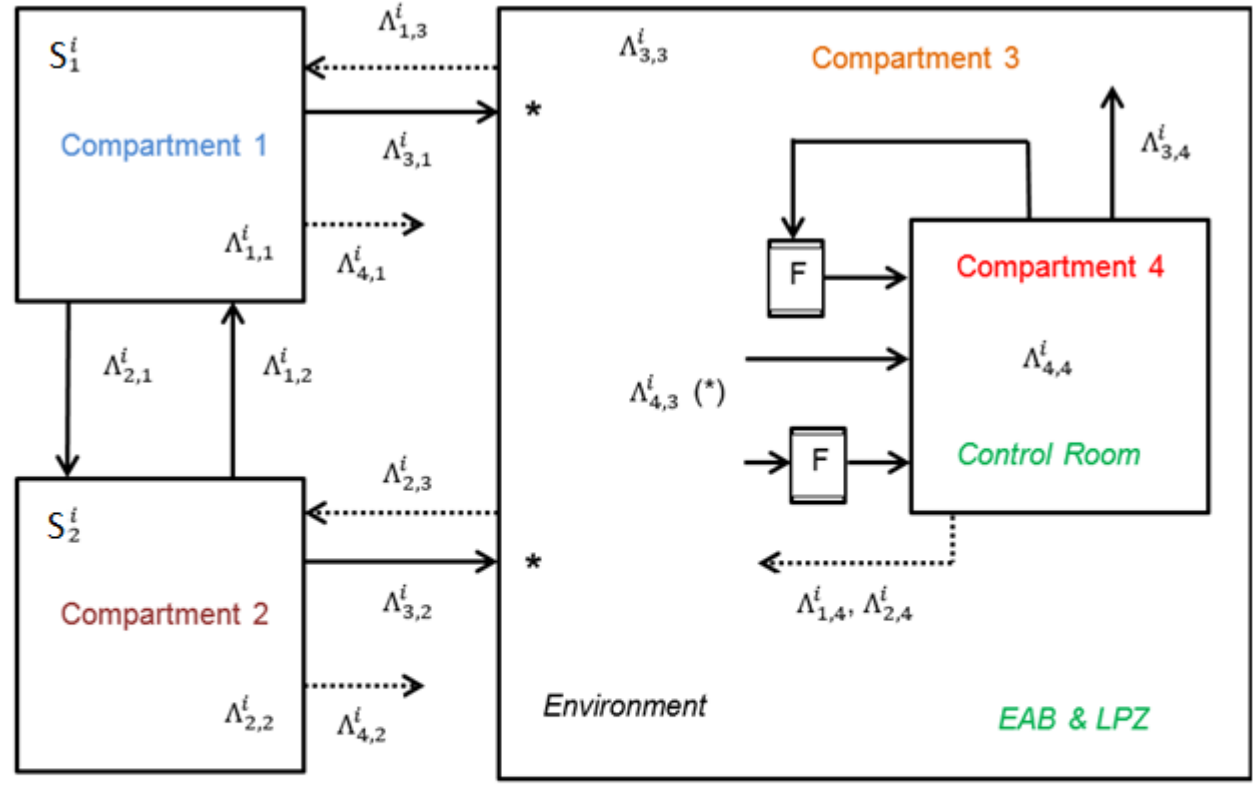
RADTRAD Governing Equations

- RADTRAD utilizes a multi-compartment model with radionuclide release to one or more compartments, flow pathways to account for transfer among compartments, and models for removal within a compartment.
- A key assumption is that the airborne activity in each non-environment compartment is assumed to be uniformly distributed or mixed.
- Because each release point and intake location has a separate X/Q value, the radionuclide inventory is not uniformly distributed in the environment compartment.
- Models for filtration and deposition within a flow pathway can be specified.
- Within a compartment, removal due to decay, natural deposition and sprays can be modeled.
- Daughter product buildup and decay can also be accounted for.

RADTRAD Governing Equations



* Denotes X/Q coupling between release points and dose points (EAB, LPZ) or control room intake.

---- Dotted lines denotes zero flowrate.

Legend:

$\Lambda_{k,j}^i$ – Inter-compartmental transfer from j to k

$\Lambda_{j,j}^i$ – Removal within a compartment j

F – Filter

S_j^i – Source release rate in compartment j

RADTRAD Governing Equations

For, compartment 1, the rate of change in the number of atoms is:

$$\dot{N}_1^i = S_1^i - \Lambda_{1,1}^i N_1^i + \Lambda_{1,2}^i N_2^i + \Lambda_{1,3}^i N_3^i + \Lambda_{1,4}^i N_4^i$$

Where:

S_1^i = the source release rate of nuclide i in compartment 1 in atoms/s
$\Lambda_{1,1}^i$ = the removal rate of nuclide i within compartment 1 in 1/s
N_1^i = the inventory of nuclide i in compartment 1 in atoms
$\Lambda_{1,2}^i$ = the transfer rate of nuclide i to compartment 1 from 2 in 1/s
N_2^i = the inventory of nuclide i in compartment 2 in atoms
$\Lambda_{1,3}^i$ = the transfer rate of nuclide i to compartment 1 from 3 in 1/s
N_3^i = the inventory of nuclide i in compartment 3 in atoms
$\Lambda_{1,4}^i$ = the transfer rate of nuclide i to compartment 1 from 4 in 1/s
N_4^i = the inventory of nuclide i in compartment 4 in atoms

RADTRAD Governing Equations

We can separate the equation into sections.

$$\dot{N}_1^i = S_1^i - \Lambda_{1,1}^i N_1^i + \Lambda_{1,2}^i N_2^i + \Lambda_{1,3}^i N_3^i - \Lambda_{1,4}^i N_4^i$$

Total change in the inventory of nuclide i in compartment 1.

Amount of nuclide i released by the source to compartment 1.

Amount of nuclide i that is removed from compartment 1.

Amount of nuclide i added to compartment 1 from compartment 2 after reduction from filters, sprays and/or deposition.

Amount of nuclide i added to compartment 1 from compartment 3 after reduction from filters, sprays and/or deposition.

Amount of nuclide i added to compartment 1 from compartment 4 after reduction from filters, sprays and/or deposition.

RADTRAD Governing Equations

For compartment 2, a similar equation is used which is:

$$\dot{N}_2^i = S_2^i - \Lambda_{2,2}^i N_2^i + \Lambda_{2,1}^i N_1^i + \Lambda_{2,3}^i N_3^i + \Lambda_{2,4}^i N_4^i$$

where

S_2^i = the source release rate of nuclide i in compartment 1 in atoms/s
$\Lambda_{2,2}^i$ = the removal rate of nuclide i within compartment 2 in 1/s
N_2^i = the inventory of nuclide i in compartment 2 in atoms
$\Lambda_{2,1}^i$ = the transfer rate of nuclide i to compartment 2 from 1 in 1/s
N_1^i = the inventory of nuclide i in compartment 1 in atoms
$\Lambda_{2,3}^i$ = the transfer rate of nuclide i to compartment 2 from 3 in 1/s
N_3^i = the inventory of nuclide i in compartment 3 in atoms
$\Lambda_{2,4}^i$ = the transfer rate of nuclide i to compartment 2 from 4 in 1/s
N_4^i = the inventory of nuclide i in compartment 4 in atoms

RADTRAD Governing Equations

More generally, the rate of change in the number of atoms in the kth compartment in a set of n interconnected compartments is given by

$$\frac{dN_k^i}{dt} = S_k^i - \sum_{j=1}^{n} \lambda_{j,j}^i N_k^i + \sum_{j=1, j\neq k}^{n} \lambda_{k,j}^i N_j^i$$

S_k^i is the source release rate of species i in compartment k in atoms/s

The first summation represents the removal terms from compartment *k* due either to removal within the compartment or transfer to another compartment. The second summation represents transfer from compartment *j* to compartment *k*.

RADTRAD Governing Equations

A matrix formulation can be used to represent the above equations for n compartments as follows:

$$\begin{bmatrix} \dot{N}_1^i \\ \dot{N}_2^i \\ \dot{N}_3^i \\ \vdots \\ \dot{N}_n^i \end{bmatrix} = \begin{bmatrix} S_1^i \\ S_2^i \\ S_3^i \\ \vdots \\ S_n^i \end{bmatrix} + \begin{bmatrix} -\Lambda_{1,1}^i & \Lambda_{1,2}^i & \Lambda_{1,3}^i & \vdots & \Lambda_{1,n}^i \\ \Lambda_{2,1}^i & -\Lambda_{2,2}^i & \Lambda_{2,3}^i & \vdots & \Lambda_{2,n}^i \\ \Lambda_{3,1}^i & \Lambda_{3,2}^i & -\Lambda_{3,3}^i & \vdots & \Lambda_{3,n}^i \\ \cdots & \cdots & \cdots & \ddots & \vdots \\ \Lambda_{n,1}^i & \Lambda_{n,2}^i & \Lambda_{n,3}^i & \cdots & -\Lambda_{n,n}^i \end{bmatrix} \begin{bmatrix} N_1^i \\ N_2^i \\ N_3^i \\ \vdots \\ N_n^i \end{bmatrix}$$

RADTRAD Governing Equations

Off-diagonal terms in the matrix are transfer terms.

- Calculated as f/V where f is the flow rate out of a compartment (vol or mass units per second) and V is the compartment volume (vol or mass units), yielding units of per second.
- This ratio is multiplied by the radionuclide inventory in the upstream connecting compartment to provide a nuclide per second source term to the connecting downstream compartment.
- Uniform mixing throughout each volume is assumed.

Diagonal terms in the matrix are removal terms.

- Idea is the same in that a removal coefficient expressed in units of per second is multiplied by the radionuclide inventory to yield a removal rate.
- Removal includes transfer of nuclides to other compartments and removal within a compartment (due to decay, deposition, spray removal, etc.)

RADTRAD Governing Equations

- The terms included in the diagonal removal coefficients each have units of 1/sec and are:

$$\Lambda^i_{j,j} = \lambda^i_{j,spr} + \lambda^i_{j,dep} + \lambda^i_{j,filter} + \sum_{\substack{k=1 \\ k \neq j}}^{n} \lambda^i_{k,j}$$

$\lambda^i_{j,spr}$ = the spray removal coefficient in 1/s
$\lambda^i_{j,dep}$ = the natural deposition removal rate in 1/s
$\lambda^i_{j,filter}$ = the filtered removal rated within compartment in 1/s
$\lambda^i_{k,j}$ = the removal rate from compartment j toward compartment k in 1/s.

RADTRAD Governing Equations

The removal rate is given by the following equation and includes a few different types of transfer between compartments.

$$\lambda_{k,j}^{i} = \lambda_{k,j,leak}^{i} + \lambda_{k,j,filter}^{i} + \frac{f_{k,j}}{V_j}$$

$\lambda_{k,j,leak}^{i}$ = the transfer via leakage paths in 1/s.
$\lambda_{k,j,filter}^{i}$ = the transfer through a filtered path in 1/s.
$f_{k,j}$ = the flow in m^3/s from *j* to *k* through a path with a DF.
V_j = the volume of compartment *j* in m^3.

RADTRAD Governing Equations

The removal rates for the off-diagonal terms, $\Lambda^i_{j,k}$ where j ≠ k, are calculated by the following:

$$\Lambda^i_{j,k} = \lambda^i_{j,k,leak} + \left(1 - \frac{\eta^j_{j,k}}{100}\right)\lambda^i_{j,k,filter} + \left(\frac{1}{DF}\right)\frac{f^i_{j,k}}{V_k}$$

$\eta^i_{j,k}$ = the percent efficiency of the filter in the path from compartment k to j.

DF = the nondimensional decontamination factor for a path with flow from compartment k to j.

RADTRAD Governing Equations

The matrix differential equation is solved in RADTRAD using a matrix exponential Taylor series expansion:

- Matrix exponential methods are used to solve systems of linear differential equations of the form $\dot{N} = S + \Lambda N$ subject to an initial condition N_0.
- Note that the coefficient matrix is invariant within a time interval. As a result, the initial condition at the start of a given time interval is adjusted based on the quantity of material in each compartment at the end of the previous time interval.

Decay is not explicitly included in the matrix equation.

- Decay is accounted for in RADTRAD by dividing the solution of the differential equations into two parts: (1) radioactive decay and daughter in-growth, and (2) radionuclide transport.
- Used to overcome the limitations of personal computers available at the time the original version of RADTRAD was developed and has been retained to the present time.

RADTRAD Governing Equations

Radioactive decay and daughter production occur within a compartment, so no intercompartmental transfer needs to be considered. The governing equation is:

$$\frac{dN_j^i}{dt} = \sum_{\nu=1}^{n-1} \beta_\nu^i \lambda_{decay}^\nu N_j^\nu - \lambda_{decay}^i N_j^i$$

n = the number of nuclides
β_ν^i = the fraction of nuclide ν that decays to nuclide i (dimensionless).
λ_{decay}^ν = the decay rate of nuclide ν in 1/s.
N_j^ν = the quantity of nuclide ν in compartment j.
λ_{decay}^i = the rate of decay of nuclide i in 1/s.

RADTRAD Governing Equations

Decay and transport calculations are performed alternately in RADTRAD.

- Code begins its integration over a time step by analyzing the effect of radioactive decay and daughter in-growth on the inventory of all compartments.
- Code then calculates the effect of radionuclide transport between compartments during that same time step.
- Process of alternating between radioactive decay and daughter in-growth and radionuclide transport continues until the specified end time is reached.
- For simulations where radioactive decay is not modeled, the solution algorithm is simplified to the single step of calculating radionuclide transport.

RADTRAD Adaptive Time Step

By default, RADTRAD uses a predetermined time step size algorithm that starts at 2 seconds and gradually increases to a maximum of 4 hours after about 12.5 hours into the simulation. The time step size can be specified manually as well.

Numerical error is a function of the time step size, and by adjusting the time step size it was found that the default time step size algorithm resulted in notable error for some simulations.

An adaptive time step algorithm was added to RADTRAD in order to control the time step size in order to reduce the numerical error associated with the default time step algorithm.