log-normal distribution for the source aerosols. The mean of the size distribution is calculated by a model based on aerodynamic fragmentation. According to this model, fragmentation of the discharging jet occurs if the Weber number, We, is greater than a critical value, which occurs when the drag force on the droplet exceeds the surface tension forces [4]. The mean droplet diameter is calculated based on the critical Weber number.

2.2.1.1.2 Liquid aerosol agglomeration

Agglomeration mechanisms are physical processes that result in the collision and adhesion of aerosol particles to form larger particles. The aerosol size distribution shifts toward large sizes as a result of agglomeration. SMART-IST models four types of agglomeration mechanisms; Brownian, gravitational, turbulent-inertial and turbulent shear, that are most commonly considered in containment safety analyses [5].

2.2.1.1.3 Gravitational settling

Aerosol particles settle onto available horizontal areas due to the force exerted on them by gravity. As the particle settles, it experiences a drag force in a direction opposite to that of the settling velocity. SMART-IST calculates the settling velocity, taking into consideration the drag force that can vary depending on the size, shape and speed of the particle and the transport properties of the surrounding gas [6].

2.2.1.1.4 Impingement

Experiments were conducted in the WALE (Wet Aerosol Leakage Experiment) facility, to study aerosol removal in a vessel, into which water jets were discharged under conditions typical to those of Loss of Coolant Accident discharges [7,8]. The overall mechanism that causes the removal of aerosols under these circumstances has been termed as “impingement”. These experiments have demonstrated that a large fraction of the water jet discharge mass is removed, and only a small fraction remains airborne in the vessel free volume. SMART-IST uses an empirical model supported by experimental data for calculation of fractional removal of the jet aerosol mass.

2.2.1.1.5 Stefan flow

Near surfaces where condensation occurs, an aerodynamic flow may occur toward the surface. This flow, called Stefan flow, may cause migration of aerosols suspended in the gas-vapour mixture toward the surface. Stefan flow may cause removal of airborne aerosols from the containment atmosphere, when steam condenses on available surfaces. SMART-IST calculates the aerosol removal rate due to Stefan flow in a given node using the condensation rate of steam and its properties.

2.2.1.1.6 Turbulent deposition

SMART-IST calculates turbulent deposition using a combination of the Liu-Agarwal model [9] for turbulent-inertial deposition, and the Davies model for turbulent-diffusion deposition [10].

2.2.1.1.7 Thermophoresis

When a temperature gradient occurs in a gas (e.g., due to heat transfer to a surface), the aerosol particles suspended in the gas experience a force in the direction of decreasing temperature [11]. The motion of the aerosol particle that results from this force is called thermophoresis. The magnitude of the thermal force depends on gas and particle properties, flow characteristics and the temperature gradient. SMART-IST calculates the removal of aerosols due to thermopheresis using a model described in reference [12].

2.2.1.2 Gaseous nuclide transport

Mass balance is the law that governs gaseous nuclide transport in containment. Processes which can cause a change in the airborne, gaseous nuclide mass in a room are:

1. convective flow through links,
2. break or dousing discharge into a room,
3. radioactive decay and build-up,
4. iodine chemical transformation and mass transfer,
5. removal in the EFADS filtering system, and
6. convective flow out of holes to the external atmosphere.

With the assumptions made in Section 2.2, and the processes identified above, the mass balance of airborne gaseous nuclides in a network of interconnected rooms can be expressed by the following set of differential equations:

$$\frac{dX_{ij}}{dt} = \text{G (Net addition due to link flows and escape path flows)}$$

$$+\text{P (Various source and sink terms)} \qquad (2)$$

where,

$$G = \sum_n \frac{W_n X_{Ij}}{TM_m} - \sum_m \frac{W_m X_{ij}}{TM_i} - \frac{W_{Hi} X_{ij}}{TM_i}$$

$$P = S_{ij} + \omega_{ij} + N_{ij} - \lambda_j X_{ij} - E_{ij}$$

Here, the symbols represent the following:

X_{ij} Quantity of gaseous nuclide j in node I (mol)

W_m flow rate in link m out of room i (kg/s)

W_n flow rate in link n into room i from donor room I (kg/s)

W_{Hi} Total flow rate through all holes connecting node i to the external atmosphere (kg/s)

λ_j Removal rate constant for the removal of nuclide j excluding decay (1/s)

ω_{ij} Net generation rate resulting from decay and build-up of nuclide j in room i (mol/s)

S_{ij} Nuclide j source term rate in node I (mol/s)

Tm_i Total mass of gas in node i (kg)

N_{ij} Iodine nuclide j source rate in node i due to chemical transformation and mass transfer (mol/s)

E_{ij} EFADS sink term (mol/s)

2.2.1.2.1 Radioactive decay and build-up

SMART-IST calculates radioactive decay and build-up of nuclides to enable calculation of Equation 2. Radioactive nuclides undergo natural decay disintegrating into other nuclides. SMART-IST models four types of decay chains (Figure 1), and calculates net rate of change due to decay and build-up using an analytical solution of the modelling differential equations.

2.2.2 EFADS engineered system

The Emergency Filtered Air Discharge System (EFADS) is an engineered system used to maintain pressure control within containments of the multi-unit CANDU stations in the long term following an accident. The EFADS consist of five components in series: a demister, a heater, a first HEPA (High Efficiency Particulate Air) filter, a charcoal filter and a second HEPA filter. As the airborne radionuclides and aerosols are transported through the EFADS, a fraction is removed within the EFADS. The resulting removal rates are coupled to the general transport Equations 1 and 2, using the net sink term, E.

2.2.3 Containment iodine chemistry model – IMOD-2

SMART-IST uses a containment iodine chemistry model, IMOD-2. This model was developed by Wren et al. [2]. The main processes modelled in IMOD-2 are the chemical transformations between non-volatile iodine species and volatile iodine species in the aqueous phase, and the partitioning of volatile iodine species among the gas, aqueous and adsorbed phases. For the purpose of implementing IMOD-2 in SMART-IST, it is assumed that the aqueous phase in each node consists of two parts. The first part is the bulk liquid pool on the floor formed by the removal of liquid aerosols from the free volume. The second part is the airborne liquid aerosols in the node. The concentration of an iodine isotope in liquid aerosols and in the gaseous state of a node may change as a result of the IMOD-2 calculations. These changes are coupled to the Equations 1 and 2 through a source term, N.

2.3 Numerical solution

The sets of differential equations 1 and 2 are of the general form:

$$\frac{d\bar{y}}{dt} = \bar{F}(\bar{y}, t) \qquad (3)$$

where,

$\bar{y} = (y_1, y_2, \ldots y_n)^T$, is a vector of dependent variables, and $\bar{F} = (F_1, F_2, \ldots F_n)^T$, is a vector of nonlinear functions of the dependent variables. The dependent variables are the airborne quantities of individual gaseous nuclides, and nuclides contained in aerosols of a spectrum of sizes within containment.

Equation (3) is solved numerically using a first-order, non-iterative, implicit method using a set of linear algebraic equations:

$$[I - [J]^t \Delta t]\Delta\bar{y} = (\bar{F}(\bar{y}, t))^t \Delta t \qquad (4)$$

where, I is the identity matrix, [J] the Jacobian, $\left[\frac{\partial \bar{F}(\bar{y}, t)}{\partial \bar{y}}\right]$, given by:

$$[J] = \begin{bmatrix} \frac{\partial F_1}{\partial y_1} & \frac{\partial F_1}{\partial y_2} & \cdots & \frac{\partial F_1}{\partial y_n} \\ \frac{\partial F_2}{\partial y_1} & \frac{\partial F_2}{\partial y_2} & \cdots & \frac{\partial F_2}{\partial y_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial F_n}{\partial y_1} & \frac{\partial F_n}{\partial y_2} & \cdots & \frac{\partial F_n}{\partial y_n} \end{bmatrix} \qquad (5)$$

Δt is the time step, and $\Delta\bar{y}$ is the incremental change of the dependent variable vector. The dependent variable vector $\bar{y}$ is updated over the time step using Equation (6) as follows:

$$\bar{y}^{t+\Delta t} = \bar{y}^{t} + \Delta\bar{y} \tag{6}$$

3. EXAMPLE PREDICTIONS

This section presents examples of typical SMART-IST calculations that are useful for safety and licensing analysis.

Figure 2 presents an example of the containment geometry modelled by SMART-IST consisting of a network of rooms (nodes) inter-connected by flow paths (links). Each node consists of a number of flow paths through which radionuclides may be released to the outside atmosphere. A high-enthalpy water discharge resulting from a Loss Of Coolant Accident (LOCA), and the associated nuclides, enter the Accident-Vault and are transported to other parts of containment through the flow paths. Figure 3 illustrates typical LOCA discharge characteristics handled by SMART-IST. The discharge initiates at time zero, and continues for approximately 30 seconds as a flashing, two-phase mixture consisting of both steam and water, and gradually changes to single-phase water. The flow remains predominantly in the single-phase mode at times greater than 30 seconds. The liquid portion of the discharge breaks up into aerosols and becomes airborne in the vault. SMART-IST calculates the size distribution of not only the aerosols, but also the distribution of the nuclides contained in these aerosols.

Figure 4 shows an example of the prediction of the time-varying, airborne size distribution of an individual nuclide, ^{127}I, in the Accident-Vault. The distribution shows a peak around 5 micrometers, which is typical of LOCA discharges. Noble gases are released with the LOCA discharge into containment. SMART-IST calculates the transport of the noble gases taking into account their radioactive decay and build-up characteristics. Figure 5 presents an example of the prediction of the quantity of a noble gas, ^{89}Kr, airborne in different nodes, as a function of time. As one would expect, ^{89}Kr spreads to different nodes from the source node 1, as a result of its transport by the carrier gas to various parts of the containment.

SMART-IST is capable of calculating individual nuclide releases to the outside atmosphere, through specific leak paths, and provides the results for use in public dose calculations. Figure 6 illustrates this capability. Here, ^{127}I is released through three paths, to the atmosphere, as a function of time. The paths are: a) leakage (through concrete and clearances around containment penetrations), b) ventilation inlet duct, and c) an arbitrary hole defined by the user. The calculated releases through leak paths are so small that they overlap the x-axis. Figure 7 presents the corresponding calculated release of a noble gas, ^{89}Kr.

The fundamental principle behind SMART calculations of nuclide transport is the mass balance. Constituent elements governing the mass balance of a nuclide are:

a) the source quantity,
b) the airborne quantity,
c) the released quantity, and
d) the removed quantity.

These four elements, together, determine the extent to which mass conservation has been achieved in SMART-IST calculations. Any numerical solution introduces truncation and round-off errors. SMART-IST continuously monitors the mass balance error (deficit) resulting from the difference between the source and the sum of the other elements in order to ensure that the error remains small at all times. Figure 8 illustrates this aspect. It presents the four constituent elements of conservation and the deficit, in the entire geometry of the model problem, as a function of time. At all times, the mass balance error remains quite small (overlays the x-axis and is of the order of 10^{-14} out of the total source quantity of the order of 10^{+5}), reinforcing confidence in the SMART-IST calculations.

4. SUMMARY

The SMART-IST computer code calculates radionuclide behaviour in CANDU reactor containments during postulated accidents. The calculations are based on solving a system of differential equations derived from the mass conservation principle, describing the transport of aerosols and gases within a network of interconnected volumes. SMART-IST obtains the required thermalhydraulic information as input data from the GOTHIC code, and provides the predicted results for use in public dose analysis. SMART-IST models radioiodine in more detail than other nuclides using the IMOD-2 model developed at AECL. SMART-IST has been developed and validated meeting the CSA N286.7 quality assurance standard, under the sponsorship of IST partners. The intended application of SMART-IST is safety and licensing analysis of public dose resulting from releases of nuclides from containment to the atmosphere.

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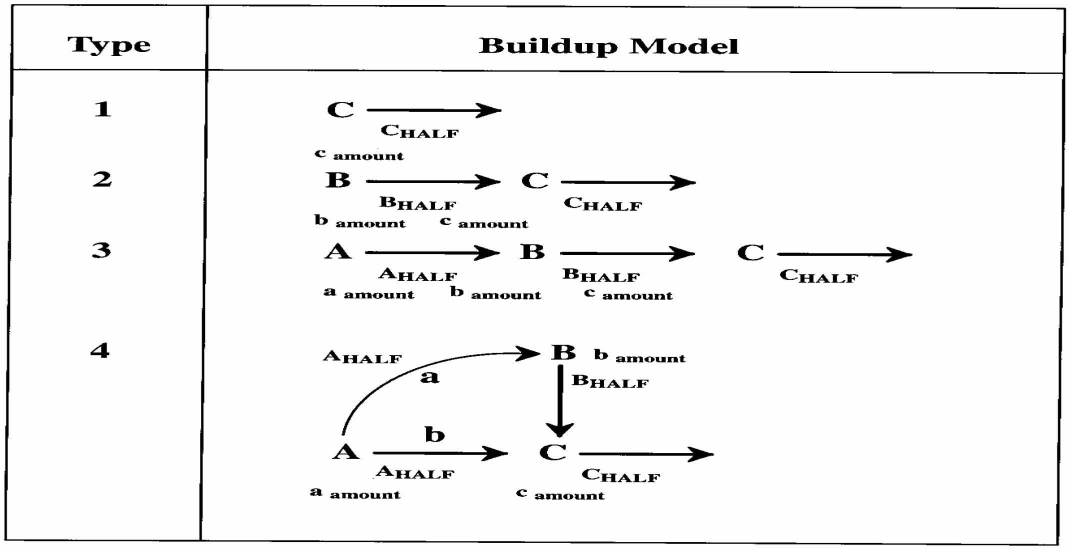

Figure 1: SMART-IST Nuclide Decay Chain Types

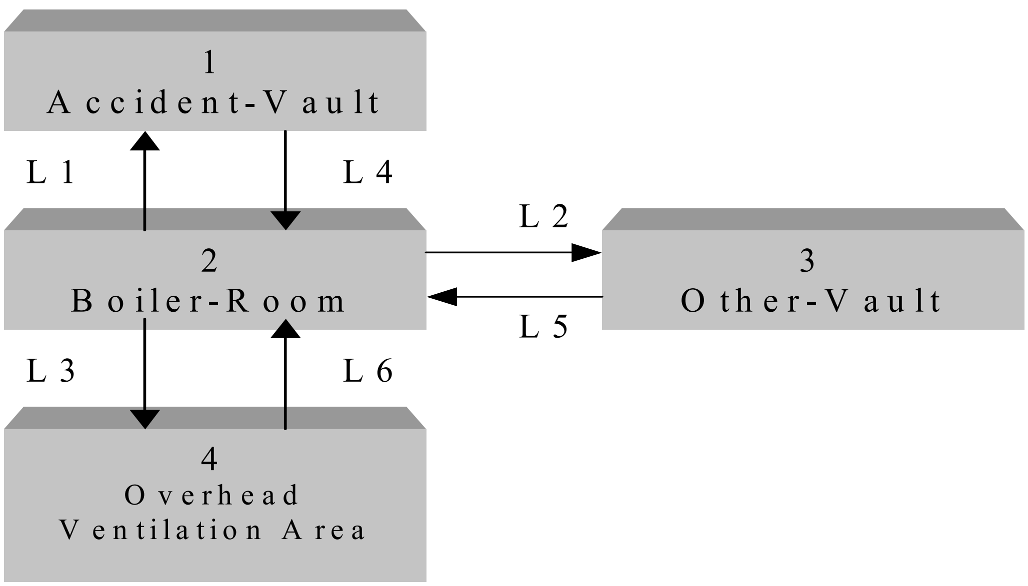

Figure 2: Containment geometry model represented by a network of rooms (nodes) inter-connected by flow paths (links)

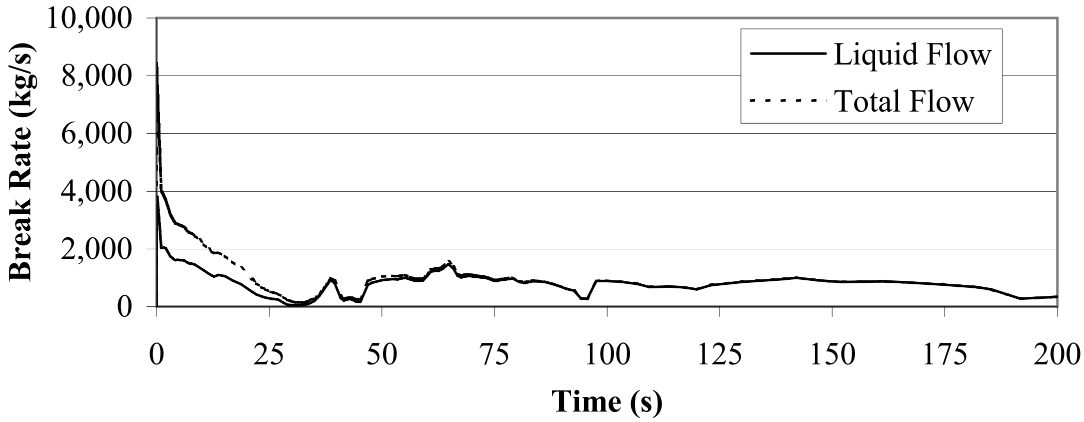

Figure 3: Break flow transients showing the total flow consisting of both water and steam and the water portion of the total flow

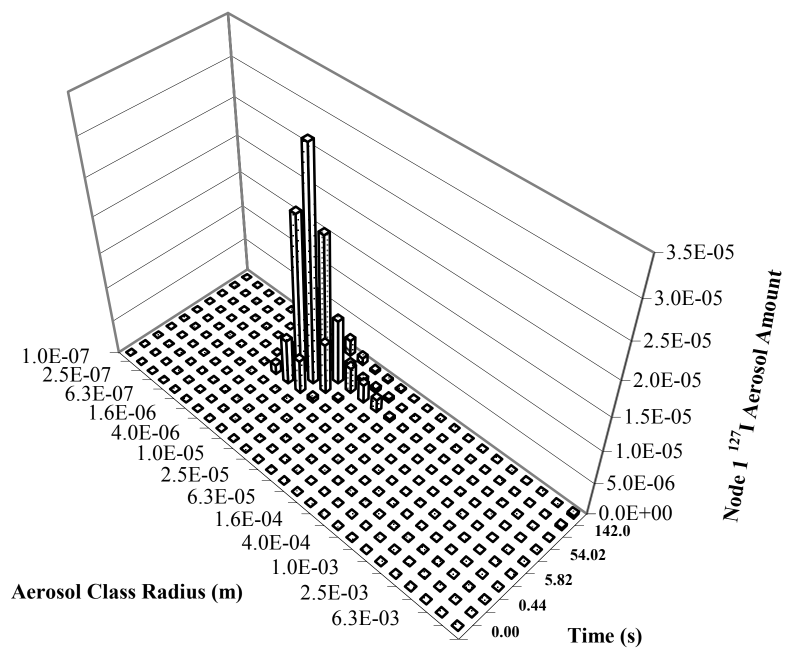

Figure 4: ^{127}I present in aerosols of different class sizes and its change with time in Accident-Vault (Node #1)

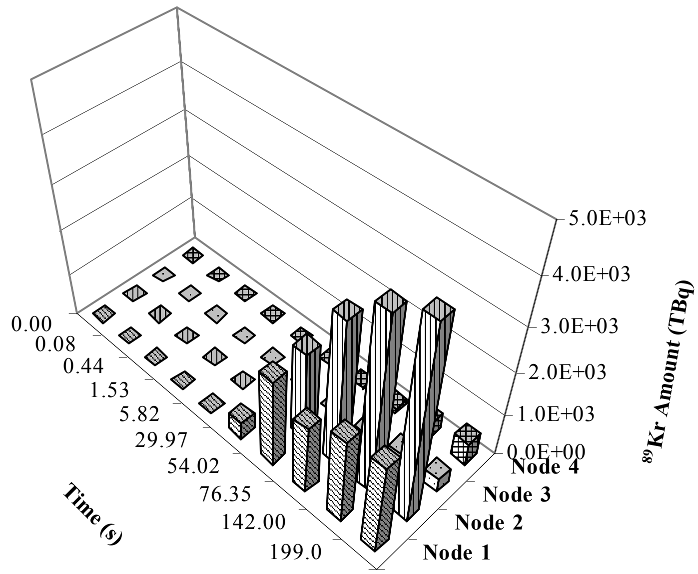

Figure 5: Distribution of airborne ^{89}Kr among nodes and its change with time

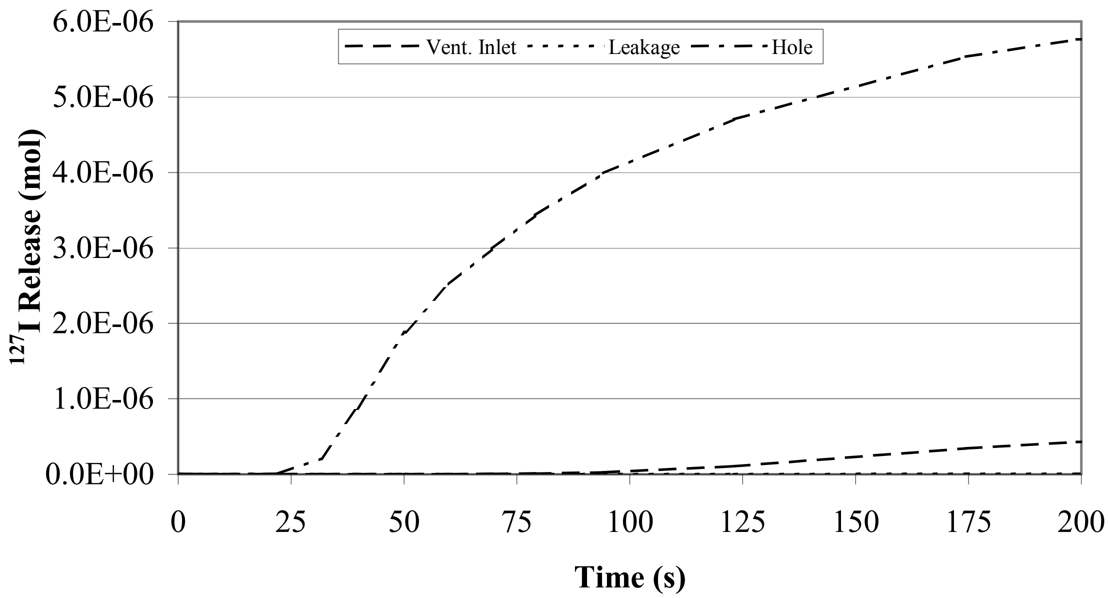

Figure 6: Cumulative quantity of ^{127}I released to the outside atmosphere through different release paths

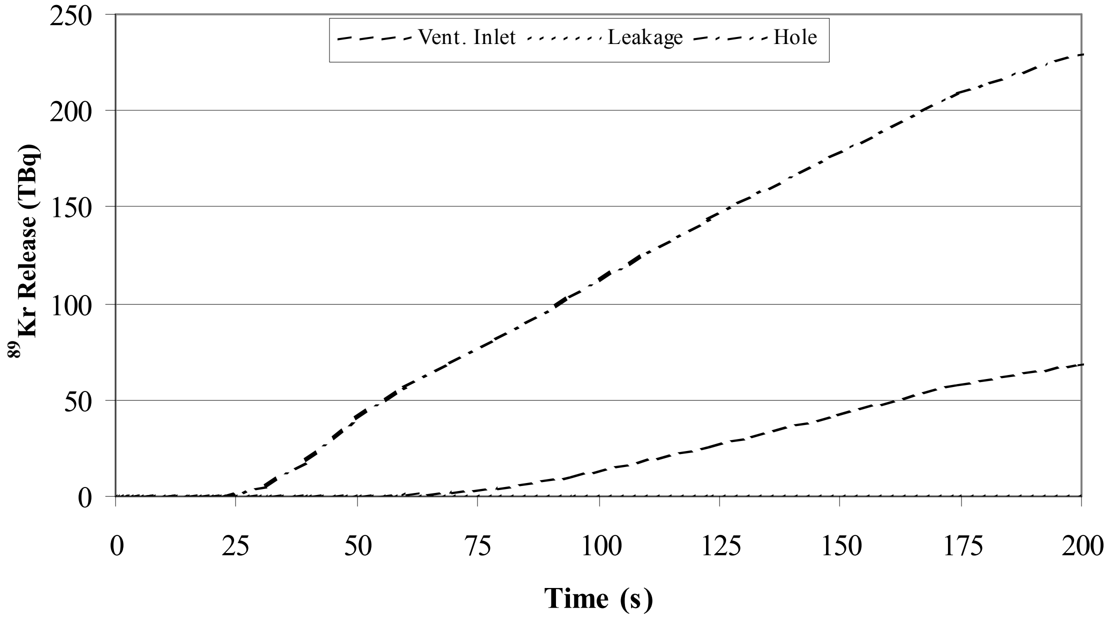

Figure 7: Cumulative quantity of ^{89}Kr released to the outside atmosphere through different release paths

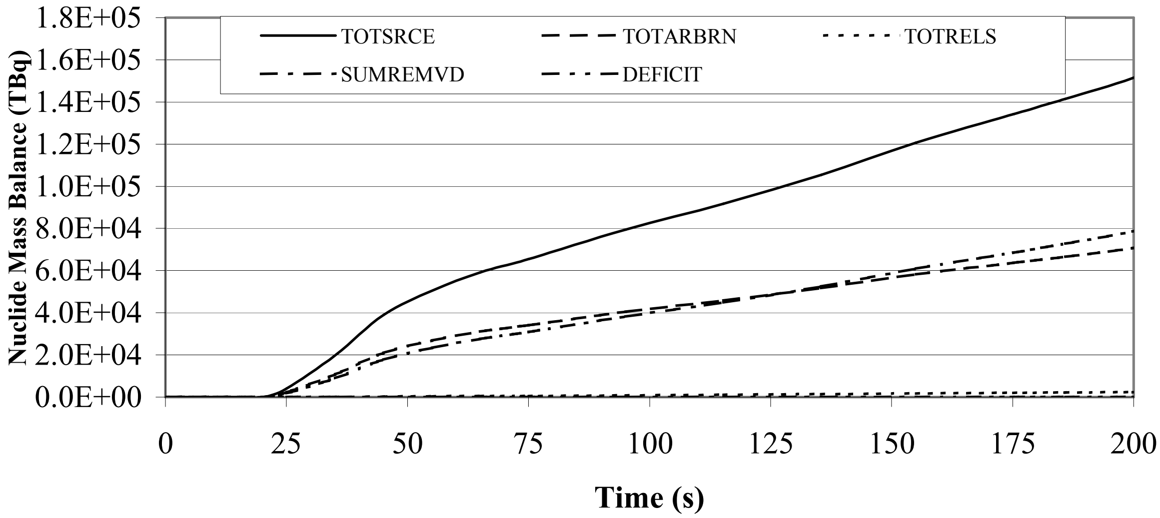

Figure 8: Mass balance of nuclides among the quantities: a) source (TOTSRCE), b) airborne in the containment atmosphere (TOTARBRN), c) escaped to the outside atmosphere (TOTRELS), d) removed from the containment atmosphere (SUMREMVD), and e) deficit.